

SHAPE SENSITIVITY ANALYSIS FOR FLOW OPTIMIZATION IN CLOSED CHANNELS

E. Rohan, R. Cimrman¹

Summary: The paper deals with the shape sensitivity analysis of the steady viscous incompressible fluid flow in a curved closed channel. The objective function which is analyzed is aimed at reducing nonuniformity of the outlet stream. The geometry of the channel is embedded in a 3D domain parametrized by splines, so that it is handled using positions of control points. This allows for simple computing the design velocity field defined inside the channel and involved in the sensitivity formulae derived using the material derivative and adjoint system technique. The sensitivity algorithm can be employed in gradient-based optimization of the channel shape. Some numerical examples are presented to illustarte performance of the implemented sensitivity formulae.

1. Introduction

Shape optimization in fluid mechanics belongs still to most challenging areas of research in the structural optimization, bringing about many difficulties in both theory and numerical implementation. At the same time, it is very attractive for engineering community due to vast industrial applications, such as wings, car bodies, jets and many others related to industrial technologies. The topic of the sensitivity analysis in flow problems has been addressed usually in the context of wing and body aerodynamics, often treated using so-called automatic differentiation of the code supplying the state problem solutions; a comprehensive survey of various methods problems was issued in [Mohammadi and Pironneau 2001].

In this paper we present the shape sensitivity analysis for flow problems defined in closed channels. We restrict ourselves to the case of steady incompressible flows described by the Stokes, or the Navier–Stokes system of equations. Although the sensitivity formulae for this situation were issued in [Mohammadi and Pironneau 2001], we use the material derivative technique in the domain approach, see e.g. [Haslinger and Neittaanmaki 1988, Haug et al. 1986]; this leads to more accurate sensitivities in comparison with boundary integral technique which requires computation of velocity gradients on the design surfaces (for other applications pursued by the authors see [Rohan and Whiteman 2000, Rohan 2003, Rohan and Miara 2006]).

¹ Doc. Dr. Ing. Eduard Rohan, Ing. Robert Cimrman, PhD., Department of Mechanics, Faculty of Applied Sciences, University of West Bohemia in Plzeň, Univerzitní22, 306 14 Plzeň, tel. +420 377 63 23 20, e-mail rohan@kme.zcu.cz

For parametrization of the channel shape we use the FFD (free-form deformation) approach based on 3D spline volumes, cf. [Menzel et al. 2005, Samareh 2000], which enables to modify the design surface and the domain FE mesh by the same handles. Since we are interested in optimization of channels with branches, we consider the 3D domain of interest as decomposed into several sub-bodies, so that the shape changes can better be localized.

In Section 2. we introduce both the state and the optimal shape problems, for which in Section 3. the sensitivity analysis is presented. The design parametrization based on the spline volumes is discussed in Section 4.. For confirmation of the theoretical results developed, in Section 5. we describe the sensitivity analysis implementation and illustrate its performance in a simple test example.

2. Problem setting

The fluid problem is defined in an open bounded domain $\Omega \subset \mathbb{R}^3$ which is decomposed in two parts

$$\overline{\Omega} = \overline{\Omega_D \cup \Omega_C} \quad \text{with} \quad \Gamma_C = \partial \Omega_D \cap \partial \Omega_C , \qquad (1)$$

where Ω_C is the *control domain* and Ω_D is the *design domain*, both separated by interface $\Gamma_C \subset \partial \Omega_C$, where in general $\partial \Omega \cap \partial \Omega_C \neq \emptyset$, see Fig. 1. The shape of Ω_D is modified exclusively through the *design boundary*, $\Gamma_D \subset \partial \Omega_D \setminus (\Gamma_{\text{in-out}} \cup \Gamma_C)$ 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, $\Gamma_{\text{in-out}} = \Gamma_{\text{in}} \cup \Gamma_{\text{out}}$.

2.1. State problem – flow through the channel

We are interested in steady state incompressible flows in domain Ω which are described by the following problem: find a velocity, \boldsymbol{u} , and pressure, p, fields in Ω such that (ν is the kinematic viscosity)

$$-\nu \nabla^2 \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \nabla p = 0 \quad \text{in } \Omega ,$$

$$\nabla \cdot \boldsymbol{u} = 0 \quad \text{in } \Omega ,$$
(2)

with the boundary conditions

$$\boldsymbol{u} = 0 \quad \text{on } \partial\Omega \setminus \Gamma_{\text{in-out}},$$

$$-p\boldsymbol{n} + \frac{\partial \boldsymbol{u}}{\partial n} = -\bar{p}\boldsymbol{n} \quad \text{on } \Gamma_{\text{in-out}},$$

$$\Gamma_{D} \qquad \Omega$$

$$\Gamma_{in} \qquad \Gamma_{D} \qquad \Gamma_{C} \qquad \Omega_{C} \qquad \Gamma_{out}$$
(3)

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

where \boldsymbol{n} is the unit outward-normal vector on $\Gamma_{\text{in-out}}$ and $\frac{\partial}{\partial n} = \boldsymbol{n} \cdot \nabla$. Note that by $(3)_2$ we prescribe the stress in the form of pressure \bar{p} (defined for Γ_{in} and Γ_{out} by \bar{p}^1 and \bar{p}^2 , respectively), 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. $\Gamma_{\text{in-out}}$.

In order to set the optimal shape problem and to derive the *sensitivity formulae*, we use the weak formulation of (2)-(3). For this we need to introduce the functional forms (i = 1, 2, 3, summation convention is employed)

$$a_{\Omega} (\boldsymbol{u}, \boldsymbol{v}) = \nu \int_{\Omega} \nabla \boldsymbol{u} : \nabla \boldsymbol{v} = \nu \int_{\Omega} \frac{\partial u_i}{\partial x_k} \frac{\partial v_i}{\partial x_k} ,$$

$$c_{\Omega} (\boldsymbol{w}, \boldsymbol{u}, \boldsymbol{v}) = \int_{\Omega} (\boldsymbol{w} \cdot \nabla \boldsymbol{u}) \cdot \boldsymbol{v} = \int_{\Omega} w_k \frac{\partial u_i}{\partial x_k} v_i ,$$

$$b_{\Omega} (\boldsymbol{u}, p) = \int_{\Omega} p \operatorname{div} \boldsymbol{u} ,$$
(4)

and the space of admissible velocities

$$\boldsymbol{V}_0 = \left\{ \boldsymbol{\nu} \in \mathbf{H}^1(\Omega) \, | \, \boldsymbol{\nu} = 0 \text{ on } \partial\Omega \setminus \Gamma_{\text{in-out}} \right\},$$
(5)

where $\mathbf{H}^1(\Omega) = [H^1(\Omega)]^3$.

With the notation just introduced we may pass to the *weak formulation* of our flow problem; on multiplication of (2) and (3) by the test functions v and q, respectively, and on integrating over Ω , we obtain the following problem: find $u \in V_0(\Omega)$ and $p \in L^2(\Omega)$ such that

$$a_{\Omega}(\boldsymbol{u},\boldsymbol{v}) + c_{\Omega}(\boldsymbol{u},\boldsymbol{u},\boldsymbol{v}) - b_{\Omega}(\boldsymbol{v},p) = -\int_{\Gamma_{\text{in-out}}} \bar{p}\,\boldsymbol{v}\cdot\boldsymbol{n}\,dS \quad \forall \boldsymbol{v}\in\boldsymbol{V}_{0},$$

$$b_{\Omega}(\boldsymbol{u},q) = 0 \quad \forall q\in L^{2}(\Omega).$$
(6)

2.2. Objective function – optimization problem

We have introduced the model of flow in channel Ω , which can be modified by changing the shape of Γ_D . Our objective of such a shape modification is to reduce the gradients of the flow velocities in domain Ω_C and thereby to enhance the flow uniformity in a neighbourhood of the outlet, where the control domain Ω_C is situated. We suggest that this merit can be pursued by minimization of the objective function $\Psi(\mathbf{u})$ by means of Γ_D :

$$\min_{\Gamma_D} \Psi(\boldsymbol{u}) ,$$
subject to: (\boldsymbol{u}, p) satisfy (6) ,
 $\Gamma_D \text{ in } \mathcal{U}_{ad}(\Omega_0) ,$
(7)
where $\Psi(\boldsymbol{u}) = \frac{\nu}{2} \int_{\Omega_C} |\nabla \boldsymbol{u}|^2 = \frac{1}{2} a_{\Omega_C} (\boldsymbol{u}, \boldsymbol{u}) .$

Above $(7)_2$ imposes the admissibility of the state, i.e. of the velocity and pressure fields, whereas $(7)_3$ 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*, $\mathcal{U}_{ad}(\Omega_0)$; we shall discus this topic later on, when reporting the domain parametrization of Ω_D . It should be noted that the

objective criterion expressed in terms of $\Psi(\mathbf{u})$ depends on the design *only in terms of the state variable*, as the control domain, Ω_C , is independent of any design modification. This point is important for feasibility of the optimal problem².

3. Sensitivity analysis – domain method

4 _

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 $\vec{\mathcal{V}}: \overline{\Omega_D} \rightarrow \mathbb{R}^3$ 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 real valued function and $f_{\Omega}(u)$ a real valued functional depending on domain Ω . The total sensitivity of f is given by

$$\delta f_{\Omega}(u) = \delta_D f_{\Omega}(u) + \delta_u f_{\Omega}(u) \circ \delta u , \qquad (8)$$

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 (7): $\vec{\mathcal{V}}$ is a feasible w.r.t. Ω_D iff the following holds:

supp
$$\mathcal{V} \subset \overline{\Omega_D}$$
 and $\mathcal{V} = 0$ on $\Gamma_{\text{in-out}} \cup \Gamma_C$,
 \mathcal{V} is differentiable in Ω_D . (9)

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 (8). We consider the Lagrangian associated with (7)

$$\mathcal{L}(\Gamma_{D}, \boldsymbol{u}, p, \boldsymbol{w}, q) = \Psi(\boldsymbol{u}) + a_{\Omega} (\boldsymbol{u}, \boldsymbol{w}) + c_{\Omega} (\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) - b_{\Omega} (\boldsymbol{w}, p) + \int_{\Gamma_{\text{in-out}}} \bar{p} \boldsymbol{v} \cdot \boldsymbol{n} \, dS + b_{\Omega} (\boldsymbol{u}, q) ,$$
(10)

where $w \in V_0$ and $q \in L^2(\Omega)$ are the Lagrange multipliers associated with state problem constraint imposed in (7). The desired sensitivity formula can be obtained using the KKT conditions concerning the "inf-sup" problem

$$\inf_{\Gamma_D, \boldsymbol{u}, p} \sup_{\boldsymbol{w}, q} \mathcal{L}(\Gamma_D, \boldsymbol{u}, p, \boldsymbol{w}, q) .$$
(11)

² Obviously, assuming bounded gradients $|\nabla u|$, their minimization as *integrated over a design-dependent domain* could lead just to annihilation of such a domain without any effect on the velocity field.

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} :

$$\delta \mathcal{L}(\Gamma_D, \boldsymbol{u}, p, \boldsymbol{w}, q) = \delta_{Da\Omega} (\boldsymbol{u}, \boldsymbol{w}) + \delta_{Dc\Omega} (\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) - \delta_{Db\Omega} (\boldsymbol{w}, p) + \delta_{Db\Omega} (\boldsymbol{u}, q) + a_{\Omega} (\delta \boldsymbol{u}, \boldsymbol{w}) + c_{\Omega} (\delta \boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) + c_{\Omega} (\boldsymbol{u}, \delta \boldsymbol{u}, \boldsymbol{w}) - b_{\Omega} (\boldsymbol{w}, \delta p) + b_{\Omega} (\delta \boldsymbol{u}, q) + \delta_{u} \Psi(\boldsymbol{u}) \circ \delta \boldsymbol{u} = \delta \Psi(\boldsymbol{u}) ,$$
(12)

where the last equality follows from the state admissibility; indeed, for a given design Γ_D , the state admissibility conditions (6) hold, so that except of $\Psi(\mathbf{u})$ all terms in (10) vanish. As a further consequence, (6) being satisfied corresponds with $\delta_{\mathbf{u},p}\mathcal{L} = 0$, as expressed by the optimality conditions

$$\delta_{\boldsymbol{u}} \mathcal{L}(\Gamma_{D}, \boldsymbol{u}, p, \boldsymbol{w}, q) = 0 = \delta_{\boldsymbol{u}} \Psi(\boldsymbol{u}) \circ \boldsymbol{v} + a_{\Omega} \left(\boldsymbol{v}, \boldsymbol{w} \right) + c_{\Omega} \left(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{w} \right) + c_{\Omega} \left(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \right) + b_{\Omega} \left(\boldsymbol{v}, q \right) , \quad (13)$$
$$\delta_{p} \mathcal{L}(\Gamma_{D}, \boldsymbol{u}, p, \boldsymbol{w}, q) = 0 = b_{\Omega} \left(\boldsymbol{w}, \eta \right) ,$$

for all $\mathbf{v} \in \mathbf{V}_0$ and for all $\eta \in L^2(\Omega)$. Problem (13) is called the *adjoint state problem* and allows for eliminating the total derivatives $\delta \mathbf{u}$, δp from sensitivity formula (12). It is readily seen that, on substituting in (13) the test functions $\mathbf{v} = \delta \mathbf{u}$, $\eta = \delta p$, in (12) we may cancel all terms except the partial design sensitivities. 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 (6),
- compute the adjoint state (w, q) by solving (13),
- compute the sensitivity w.r.t. given design velocity field $\vec{\mathcal{V}}$ using

$$\delta \Psi(\boldsymbol{u}) = \delta_D a_\Omega(\boldsymbol{u}, \boldsymbol{w}) + \delta_D c_\Omega(\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) - \delta_D b_\Omega(\boldsymbol{w}, p) + \delta_D b_\Omega(\boldsymbol{u}, q) \quad .$$
(14)

Below we shall derive the particular partial design sensitivities employed in (14), which depend on $\vec{\mathcal{V}}$. It is worth noting that the r.h.s. functional of the adjoint state problem is constituted by $-\delta_u \Psi(\boldsymbol{u}) \circ \boldsymbol{v} = -a_{\Omega_C}(\boldsymbol{u}, \boldsymbol{v})$, which is integrated only over Ω_c , however, the adjoint state is defined in the entire Ω .

3.2. Partial shape derivative

Once the design velocity field is defined, the design domain can be parametrized by means of a scalar parameter τ : let \vec{V} is feasible according to (9), we introduce

$$\overline{\Omega_D}(\tau) = \{y\} \quad \text{where} \quad y_i(x,\tau) = x_i + \tau \mathcal{V}_i(x) , \quad x \in \overline{\Omega_D}, \ \tau \in \mathbb{R} .$$
(15)

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 (8), we define the *partial shape derivative* of $f_{\Omega}(u)$

$$\delta_D f_\Omega(u) = \frac{\mathrm{d}}{\mathrm{d}\,\tau} \left(f_{\Omega_D(\tau)}(u) \right)_{\tau=0} \,. \tag{16}$$

In order to compute the partial shape derivative involved in (14), we need the following preliminaries, which are easy to verify $(J(y(x, \tau)) = \det[\partial y_i(x, \tau)/\partial x_i])$:

$$\delta_{D} \left(\frac{\partial y_{i}}{\partial x_{j}} \right) = \frac{\mathrm{d}}{\mathrm{d} \tau} \left(\frac{\partial y_{i}(x,\tau)}{\partial x_{j}} \right)_{\tau=0} = \frac{\partial \mathcal{V}_{i}(x)}{\partial x_{j}} ,$$

$$\delta_{D} \left(\frac{\partial x_{k}}{\partial y_{j}} \right) = \frac{\mathrm{d}}{\mathrm{d} \tau} \left(\frac{\partial x_{k}}{\partial y_{j}(x,\tau)} \right)_{\tau=0} = -\frac{\partial \mathcal{V}_{k}(x)}{\partial x_{j}} ,$$

$$\delta_{D} \left(J(y) \right) = \frac{\mathrm{d}}{\mathrm{d} \tau} \left(J(y(x,\tau)) \right)_{\tau=0} = \frac{\partial \mathcal{V}_{i}(x)}{\partial x_{i}} = \mathrm{div} \vec{\mathcal{V}} .$$
(17)

We are now ready to apply (16) to variation of $a_{\Omega}(\boldsymbol{u}, \boldsymbol{w})$; note that only Ω_D is being perturbed because of restricted support of $\vec{\mathcal{V}}$, so that $\delta_D a_\Omega(\boldsymbol{u}, \boldsymbol{w}) = \delta_D a_{\Omega_D}(\boldsymbol{u}, \boldsymbol{w})$. Therefore, we consider

$$a_{\Omega_{D(\tau)}}(\boldsymbol{u}, \boldsymbol{w}) = \nu \int_{\Omega_{D}(\tau)} \frac{\partial u_{i}}{\partial y_{k}(\tau)} \frac{\partial w_{i}}{\partial y_{k}(\tau)} dy$$

$$= \nu \int_{\Omega_{D}} \frac{\partial u_{i}(x)}{\partial x_{j}} \frac{\partial x_{j}}{\partial y_{k}(x,\tau)} \frac{\partial w_{i}(x)}{\partial x_{l}} \frac{\partial x_{l}}{\partial y_{k}(x,\tau)} J(y(x,\tau)) dx .$$
(18)

On differentiating above w.r.t. τ , using (17) we get the desired expression

$$\delta_D a_\Omega \left(\boldsymbol{u}, \, \boldsymbol{w} \right) = \nu \int_{\Omega_D} \left[\frac{\partial u_i}{\partial x_k} \frac{\partial w_i}{\partial x_k} \mathrm{div} \mathcal{V} - \frac{\partial \mathcal{V}_j}{\partial x_k} \frac{\partial u_i}{\partial x_j} \frac{\partial w_i}{\partial x_k} - \frac{\partial u_i}{\partial x_k} \frac{\partial \mathcal{V}_l}{\partial x_k} \frac{\partial w_i}{\partial x_l} \right] \,. \tag{19}$$

In much the same way one finds the formulae for other sensitivities involved in (14):

$$\delta_D c_\Omega \left(\boldsymbol{u}, \, \boldsymbol{u}, \, \boldsymbol{w} \right) = \int_{\Omega_D} \left[u_k \frac{\partial u_i}{\partial x_k} \, w_i \, \mathrm{div} \mathcal{V} - u_k \frac{\partial \mathcal{V}_j}{\partial x_k} \frac{\partial u_i}{\partial x_j} \, w_i \right] \,, \tag{20}$$

$$\delta_D b_\Omega \left(\boldsymbol{u}, \, q \right) = \int_{\Omega_D} q \, \left[\operatorname{div} \boldsymbol{u} \, \operatorname{div} \mathcal{V} - \frac{\partial \mathcal{V}_k}{\partial x_i} \frac{\partial u_i}{\partial x_k} \right] \,. \tag{21}$$

We may conclude that using (19)-(21) applied in (14), the total shape derivative can be recovered for any feasible $\vec{\mathcal{V}}$; construction of such $\vec{\mathcal{V}}$ for our specific design parametrization is addressed in the next section.

4. Domain parametrization

The sensitivity analysis developed in previous sections is based on the directional derivatives of given functionals, see (14), w.r.t. a given design velocity field $\vec{\mathcal{V}}$. In this section we introduce a parametrization of $\vec{\mathcal{V}}$ which is based on the free-form deformation (FFD) approach, as reported e.g. in [Samareh 2000].

The FFD method of parametrization is based on the domain parametrization using B-spline, or Bezier volumes. As we stem for treatment of complex channels with many branches, we use splitting of Ω into several subdomains, each one handled by one B-spline volume, so that we need to introduce some continuity conditions.

Let Ω_0 be a reference (initial) domain embedded in the box $\mathcal{B}_0 \subset \mathbb{R}_3$; we consider a nonoverlapping decomposition

$$\Omega_0 \subset \mathcal{B}_0 = \Pi_{k=1,2,3}]a_k, b_k [,$$

$$\mathcal{B}_0 = \sum_{I=1}^{NSB} \mathcal{B}_0^I, \quad \mathcal{B}_0^I =]a_k^I, b_k^I [$$

such that

$$\mathcal{B}_{0}^{I} \cap \mathcal{B}_{0}^{J} = \emptyset \quad \text{for } I \neq J ,$$

and for $I \neq J : \overline{\mathcal{B}_{0}^{I}} \cap \overline{\mathcal{B}_{0}^{J}} \equiv \mathcal{S}_{0}^{IJ} \neq \emptyset \quad \text{iff } \exists k, l, m \in \{1, 2, 3\} : \mathcal{S}_{0}^{IJ} = x_{m} \times [a_{k}^{I}, b_{k}^{I}] \times [a_{l}^{I}, b_{l}^{I}]$
where $x_{m} = a_{m}^{I} = b_{m}^{J}, \text{ or } x_{m} = b_{m}^{I} = a_{m}^{J} .$
(22)

Thus, the domain of interest is embedded in the box \mathcal{B}_0 which is then partitioned into sub-boxes \mathcal{B}_0^I by planar cuts, so that their closures (i.e. including the boundary) have common entire faces \mathcal{S}_0^{IJ} . Each sub-box \mathcal{B}^I is parametrized and "shaped" by the B-spline volume S^I which is defined in terms of the control vertices $b^{ijk} = (b_r^{ijk}) \in \mathbb{R}^3$ and the spline basis functions $N^i(t), t \in \mathbb{R}$ (in our case we use the cubic splines)

$$\mathcal{B}^{I} \ni x = S^{I}(\{b\}, \{N\}, t) \equiv \left[\sum_{i=1}^{\bar{i}} \sum_{j=1}^{\bar{j}} \sum_{k=1}^{\bar{k}} b^{ijk} N^{i}(t_{1}) N^{j}(t_{2}) N^{k}(t_{3})\right]_{I}, \quad t = (t_{r}) \in \mathcal{B}_{0}^{I},$$
(23)

where the bracketed notation $[\cdot]_I$ refers to the data associated with \mathcal{B}^I . It is worth noting that the initial boxes \mathcal{B}_0^I serve for the domain of spline parametrization, so that on selecting b^{ijk} as the Greville abscissae g^{ijk} , cf. [Hoschek and Lasser 1992], we recover the initial sub-boxes, i.e. we have the *identity property* $\mathcal{B}_0^I = S^I(\{g\}, \{N\}, \mathcal{B}_0^I)$

$$\mathcal{B}_{0}^{I} \ni t = x = \left[\sum_{i=1}^{\bar{i}} \sum_{j=1}^{\bar{j}} \sum_{k=1}^{\bar{k}} g^{ijk} N^{i}(t_{1}) N^{j}(t_{2}) N^{k}(t_{3})\right]_{I} .$$
 (24)

Let $\overline{\Omega_0^I} = \overline{\Omega_0 \cap \mathcal{B}_0^I}$, so that we have $\overline{\Omega_0} = \sum_{I=1}^{NSB} \overline{\Omega_0^I}$ and $\Omega_0^I = S^I(\{g\}, \{N\}, \Omega_0^I)$ due to the identity property. Obviously, the domain Ω_0 (or merely its subdomain) is modified in terms of control points $\{[b]_I\}_{I=1}^{NSB}$ which are subject to the interface conditions:

$$P^{IJ}[b]_J = P^{JI}[b]_I \quad \text{for any } I, J : \quad \mathcal{S}_0^{IJ} \cap \Omega_0 \neq \emptyset ,$$
(25)

where P^{IJ} and P^{JI} are the coupled continuity operators which make the links between the control points of neighbouring sub-boxes; the details concerning these operators are beyond the scope of this paper. For any $\{[b]_I\}_{I=1}^{NSB}$ such that (25) holds we obtain an image Ω of Ω_0 by a one-to-one mapping:

$$\overline{\Omega} = \sum_{I=1}^{NSB} S^{I}(\{b\}, \{N\}, \overline{\Omega_{0}^{I}}) \quad \text{such that:}$$

$$\forall \mathcal{S}_{0}^{IJ}: \text{ if } \Omega_{0} \ni x \in \mathcal{S}_{0}^{IJ} \Rightarrow S^{I}(\{b\}, \{N\}, x) = S^{J}(\{b\}, \{N\}, x) \quad \text{for any } \{[b]_{I}\}_{I=1}^{NSB} \text{ satisfying } (25).$$

$$(26)$$

Obviously, property (26) can be expressed in terms of a (matrix) operator as

$$B(\{b\}) = 0 \quad \Leftrightarrow \ (25) \text{ holds.} \tag{27}$$

The design variables γ_{α} , $\alpha = 1, ..., \bar{\alpha}$ can be introduced as multipliers associated with the elements of the kernel of operator *B*:

$$\{b\} = \{g\} + \sum_{\alpha=1}^{\alpha} \gamma^{\alpha} \{d\}^{\alpha} , \quad \text{where } \{d\}^{\alpha} \in \text{Ker}B \text{ and } \bar{\alpha} \leq \text{card}(\text{Ker}B) , \qquad (28)$$

so that for any $\gamma = (\gamma^{\alpha})$ using the Greville abscissae $\{g\}$ we define control points $\{b\}$ which satisfy (27); note that also $\{g\} \in \text{Ker}B$ by (24). On the other hand, as we impose some smoothness properties on the shape $\Gamma_D \in \mathcal{U}_{ad}$, we still must confine the design variability by introducing an admissibility set D_{ad} . Moreover, for protecting the control domain, Ω_C , as well as the input and output boundaries, $\Gamma_{\text{in-out}}$, from the design modification, we have further restriction on the selection of those design variables which can actually be manipulated. Thus, we define D_{ad} in an "implicit way" as the set of all γ^{β} , $\beta \in I_{ad} \subset [1, \bar{\alpha}]$ such that

$$\gamma^{\beta} \in [\underline{\gamma}^{\beta}, \overline{\gamma}^{\beta}] \quad \forall \beta \in I_{ad},$$

$$\overline{\Omega_{C0}} \stackrel{!}{=} \sum_{I=1}^{NSB} S^{I}(\{g\} + \gamma^{\beta}\{d\}^{\beta}, \{N\}, \overline{\Omega_{C0}^{I}}), \quad \forall \beta \in I_{ad},$$

$$\Gamma_{\text{in-out}_{0}} \stackrel{!}{=} \sum_{I=1}^{NSB} S^{I}(\{g\} + \gamma^{\beta}\{d\}^{\beta}, \{N\}, \Gamma_{\text{in-out}_{0}}^{I}) \quad \forall \beta \in I_{ad},$$

$$\mathcal{U}_{ad} \stackrel{!}{=} \Gamma_{D} = \sum_{I=1}^{NSB} S^{I}(\{g\} + \sum_{\beta \in I_{ad}} \gamma^{\beta}\{d\}^{\beta}, \{N\}, \Gamma_{D0}^{I}),$$

$$(29)$$

where Γ_{D0}^{I} and Ω_{C0}^{I} are the *I*-th sub-box restrictions of Γ_{D} and Ω_{C} , respectively, in the "initial configuration" Ω_{0} . Above in (29)₁, as usually, we impose box constraints, whereas in (29)₄ we constrain the design variables to obtain admissible variation of Γ_{D} .

Having defined the design variables and the admissibility set, D_{ad} , we can introduce the design velocity field associated with a change in γ (denoted by $\delta\gamma$):

$$\vec{\mathcal{V}} = \sum_{I=1}^{NSB} S^{I}(\sum_{\alpha \in I_{ad}} \delta \gamma^{\alpha} \{d\}^{\alpha}, \{N\}, \overline{\Omega_{0}^{I}}) , \qquad (30)$$

so that by virtue of (29), $\vec{\mathcal{V}}$ is admissible according to (9). So, for each variable γ^{α} , $\alpha \in I_{ad}$ we can obtain easily the α -th basic velocity, $\vec{\mathcal{V}}^{\alpha}$ which allows for computing the *design gradients* of $\Psi(\boldsymbol{u})$. We define

$$\vec{\mathcal{V}}^{\alpha} = \sum_{I=1}^{NSB} S^{I}(\{d\}^{\alpha}, \{N\}, \overline{\Omega_{0}^{I}}) , \qquad (31)$$

and evaluate (19)-(21) for this $\vec{\mathcal{V}}^{\alpha}$. Then, on substituting the partial sensitivities into (14), we obtain $\partial \Psi(\boldsymbol{u})/\partial d_{\alpha}$, the α -th component of the design gradient.





Fig. 3. Perturbation of the initial shape of Ω .

Fig. 2. The decomposition of Ω .

5. Numerical examples

For the purposes of the numerical simulations only the Stokes problem will be considered, as the full Navier-Stokes code was not finished at the time of writing the article. In this case the weak formulation of the direct flow problem (see (6)) reads: find $\boldsymbol{u} \in V_0(\Omega)$ and $p \in L^2(\Omega)$ such that

$$a_{\Omega} (\boldsymbol{u}, \boldsymbol{v}) - b_{\Omega} (\boldsymbol{v}, p) = 0 \quad \forall \boldsymbol{v} \in \boldsymbol{V}_{0} ,$$

$$b_{\Omega} (\boldsymbol{u}, q) = 0 \quad \forall q \in L^{2}(\Omega) ,$$

$$\boldsymbol{u} = \boldsymbol{u}_{0} \text{ on } \Gamma_{\text{in}} ,$$

$$\boldsymbol{u} = 0 \text{ on } \partial \Omega \setminus \Gamma_{\text{out}} ,$$
(32)

the corresponding adjoint problem (see (13)) is

$$a_{\Omega} (\boldsymbol{\nu}, \boldsymbol{w}) + b_{\Omega} (\boldsymbol{\nu}, q) = -a_{\Omega_{C}} (\boldsymbol{u}, \boldsymbol{\nu}) \quad \forall \boldsymbol{\nu} \in \boldsymbol{V}_{0} ,$$

$$b_{\Omega} (\boldsymbol{w}, \eta) = 0 \quad \forall \eta \in L^{2}(\Omega) ,$$

$$\boldsymbol{w} = 0 \text{ on } \partial\Omega \setminus \Gamma_{\text{in-out}} ,$$
(33)

and finally the sensitivity formula (14) takes the simplified form

$$\delta \Psi(\boldsymbol{u}) = \delta_D a_\Omega(\boldsymbol{u}, \boldsymbol{w}) - \delta_D b_\Omega(\boldsymbol{w}, p) + \delta_D b_\Omega(\boldsymbol{u}, q) .$$
(34)

The equations (32)-(34) were discretized by the standard P1+/P1 finite elements, using P1 pressure and P1 enriched with bubble functions velocity approximations.

The purpose of the examples shown below was to verify the shape sensitivities obtained by our code and to see the effects of a domain shape perturbation on the objective function (7).

In the following, the actual units are not important and thus they will not be written explicitly; any consistent set could be used. Our test domain was a cylinder 0.1 long of the radius 0.02, whose longitudinal cut is shown in Fig. 2, with the control domain Ω_C a smaller cylinder embedded in the domain Ω , visualized as the missing elements in the Figure. The kinematic viscosity ν was set to 12.5.

The initial geometry was then perturbed by a design velocity field $\vec{\mathcal{V}}_{pert}$ satisfying (9) as shown in Fig. 3. It was obtained by solving an auxiliary linear elasticity problem; the domain parametrization introduced above was not used here.

We proceeded as follows:

1. solve the direct problem (32) on the perturbed domain

$$\Omega_P := \Omega + \{ \vec{\mathcal{V}}_{\text{pert}} \}_{x \in \Omega} \equiv \{ x + \vec{\mathcal{V}}_{\text{pert}}(x), x \in \Omega \} ,$$

- 2. compute the objective function $\Psi(\boldsymbol{u})$ using (7) on the perturbed domain Ω_P ,
- 3. compute the sensitivity w.r.t. $-\vec{\mathcal{V}}_{pert}$ using (34) on the perturbed domain Ω_P ,
- 4. verify the sensitivity by evaluating the objective function on

$$\Omega_{+\varepsilon} := \Omega + \{\varepsilon \vec{\mathcal{V}}_{\text{pert}}\}_{x \in \Omega} , \quad \Omega_{-\varepsilon} := \Omega - \{\varepsilon \vec{\mathcal{V}}_{\text{pert}}\}_{x \in \Omega}$$

and comparing $\delta \Psi(\boldsymbol{u})$ with

$$\delta \bar{\Psi}(\boldsymbol{u}) := \frac{1}{2\varepsilon} \left(\Psi_{\Omega_{+\varepsilon}}(\boldsymbol{u}) - \Psi_{\Omega_{-\varepsilon}}(\boldsymbol{u}) \right) , \qquad (35)$$

- 5. solve the direct problem (32) on the original domain Ω ,
- 6. and finally compute the objective function, as well as test the sensitivity w.r.t. $\vec{\mathcal{V}}_{pert}$ on the original domain Ω .

Domain	Ψ	$\delta \Psi$	$\delta ar{\Psi}$	$\delta\Psi/\delta\bar{\Psi}$	$ec{\mathcal{V}}$
Ω_P	0.4065	-0.11381941	-0.11389113	0.9993702	$-ec{\mathcal{V}}_{ m pert}$
Ω	0.3528	-0.06780651	-0.06780651	1.	$ec{\mathcal{V}}_{ ext{pert}}$



Tab. 1.

Fig. 4. Ω_C .



Fig. 5. Adjoint problem, Ω .

Ľ

The sensitivity w.r.t. $\vec{\mathcal{V}}_{pert}$ of the objective function for the original domain Ω is also negative — it seems that, although the objective function ultimately increases in the direction of $\varepsilon \vec{\mathcal{V}}_{pert}$, see Tab. 1, there is a local minimum for some $\varepsilon \in [0, 1]$. Indeed, Tab. 2 proves that: Having $\Psi(\Omega) = 0.3513^3$, we have performed the step 4 for various ε and noted by \pm whether the objective functions on the perturbed domains $\Omega_{+\varepsilon}$, $\Omega_{-\varepsilon}$ increased or decreased w.r.t. $\Psi(\Omega)$. The remaining columns show the accuracy of the finite difference approximation of the sensitivity $\delta \Psi$ — it is satisfactory already for $\varepsilon = 0.01$.

 $^{^{3}}$ A little discrepancy of values in the two tables was caused by the different starting meshes which were stored in a format not using the full double precision and thus introducing round-off errors.

Overall the numerical experiments with various design velocity fields $\vec{\mathcal{V}}$ show a very good agreement of the analytical sensitivity formula (34) for the Stokes problem. In the examples presented we used an artificially constructed design velocities; however, to be able to perform the shape optimization, it should be parametrized as discussed in Section 4.. For real world applications, using the full Navier-Stokes equations will be necessary.





Fig. 6. Direct problem solution, Ω .

Fig. 7. Direct problem solution, Ω_P .

ε	$\Psi(\Omega_{+\varepsilon}):\pm$	$\Psi(\Omega_{-\varepsilon}):\pm$	$\delta \Psi$	$\delta \bar{\Psi}$	$\delta\Psi/\delta\bar{\Psi}$
1.0	0.4047 : +	1.6464 : +	-0.06780651	-0.62083869	0.1092176
0.5	0.3593 : +	0.5163 : +	-0.06780651	-0.15705514	0.43173698
0.25	0.3473 : -	0.3912 : +	-0.06780651	-0.08771283	0.77305118
0.1	0.3469 : -	0.3611 : +	-0.06780651	-0.07090143	0.95634897
0.05	0.3485 : -	0.3554 : +	-0.06780651	-0.06857715	0.9887624
0.01	0.3506 : -	0.3519 : +	-0.06780651	-0.0678373	0.99954617



6. Conclusion

In this paper we presented sensitivity analysis for steady incompressible flow problems. The shape sensitivity formulae were derived using the domain approach based on the material derivative, so that computation of gradients of velocities on boundaries is avoided. This allows for using lower order finite element approximation for achieving standard accuracy in the design gradients with respect to usual comparison with the finite difference calculations. We implemented the sensitivity procedures within our in-house code, however the testing was performed and is presented for the Stokes problem only; to overcome this temporary restriction we need to improve further our algebraic solver for the Navier-Stokes system.

We have suggested to use the Free-Form Deformation (FFD) technique for manipulating the design boundary and the mesh deformation at the same time (examples to be presented at the conference). This approach enables to obtain in an easy way the design velocity fields employed in evaluating the sensitivity formulae. As another advantage, such treatment is independent of the geometrical description of the "original" (initial) body, i.e. the surface of the channel in our case. Moreover, we have developed further the FFD approach in the sense of decomposing the design space (in 3D) into so-called sub-boxes which make possible to localize the design changes with a reduced number of design variables. On the other hand, it requires some more care regarding the continuity and smoothness constraints imposed on the design variables. Therefore, further research will be focused in this respect, which may bring this tool in industrial application (an engine exhaust piping).

Acknowledgment

This research was supported by the project "Materiály a komponenty pro ochranu životního prostředí", MSMT 1M06031.

References

- [Haslinger and Neittaanmaki 1988] Haslinger, J., Neittaanmaki, P. (1988) *Finite Element Approximation for Optimal Shape Design.* J. Wiley, Chichester.
- [Haug et al. 1986] Haug, E.J, Choi, K.K., Komkov, V. (1986) *Design Sensitivity Analysis of Structural Systems*, vol. 177, Math. in Sci. and Engrg., Academic Press.
- [Hoschek and Lasser 1992] Hoschek, J., Lasser, D. (1989) Grundlangen der geometrischen Datenverarbeitung. Teubner Verlag, Stuttgart.
- [Menzel et al. 2005] Menzel, S., Olhofer, M., Sendhoff, B. (2005) Application of free form deformation techniques in evolutionary design optimization, 6th World Congress on Structural and Multidisciplinary Optimization, Rio de Janeiro, Brazil.
- [Mohammadi and Pironneau 2001] Mohammadi, B., Pironneau, O. (2001) *Applied Shape Optimization for Fluids*, Oxford Science Publications, Oxford.
- [Rohan and Whiteman 2000] Rohan, E., Whiteman, J.R. (2000) Shape optimization of elastoplastic structures and continua. *Comput. Methods Appl. Mech. Engrg.*, 187:261–288.
- [Rohan 2003] Rohan, E. (2003) Sensitivity strategies in modelling heterogeneous media undergoing finite deformation. *Math. and Computers in Simul.*, 61:261–270.
- [Rohan and Miara 2006] Rohan, E., Miara, B. (2006) Homogenization and shape sensitivity of microstructures for design of piezoelectric bio-materials. (accepted for publication in *Mechanics of Advanced Materials and Structures*).
- [Samareh 2000] Samareh, J. A. (2000). Multidisciplinary Aerodynamic-Structural Shape Optimization Using Deformation (MASSOUD), AIAA-2000-4911. (8th AIAA/NASA/USAF/ISSMO Symposium on Multidisciplinary Analysis and Optimization, September 6-8, 2000/Long Beach, CA.)