Shape sensitivity analysis for fluids with shear-dependent viscosity

Jan Stebel

Institute of Mathematics AS CR, v.v.i.,
Technical university of Liberec

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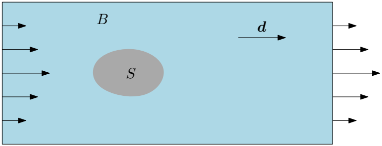
Joint work with Jan Sokołowski (Nancy)

Introduction

Goal: Sensitivity analysis of a functional which depends on the flow of a non-Newtonian fluid.

Geometry: bounded domain $\Omega := B \setminus S \subset \mathbb{R}^2$ containing an obstacle S.



We investigate the sensitivity of the drag functional

$$J(\Omega) = \int_{\partial S} (-p\mathbb{I} + \mathbb{S})\mathbf{n} \cdot \mathbf{d}, \ |\mathbf{d}| = 1,$$

with respect to smooth perturbations of the shape of S.

Flow equations

Fluid motion is described by the generalized Navier-Stokes equations:

$$\operatorname{div}(\mathbf{v} \otimes \mathbf{v}) - \operatorname{div} \mathbb{S}(\mathbb{D}\mathbf{v}) + \nabla p + \mathbb{C}\mathbf{v} = \mathbf{f} \quad \text{in } \Omega, \tag{1a}$$

$$\operatorname{div} \mathbf{v} = 0 \quad \text{in } \Omega, \tag{1b}$$

$$\mathbf{v} = \mathbf{g} \quad \text{on } \partial\Omega. \tag{1c}$$

Ω	bounded domain in $\mathbb{R}^2$
$\mathbb{S}$	deviatoric part of Cauchy stress tensor
$\mathbb{D}\mathbf{v}$	symmetric part of $\nabla\mathbf{v}$
$\mathbb{C}$	Coriolis force (constant skew-symmetric matrix)
$\mathbf{g}$	Dirichlet b.c., vanishing in the vicinity of S

Constitutive law for the fluid:

$$\mathbb{S}(\mathbb{D}\mathbf{v}) = 2\mu_0(1 + |\mathbb{D}\mathbf{v}|^2)^{\frac{r-2}{2}}\mathbb{D}\mathbf{v}, \quad r \in [2, 4).$$

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Shape derivative of a functional

Let $\{\Omega_\varepsilon\}_{\varepsilon>0}$ be a sequence of domains approaching Ω. On Ω_ε we consider the problem

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and the functional

$$J(\Omega_\varepsilon) := \int_{\partial S_\varepsilon} (-\bar{p}_\varepsilon\mathbb{I} + \mathbb{S}(\mathbb{D}\bar{\mathbf{v}}_\varepsilon))\mathbf{n}\cdot\mathbf{d}.$$

Our aim is:

- to show the existence of shape gradient of J:

$$dJ = \lim_{\varepsilon\to 0} \frac{J(\Omega_\varepsilon) - J(\Omega)}{\varepsilon}$$

- derive a formula to compute dJ.

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Remarks on the shape sensitivity analysis

Why shape sensitivity analysis

- numerical methods of shape optimization – gradient based minimization, level-set method
- stability of solutions with respect to geometry

Numerical methods of shape optimization

- **discretize-then-differentiate**

  continuous problem $\rightarrow$ approximate problem $\rightarrow$ shape gradient

  $+$ exact derivative of the approximate solution
- **differentiate-then-discretize**

  continuous problem $\rightarrow$ shape gradient $\rightarrow$ approximation

  $+$ independence of the approximation of the state problem

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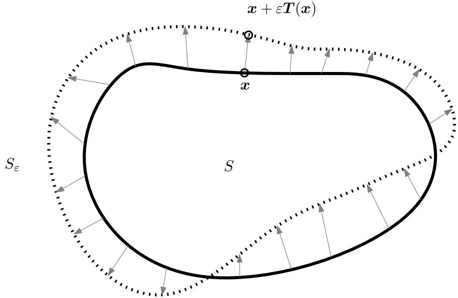
  $+$ independence of the approximation of the state problem

Parameterization of the boundary perturbation S

Let $\mathbf{T} \in \mathcal{C}^2(\mathbb{R}^2, \mathbb{R}^2)$ be a vector field vanishing in the vicinity of ∂B. We define the mapping

$$\mathbf{y}_\varepsilon = \mathbf{x} + \varepsilon \mathbf{T}(\mathbf{x}),$$

describing the deviation of material points. For small $\varepsilon > 0$ the map $\mathbf{x} \mapsto \mathbf{y}_\varepsilon$ is a diffemorphism of Ω onto $\Omega_\varepsilon = B \setminus S_\varepsilon$, where $S_\varepsilon = \mathbf{y}_\varepsilon(S)$.



Shape and material derivative of solutions

For differentiation of J we need the derivatives of solutions to (3) with respect to shape.
For formal derivation of the formula for dJ one usually uses the **shape derivative**

$$\mathbf{v}' := \lim_{\varepsilon\to 0} \frac{\bar{\mathbf{v}}_\varepsilon - \mathbf{v}}{\varepsilon}.$$

For the proof of existence of dJ the **material derivative** is useful.

$$\dot{\mathbf{v}} := \lim_{\varepsilon\to 0} \frac{\bar{\mathbf{v}}_\varepsilon \circ \mathbf{y}_\varepsilon - \mathbf{v}}{\varepsilon} = \mathbf{v}' + (\nabla\mathbf{v})\mathbf{T}.$$

We will also need a modified material derivative

$$\tilde{\mathbf{v}} := \lim_{\varepsilon\to 0} \frac{\det(\nabla\mathbf{y}_\varepsilon)\nabla\mathbf{y}_\varepsilon^{-1}(\bar{\mathbf{v}}_\varepsilon \circ \mathbf{y}_\varepsilon) - \mathbf{v}}{\varepsilon},$$

which satisfies $\operatorname{div}\tilde{\mathbf{v}} = 0$.

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Calculus for the shape and material derivatives

Let f, f_ε be defined in Ω and Ω_ε, respectively. Denote

$$f' := \lim_{\varepsilon\to 0} \frac{f_\varepsilon - f}{\varepsilon}, \quad \dot{f} := \lim_{\varepsilon\to 0} \frac{f_\varepsilon \circ \mathbf{y}_\varepsilon - f}{\varepsilon}.$$

Then it holds:

$$\begin{aligned} \frac{d}{d\varepsilon} \int_{\Omega_\varepsilon} f_\varepsilon \Big|_{\varepsilon=0} &= \int_\Omega \dot{f} + \int_\Omega f \operatorname{div} \mathbf{T} \\ &= \int_\Omega f' + \int_{\partial\Omega} f \mathbf{T}\cdot\mathbf{n}. \end{aligned}$$

General theory of shape sensitivity analysis

- under some assumptions, the shape gradient is a distribution supported on the boundary

$$dJ(\Omega; \mathbf{T}) = \langle \mathbf{G}, \mathbf{T} \cdot \mathbf{n} \rangle_{\partial S}$$

- linear elliptic problems are relatively easy to handle
- nonlinear problems: non-trivial
  - lipschitz estimates
  - regularity
  - uniqueness

Related results

Non-Newtonian fluids

- **Slawig** (2005): optimal control, stationary problem
- **Wachsmuth and Roubíček** (2010): optimal control, non-stationary problem
- **Abraham, Behr and Heinkenschloss** (2005): numerical shape optimization

Sensitivity analysis for Navier-Stokes and related systems

- **Consiglieri, Nečasová and Sokołowski** (2010): N-S + Maxwell
- **Plotnikov and Sokołowski** (2010): compressible N-S equations

General reference

- **Sokołowski and Zolésio** (1992)

Main result

Theorem

Let $\mathbf{f} \in \mathbf{W}^{1,2}(B)$, $\|\mathbf{f}\|_2 + \|\mathbf{g}\|_{3,2+\delta} \ll C$. *Then the shape gradient of* J *exists and satisfies:*

$$dJ(\Omega;\mathbf{T}) = -\int_{\partial S}\left[\left(\mathbb{S}'(\mathbb{D}\mathbf{v})^\top\mathbb{D}\mathbf{w} - s\mathbb{I}\right) : \frac{\partial\mathbf{v}}{\partial\mathbf{n}}\otimes\mathbf{n} + \mathbf{f}\cdot\mathbf{d}\right]\mathbf{T}\cdot\mathbf{n},$$

where $(\mathbf{w}, s)$ *is the solution of the linearized adjoint problem*

$$\begin{aligned} -2(\mathbb{D}\mathbf{w})\mathbf{v} - div(\mathbb{S}'(\mathbb{D}\mathbf{v})^\top\mathbb{D}\mathbf{w}) + \nabla s - \mathbb{C}\mathbf{w} &= \mathbf{0} && \text{in } \Omega,\\ div\,\mathbf{w} &= 0 && \text{in } \Omega,\\ \mathbf{w} &= \mathbf{d} && \text{on } \partial\Omega. \end{aligned}$$

Main steps of the proof

1. formal derivation of the result
2. well-posedness of the nonlinear and linearized problem
3. existence of the material derivative of weak solutions
4. differentiability of J

Formal results: distributed representation of the functional

Let $\boldsymbol{\xi} \in \mathcal{C}^{\infty}_{0,\sigma}(B)$ satisfy $\boldsymbol{\xi}_{|\partial S} = \mathbf{d}$. Applying the Green theorem we get:

$$J(\Omega) = \int_{\partial\Omega} (\mathbb{S}(\mathbb{D}\mathbf{v}) - p\mathbb{I})\boldsymbol{\xi} \cdot \mathbf{n} = \int_{\Omega} \operatorname{div} ((\mathbb{S}(\mathbb{D}\mathbf{v}) - p\mathbb{I})\boldsymbol{\xi})$$
$$= \int_{\Omega} \operatorname{div} (\mathbb{S}(\mathbb{D}\mathbf{v}) - p\mathbb{I}) \cdot \boldsymbol{\xi} + \int_{\Omega} \mathbb{S}(\mathbb{D}\mathbf{v}) : \nabla\boldsymbol{\xi}. \quad (2)$$

First term on the right of (2) can be rewritten using $(3)_1$:

$$\int_{\Omega} \operatorname{div} (\mathbb{S}(\mathbb{D}\mathbf{v}) - p\mathbb{I}) \cdot \boldsymbol{\xi} = \int_{\Omega} (\operatorname{div} (\mathbf{v} \otimes \mathbf{v}) + \mathbb{C}\mathbf{v} - \mathbf{f}) \cdot \boldsymbol{\xi}$$
$$= -\int_{\Omega} \mathbf{v} \otimes \mathbf{v} : \nabla\boldsymbol{\xi} + \int_{\Omega} (\mathbb{C}\mathbf{v} - \mathbf{f}) \cdot \boldsymbol{\xi},$$

which together with (2) yields:

$$J(\Omega) = \int_{\Omega} [(\mathbb{C}\mathbf{v} - \mathbf{f}) \cdot \boldsymbol{\xi} + (\mathbb{S}(\mathbb{D}\mathbf{v}) - \mathbf{v} \otimes \mathbf{v}) : \nabla\boldsymbol{\xi}] .$$

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Applying the rules for differentiation with respect to shape we get:

$$dJ(\Omega;\mathbf{T}) := \left.\frac{dJ}{d\varepsilon}\right|_{\varepsilon=0} = \int_{\partial S} (\mathbb{S}'(\mathbb{D}\mathbf{v})\mathbb{D}\mathbf{v}' - p'\mathbb{I}) : \mathbf{d}\otimes\mathbf{n} - (\mathbf{f}\cdot\mathbf{d})\mathbf{T}\cdot\mathbf{n}.$$

Shape derivatives $(\mathbf{v}', p')$ satisfy the linearized problem:

$$\begin{aligned} \operatorname{div}(\mathbf{v}'\otimes\mathbf{v}+\mathbf{v}\otimes\mathbf{v}') - \operatorname{div}(\mathbb{S}'(\mathbb{D}\mathbf{v})\mathbb{D}\mathbf{v}') + \nabla p' + \mathbb{C}\mathbf{v}' &= \mathbf{0} && \text{in } \Omega,\\ \operatorname{div}\mathbf{v}' &= 0 && \text{in } \Omega,\\ \mathbf{v}' &= -\frac{\partial\mathbf{v}}{\partial\mathbf{n}}\mathbf{T}\cdot\mathbf{n} && \text{on } \partial\Omega. \end{aligned}$$

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Formal results: adjoint problem

Using the adjoint system we can eliminate the shape derivatives. Let $(\mathbf{w}, s)$ be the solution to

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Well-posedness of the nonlinear problem

We can assume more general $\mathbb{S}$, satisfying for $r \in [2,4)$:

$$C_1(1+|\mathbb{A}|^{r-2})|\mathbb{B}|^2 \le \mathbb{S}'(\mathbb{A}) :: (\mathbb{B}\otimes\mathbb{B}) \le C_2(1+|\mathbb{A}|^{r-2})|\mathbb{B}|^2,$$
$$|\mathbb{S}''(\mathbb{A})| \le C_3(1+|\mathbb{A}|^{r-3}) \quad \forall 0 \ne \mathbb{A},\mathbb{B} \in \mathbb{R}^{2\times 2},$$

from which it follows:

- $\mathbb{S}$ is strongly monotone;
- $\mathbb{D} \mapsto \mathbb{S}(\mathbb{D})$ and $\mathbb{D} \mapsto \mathbb{S}'(\mathbb{D})$ is continuous from L^r to L^{r-1} and L^{r-2}, respectively.

$$\operatorname{div}(\mathbf{v}\otimes\mathbf{v}) - \operatorname{div}\mathbb{S}(\mathbb{D}\mathbf{v}) + \nabla p + \mathbb{C}\mathbf{v} = \mathbf{f} \quad \text{in } \Omega, \tag{3a}$$
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Theorem (Kaplický, Málek, Stará, 1999)

Let $\Omega \in \mathcal{C}^2$, $\mathbf{f} \in \mathbf{L}^{2+\delta}(\Omega)$ and $\|\mathbf{g}\|_{3,2+\delta,\Omega}$ be sufficiently small (for certain

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Let $\Omega \in \mathcal{C}^2$, $\mathbf{f} \in \mathbf{L}^{2+\delta}(\Omega)$ and $\|\mathbf{g}\|_{3,2+\delta,\Omega}$ be sufficiently small (for certain $\delta > 0$). Then (3) has a unique weak solution that satisfies $\mathbf{v} \in \mathbf{W}^{2,q}(\Omega)$, $q > 2$.

Well-posedness of the linearized problem

$$\operatorname{div}(\mathbf{b}\otimes\mathbf{u}+\mathbf{u}\otimes\mathbf{b})-\operatorname{div}(\mathbb{A}\nabla\mathbf{u})+\nabla q=\mathbf{f} \quad \text{in } \Omega, \tag{4a}$$

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Theorem

Let $\mathbb{A}\in L^\infty(\Omega,\mathbb{R}^{2^4})$ *be symmetric positive definite,* $\mathbf{f}\in L^2(\Omega)$, $\mathbf{b}\in\mathbf{W}^{1,2}_{0,div}$ *and* $\|\nabla\mathbf{b}\|_2\ll C$. *Then (4) has a unique weak solution.*

Smallness of $\mathbf{b}$ is required in the estimate of the convective term:

$$\int_\Omega \operatorname{div}(\mathbf{b}\otimes\mathbf{u}+\mathbf{u}\otimes\mathbf{b})\cdot\mathbf{u}=\int_\Omega \nabla\mathbf{b}:\mathbf{u}\otimes\mathbf{u}\le\|\nabla\mathbf{b}\|_2\|\nabla\mathbf{u}\|_2^2.$$

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Smallness of **b** is required in the estimate of the convective term:

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Transformation from Ω_ε to Ω

Denote

$$\mathbb{M} := \mathbb{I} + \varepsilon \nabla \mathbf{T}^\top, \ \mathfrak{g} := \det \mathbb{M}, \ \mathbb{N} := \mathfrak{g}\mathbb{M}^{-1},$$
$$\mathbf{v}_\varepsilon := \mathbb{N}^\top (\bar{\mathbf{v}}_\varepsilon \circ \mathbf{y}_\varepsilon), \quad p_\varepsilon := \bar{p}_\varepsilon \circ \mathbf{y}_\varepsilon.$$

Then the new functions $(\mathbf{v}_\varepsilon, p_\varepsilon)$, defined in Ω, satisfy:

Problem for $(\mathbf{v}_\varepsilon, p_\varepsilon)$

$$\begin{aligned} \operatorname{div}(\mathbf{v}_\varepsilon \otimes \mathbf{v}_\varepsilon) - \mathbb{N}^{-1}\operatorname{div}(\mathbb{N}^\top \mathbb{S}(\mathbb{D}_\varepsilon \mathbf{v}_\varepsilon)) + \nabla p_\varepsilon + \mathbb{C}\mathbf{v}_\varepsilon &= \mathbf{f} + \mathbf{A}^1_\varepsilon && \text{in } \Omega, \\ \operatorname{div} \mathbf{v}_\varepsilon &= 0 && \text{in } \Omega, \\ \mathbf{v}_\varepsilon &= \mathbf{g} && \text{on } \partial\Omega. \end{aligned}$$

Here $\mathbb{D}_\varepsilon \mathbf{v}_\varepsilon := \mathfrak{g}^{-1}(\mathbb{N}\nabla(\mathbb{N}^{-\top}\mathbf{v}_\varepsilon))_{sym}$, and $\mathbf{A}^1_\varepsilon \in \mathbf{W}^{1,2}_{0,div}(\Omega)^*$ is of order ε:

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Transformation from Ω_ε to Ω

Denote

$$\mathbb{M} := \mathbb{I} + \varepsilon \nabla \mathbf{T}^\top, \ \mathfrak{g} := \det \mathbb{M}, \ \mathbb{N} := \mathfrak{g}\mathbb{M}^{-1},$$
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Using the standard technique of the theory of Navier-Stokes equations we get from the equation for $\mathbf{v}_\varepsilon$:

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Thus, there exists a weak limit $\bar{\mathbf{v}}$ of a subsequence of $\{\mathbf{v}_\varepsilon\}$ in the above spaces. From strong monotonicity of $\mathbb{S}$ it follows:

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System for the differences

Next we want to estimate the differences

$$(\mathbf{u}_\varepsilon, q_\varepsilon) := \left(\frac{\mathbf{v}_\varepsilon - \mathbf{v}}{\varepsilon}, \frac{p_\varepsilon - p}{\varepsilon} \right).$$

System for differences $(\mathbf{u}_\varepsilon, q_\varepsilon)$

$$\operatorname{div}(\mathbf{v}_\varepsilon \otimes \mathbf{u}_\varepsilon + \mathbf{u}_\varepsilon \otimes \mathbf{v}) - \mathbb{N}^{-1}\operatorname{div}\left(\mathbb{N}^\top \frac{\mathbb{S}(\mathbb{D}_\varepsilon \mathbf{v}_\varepsilon) - \mathbb{S}(\mathbb{D}_\varepsilon \mathbf{v})}{\varepsilon}\right)$$

$$+\nabla q_\varepsilon + \mathbb{C}\mathbf{u}_\varepsilon = \frac{1}{\varepsilon}\mathbf{A}_\varepsilon \quad \text{in } \Omega,$$

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Lipschitz estimates

Thanks to the regularity of **v** it holds:

$$\left\{\frac{1}{\varepsilon}\mathbf{A}_\varepsilon\right\}_{\varepsilon>0} \quad \text{is bounded in } \mathbf{W}^{1,2}_{0,div}(\Omega)^*.$$

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Convergence to the material derivative

Using strong convergence of $\mathbb{D}\mathbf{v}_\varepsilon$ and the Lipschitz estimates we have:

$$\mathbf{u}_\varepsilon \rightharpoonup \tilde{\mathbf{v}},$$
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where $\tilde{\mathbf{v}}$ is a solution to the linearized problem:

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This problem has for small $\|\nabla\mathbf{v}\|_2$ a unique weak solution, we have therefore proved the existence of the material and shape derivative of $\mathbf{v}$.

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Differentiability of the functional J

Volume representation of $J(\Omega)$ and $J(\Omega_\varepsilon)$:

$$J(\Omega) = \int_\Omega [(\mathbb{C}\mathbf{v} - \mathbf{f}) \cdot \boldsymbol{\xi} + (\mathbb{S}(\mathbb{D}\mathbf{v}) - \mathbf{v} \otimes \mathbf{v})] : \nabla \boldsymbol{\xi}.$$

$$J(\Omega_\varepsilon) = \int_\Omega \Big[\mathfrak{g} \left(\mathbb{N}^{-1} \mathbb{C} \mathbb{N}^{-\top} \mathbf{v}_\varepsilon - \mathbb{N}^{-1} (\mathbf{f} \circ \mathbf{y}_\varepsilon) \right) \cdot \boldsymbol{\xi} + \left(\mathbb{N}^\top \mathbb{S}(\mathbb{D}_\varepsilon \mathbf{v}_\varepsilon) - \mathbf{v}_\varepsilon \otimes (\mathbb{N}^{-\top} \mathbf{v}_\varepsilon) \right) : \nabla (\mathbb{N}^{-\top} \boldsymbol{\xi}) \Big].$$

Differentiability of the functional J

Using the derived convergence of $\mathbf{v}_\varepsilon$, $\mathbf{u}_\varepsilon$ one can show that

$$\frac{J(\Omega_\varepsilon) - J(\Omega)}{\varepsilon} \to dJ(\Omega; \mathbf{T}) = J_D(\tilde{\mathbf{v}}) + J_G(\mathbf{T}),$$

where J_D and J_G are bounded linear functions of $\tilde{\mathbf{v}}$, resp. $\mathbf{T}$. Since $\tilde{\mathbf{v}}$ depends continuously on the $\mathcal{C}^2$-norm of $\mathbf{T}$,

$$\mathbf{T} \mapsto dJ(\Omega; \mathbf{T})$$

is a bounded linear functional on $\mathcal{C}^2(\mathbb{R}^2, \mathbb{R}^2)$. This justifies the formal calculation of dJ.

Numerical computation of shape gradient of J

1. **Computation of $(\mathbf{v}, p)$ and J**
   - FEM, P2/P1 approximation on simplices
   - Linearization by Newton-Raphson method
   - Jacobian computed with help of automatic differentiation
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2. **Computation of dJ: differences**
   - Compute $(\mathbf{v}, p)$ and $J(\Omega)$
   - For each node on ∂S: shift by δ in the normal direction, on the new domain compute $(\mathbf{v}_\varepsilon, p_\varepsilon)$, $J(\Omega_\varepsilon)$
   - $dJ_i \approx \frac{J(\Omega_\varepsilon)-J(\Omega)}{\delta}$
3. **Computation of dJ: sensitivity analysis**
   - Compute $(\mathbf{v}, p)$
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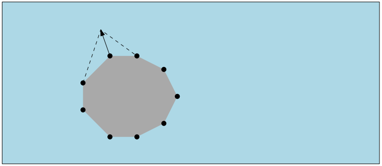

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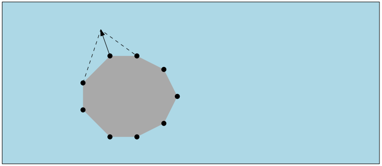

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Comparison of methods for computing the shape gradient

Differences

+ easy implementation
+ easy parallelization
- computationally expensive: $n+1$ nonlinear problems
- limited accuracy, sensitivity w.r.t. the choice of δ

Sensitivity analysis

+ efficient computation: 1 nonlinear and 1 linear problem
- difficult derivation of the formula and its proof
- possible discrepancy between continuous and approximate problem

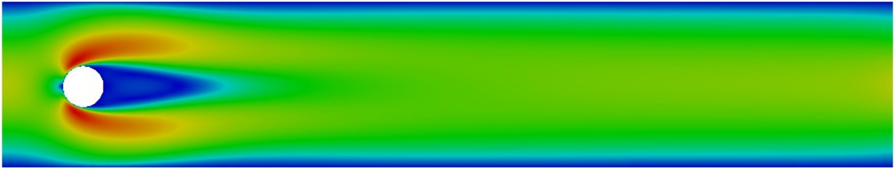
Numerical computation of shape gradient

Flow around a cylinder

$$\mathbb{S}(\mathbb{D}\mathbf{v}) = \mu_0(1 + |\mathbb{D}\mathbf{v}|^2)^{\frac{r-2}{2}}\mathbb{D}\mathbf{v}, \ \mu_0 = 2 \times 10^{-3}$$

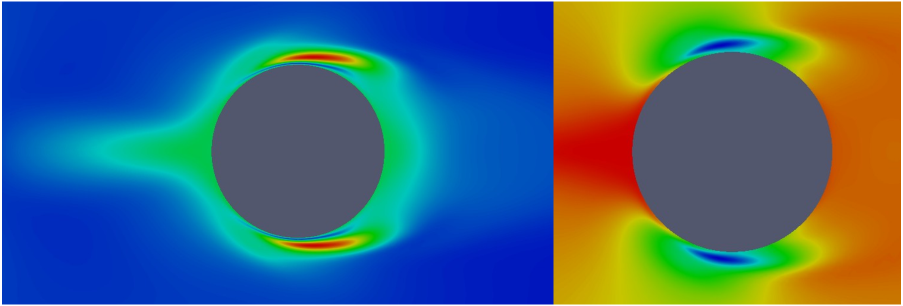
$$\mathbb{C} = 0$$

Inflow and outflow velocity given by the parabolic profile.



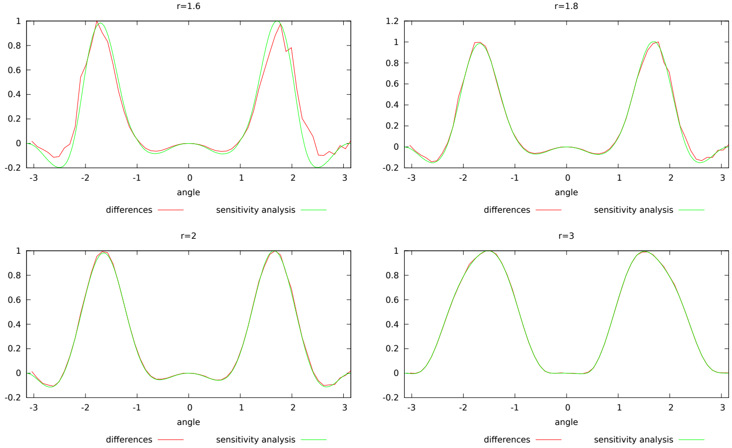
Velocity magnitude, $r = 1.4$.

Numerical computation of shape gradient



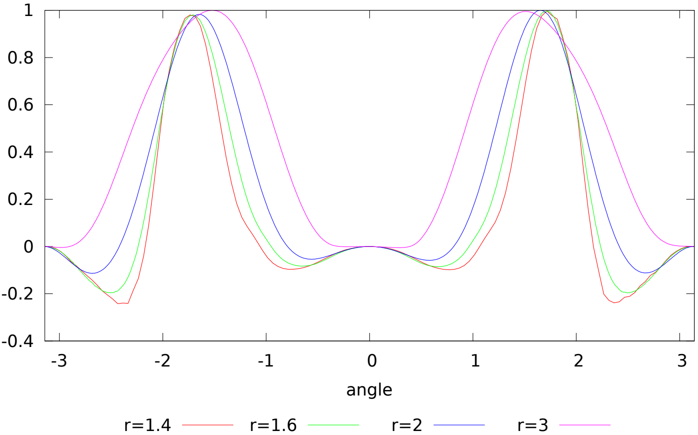
Adjoint velocity and pressure in the vicinity of the cylinder, $r = 1.4$.

Numerical computation of shape gradient



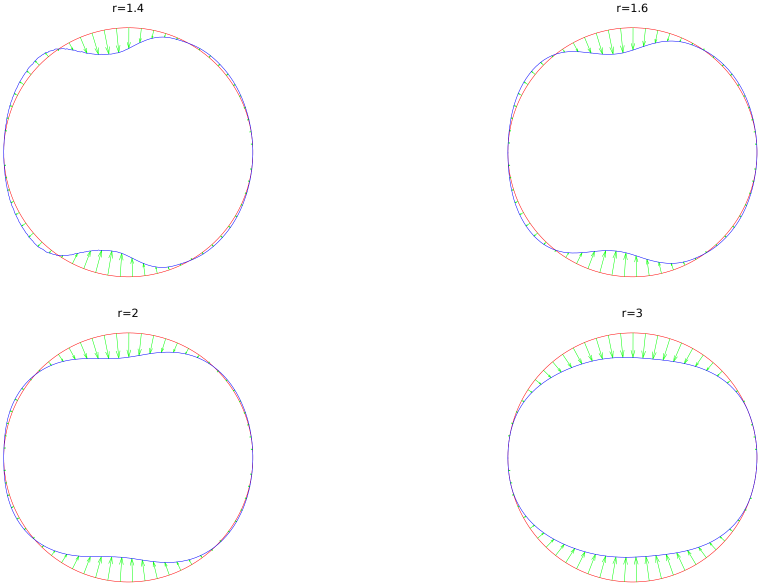
Comparison of the results (differences vs. sensitivity analysis).

Numerical computation of shape gradient



Shape gradient of J around the cylinder.

Numerical computation of shape gradient



Thank you for attention!