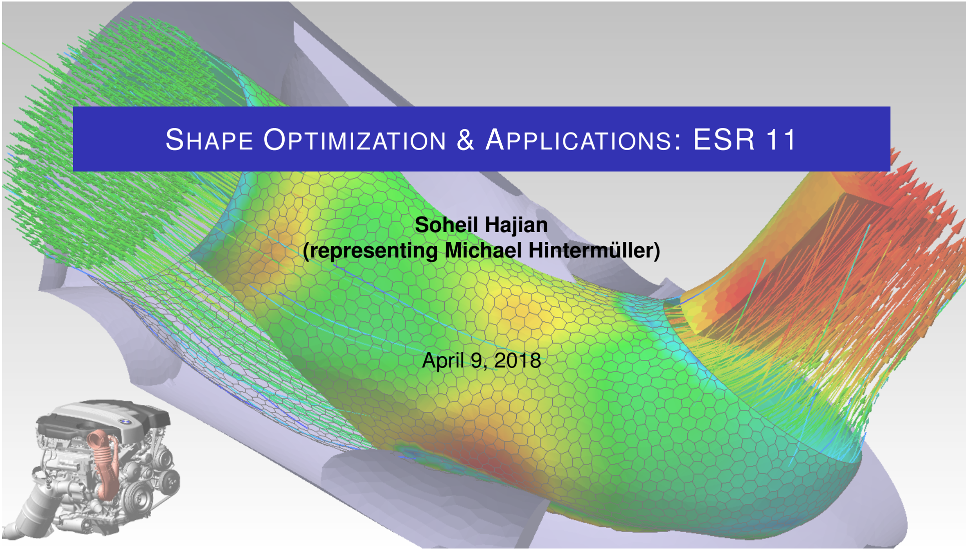

Shape Optimization & Applications: ESR 11

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(representing Michael Hintermüller)

April 9, 2018

Weierstrass Institute for Applied Analysis and Stochastics

- Founded in 1992
- project oriented research in applied mathematics with the aim of solving complex problems in technology, science and the economy.
- 156 employees, including 125 scientists (as at end of 2016)
- Scientifically independent non-university research institute
- Part of Forschungsverbund Berlin e.V. (joint administration for eight institutes) and a member of Leibniz Association
- Leibniz Association connects 91 research institutions that range in focus from the natural, engineering and environmental sciences via economics, spatial and social sciences to the humanities.

Scientific structure

RG1	RG2	RG3	RG4
PARTIAL DIFFERENTIAL EQUATIONS Prof. Dr. Alexander Mielke	LASER DYNAMICS PD Dr. Uwe Bandelow	NUMERICAL MATHEMATICS AND SCIENTIFIC COMPUTING Prof. Dr. Volker John	NONLINEAR OPTIMIZATION AND INVERSE PROBLEMS Prof. Dr. Dietmar Hömberg

RG5	RG6	RG7	RG8
INTERACTING RANDOM SYSTEMS Prof. Dr. Wolfgang König Partial Differential	STOCHASTIC ALGORITHMS AND NONPARAMETRIC STATISTICS Prof. Dr. Vladimir Spokoiny	THERMODYNAMIC MODELING AND ANALYSIS OF PHASE TRANSITIONS Prof. Dr. Barbara Wagner (acting head)	NONSMOOTH VARIATIONAL PROBLEMS AND OPERATOR EQUATIONS Prof. Dr. Michael Hintermüller

and three flexible research platforms

- **Weierstrass Group:** Modeling, Analysis, and Scaling Limits for Bulk-Interface Processes (until 07/20)
  Dr. Marita Thomas
- **Leibniz Group:** Probabilistic Methods for Mobile Ad-hoc Networks (until 12/17)
  Prof. Dr. Wolfgang König
- **Fokus Platform:** Quantitative Analysis of Stochastic and Rough Systems
  Prof. Dr. Peter K. Friz and Dr. Christian Bayer

MATH+TEC

- Established in 2009
- Expertise in warehouse logistics, production logistics, transport logistics and industry optimization as well as numerical simulation of fluids
- Main products:
  1. MATH.TOUR (mathematical route optimisation)
  2. MATH.PICK (warehouse optimisation software)
  3. MATH.PACK (3D packing calculation for load carriers)

Shape optimization of air ducts

Navier-Stokes equations

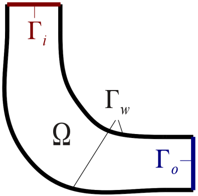
Stationary regime for the velocity $\boldsymbol{u}$ and the kinematic pressure p:

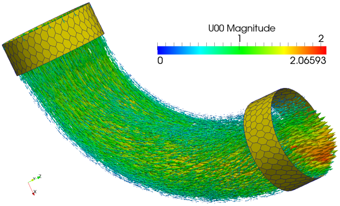
$$
\begin{aligned}
(\boldsymbol{u}\cdot\nabla)\,\boldsymbol{u} - \nu\Delta\boldsymbol{u} + \nabla p &= \mathbf{0} \quad \text{in } \Omega,\\
\nabla\cdot\boldsymbol{u} &= 0 \quad \text{in } \Omega,\\
\boldsymbol{u} &= \boldsymbol{g} \quad \text{on } \Gamma_i,\\
\boldsymbol{u} &= \mathbf{0} \quad \text{on } \Gamma_w,\\
-\nu\partial_n\boldsymbol{u} + p\boldsymbol{n} &= \mathbf{0} \quad \text{on } \Gamma_o.
\end{aligned}
$$

$\boldsymbol{g}$: inflow profile

ν : kinematic viscosity

$\boldsymbol{n}$: outer normal vector





To achieve **uniform outflow** at the outlet the cost functional

$$\mathcal{J}_1\left(\boldsymbol{u}(\Omega)\right) = \frac{1}{2}\int_{\Gamma_o} \left(\boldsymbol{u}\cdot\boldsymbol{n} - \bar{u}\right)^2 \qquad \text{mit} \quad \bar{u} = \frac{1}{|\Gamma_o|}\int_{\Gamma_i} -\boldsymbol{g}\cdot\boldsymbol{n}. \tag{1}$$

is used. To minimize the **total pressure loss** we use

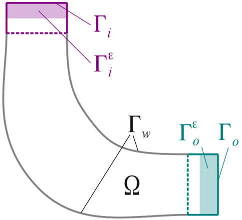
$$\mathcal{J}_2\left(\boldsymbol{u}(\Omega)\right) = -\frac{|\Gamma_i|}{|\Gamma_i^\varepsilon|}\int_{\Gamma_i^\varepsilon}\left(p + \frac{1}{2}|\boldsymbol{u}|^2\right)\boldsymbol{u}\cdot\boldsymbol{n} - \frac{|\Gamma_o|}{|\Gamma_o^\varepsilon|}\int_{\Gamma_o^\varepsilon}\left(p + \frac{1}{2}|\boldsymbol{u}|^2\right)\boldsymbol{u}\cdot\boldsymbol{n}. \tag{2}$$

Mixed cost functional

$$\mathcal{J}_{12}\left(\boldsymbol{u}(\Omega)\right) = (1-\gamma)\,\mathcal{J}_1\left(\boldsymbol{u}(\Omega)\right) + \gamma\rho\mathcal{J}_2\left(\boldsymbol{u}(\Omega)\right) \tag{3}$$

with weighting parameter $\gamma \in [0,1]$ and

$$\rho = \begin{cases} \dfrac{\left\|\partial\mathcal{J}_1\left(\boldsymbol{u}\left(\Omega^0\right)\right)\right\|_{L^2\left(\Gamma_w^0\right)}}{\left\|\partial\mathcal{J}_2\left(\boldsymbol{u}\left(\Omega^0\right)\right)\right\|_{L^2\left(\Gamma_w^0\right)}} & \text{, if } \gamma \in (0,1)\,, \\ 1 & \text{, if } \gamma \in \{0,1\}. \end{cases}$$



Weighted shape gradient

Adjoint equation:

$$
\begin{aligned}
-\nu\Delta \boldsymbol{v} - (\nabla \boldsymbol{v})^T \cdot \boldsymbol{u} - \nabla \boldsymbol{v}\cdot \boldsymbol{u} + \nabla q &= \gamma\, \nu k_\varepsilon \left[(\boldsymbol{u}\cdot\boldsymbol{n})\boldsymbol{u} + \left(p + \frac{1}{2}|\boldsymbol{u}|^2 \right) \boldsymbol{n} \right] \text{ in } \Omega,\\
\nabla \cdot \boldsymbol{v} &= -\gamma \nu k_\varepsilon \boldsymbol{u}\cdot\boldsymbol{n} \quad \text{in } \Omega,\\
\boldsymbol{v} &= 0 \quad \text{auf } \Gamma_i \cup \Gamma_w,\\
-\nu\partial_n \boldsymbol{v} - \boldsymbol{n}\,(\boldsymbol{u}\cdot\boldsymbol{v}) - (\boldsymbol{u}\cdot\boldsymbol{n})\,\boldsymbol{v} + q\boldsymbol{n} &= -(1-\gamma)\,\nu\,(\boldsymbol{u}\cdot\boldsymbol{n} - \bar{u})\,\boldsymbol{n} \quad \text{auf } \Gamma_o
\end{aligned}
$$

with $$k_\varepsilon(x) = \begin{cases} -\frac{|\Gamma_i|}{|\Gamma_i^\varepsilon|} & \text{if } x \in \Gamma_i^\varepsilon,\\ -\frac{|\Gamma_o|}{|\Gamma_o^\varepsilon|} & \text{if } x \in \Gamma_o^\varepsilon,\\ 0 & \text{else.} \end{cases}$$

Euler-semiderivative:

$$\partial \mathcal{J}_{12}^{\gamma}(\Omega; V) = \int_{\Gamma_w} [\partial_n \boldsymbol{v} \cdot \partial_n \boldsymbol{u}]\; V\cdot\boldsymbol{n}.$$

Shape gradient:

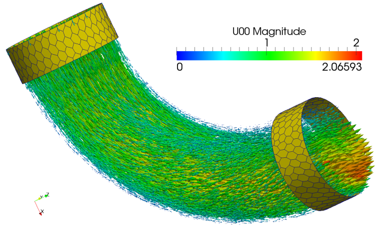
$$D\mathcal{J}_{12}^{\gamma}(\Omega) = (\partial_n \boldsymbol{v} \cdot \partial_n \boldsymbol{u})\,|_{\Gamma_w}.$$

Adjoint solution and shape gradient

Shape gradient on a simple 3D geometry with Reynolds number 150:

The solution $\boldsymbol{u}$ of the Navier-Stokes equations is shown in the upper right figure.

The corresponding adjoint solution and the **negative shape gradient** coloured on the surface are presented in the figures below.



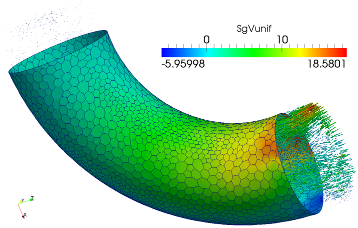


Figure 1: Uniform outflow.

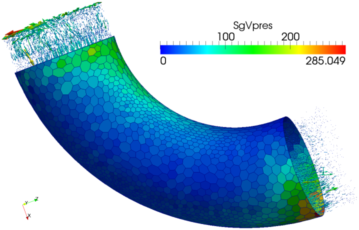
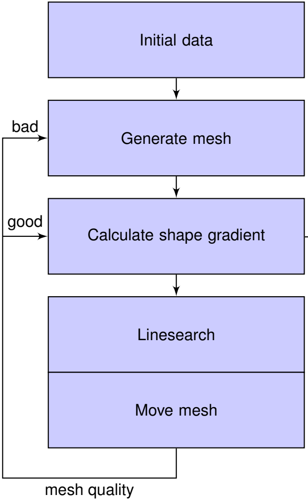


Figure 2: Total pressure loss.

Descent algorithm: calculation of the shape gradient

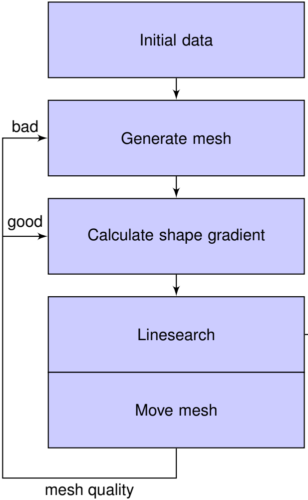


- Solve primal equation in $\Omega^k \to (\boldsymbol{u}, p)$.
- Solve adjoint equation in $\Omega^k \to (\boldsymbol{v}, q)$.
- Calculate shape gradient:

$$\mathcal{D}\mathcal{J}_{12}^{\alpha}\left(\Omega^k; \boldsymbol{x}\right) = \partial_n \boldsymbol{v}\left(\Omega^k; \boldsymbol{x}\right) \cdot \partial_n \boldsymbol{u}\left(\Omega^k; \boldsymbol{x}\right) + \alpha\, \ell\,(\boldsymbol{x})$$

for $\boldsymbol{x}$ on Γ_w.

Descent algorithm: usage of Armijo linesearch



Armijo - linesearch:

$$\mathcal{J}_{12}^{\alpha}\left(\Omega^{k+1}\right) \leq \mathcal{J}_{12}^{\alpha}\left(\Omega^{k}\right) - \mu s_k \|\mathcal{D}\mathcal{J}_{12}^{\alpha}\left(\Omega^{k}\right)\|_{L^2\left(\Gamma_w^k\right)}$$

with $0 < \mu < 1$ and $\Omega^{k+1} = \mathcal{T}_{D\left(s_k,\Omega^k\right)}\left(\Omega^k\right)$

We need to evaluate the cost functional in Ω_{k+1}. This requires to solve the primal equation, therefore:

- ensure mesh quality of Ω_{k+1} (by reduction of the step length),
- guarantee efficiency by avoiding unnecessary recalculations of the primal solution.

Geometrical constraint: design space

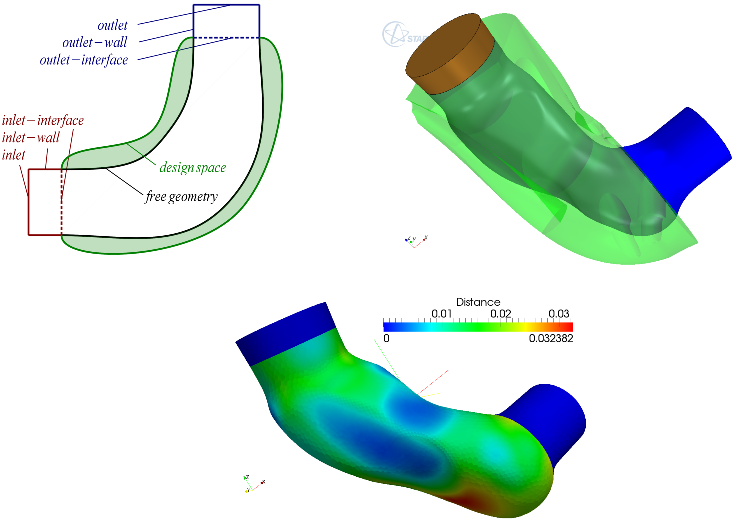


Figure 3: Sketch, geometry with transparent design space, geometry with distance values to the design space.

The minimization problem with geometrical constraint

$$\text{minimize} \mathcal{J}_{12}\left(\boldsymbol{u}\left(\Omega\right)\right) \qquad \text{s.t.} \quad \Omega \subset K \tag{4}$$

can be reformulated as

$$\text{minimize} \mathcal{J}_{12}\left(\boldsymbol{u}\left(\Omega\right)\right) + \alpha \mathcal{L}\left(\Omega\right) \tag{5}$$

with $\alpha > 0$ and $\mathcal{L}\left(\Omega\right) = \int_\Omega \ell\left(\Omega\right)$.

We are using two approaches:
barrier method:

$$\ell\left(\Omega\right) = \left|\ln d\left(x, K^c\right)\right|, \tag{6}$$

penalty method:

$$\ell\left(\Omega\right) = \left(d\left(x, K\right)\right)^\beta, \tag{7}$$

with $\beta \geq 1$, $K^c = \mathbb{R}^n \setminus K$ and the distance function $d\left(x, K\right) = \min_{y \in K} |x - y|$.

The sensitivity is calculated by

$$\partial \mathcal{L}\left(\Omega, V\right) = \int_\Omega \ell'\left(\Omega, V\right) dx + \int_\Gamma \ell\left(\Omega\right) \left\langle V\left(0\right), \boldsymbol{n}\right\rangle = \int_\Gamma \ell\left(\Omega\right) \left\langle V\left(0\right), \boldsymbol{n}\right\rangle. \tag{8}$$

Geometrical constraint: fixed interface

To avoid kinks between the fixed geometry and the geometry, which needs to be optimized, we add a penalty functional (green) to the cost functional

$$\mathcal{J}_{12}^{\alpha,\varphi}\left(\boldsymbol{u}\left(\Omega\right)\right) = \mathcal{J}_{12}\left(\boldsymbol{u}\left(\Omega\right)\right) + \alpha\mathcal{L}\left(\Omega\right) + \varphi\mathcal{L}_F\left(\Omega\right)$$

with $\mathcal{L}_F\left(\Omega\right) = \int_\Omega (d(x, K_F))^2$, weight φ, distance function d and valid domain K_F.

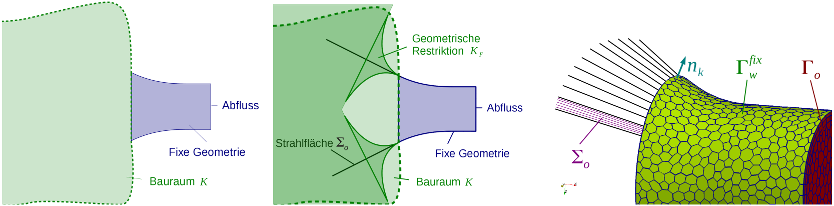


Figure 4: Left: fixed geometry (blue) and design space (green). Middle: additional valid domain. Right: continuation of the fixed geometry.

The sensitivity is calculated by

$$\partial\mathcal{L}_F\left(\Omega, V\right) = \int_\Gamma \ell_F\left(\Omega\right)\left\langle V\left(0\right), \boldsymbol{n}\right\rangle \quad \text{with } \ell_F = (d(x, K_F))^2.$$

Turbulence modelling for high Reynolds numbers

For applications with high Reynolds numbers (200.000) we use a K-epsilon turbulence model. The kinematic viscosity ν in the Navier-Stokes equations is replaced by the effective viscosity, which is the sum of kinematic and turbulent viscosity:

$$\nu_{eff} = \nu + \nu_t.$$

Instead of the convection equation

$$\boldsymbol{u}_t + \nabla \cdot \left(\boldsymbol{u}\boldsymbol{u}^T\right) - \nu\Delta\boldsymbol{u} + \nabla p = \boldsymbol{0} \tag{9}$$

the equation

$$\boldsymbol{u}_t + \nabla \cdot \left(\boldsymbol{u}\boldsymbol{u}^T\right) - \nabla \cdot \left(\left(\nu + \nu_t\right)\nabla\boldsymbol{u}\right) + \nabla\left(p + \frac{2}{3}k\right) = \boldsymbol{0} \tag{10}$$

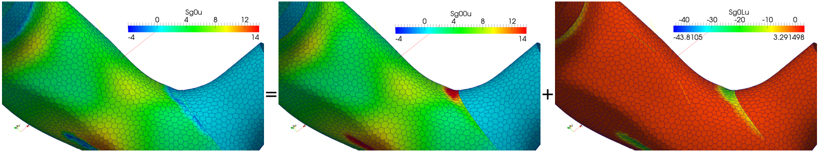
is solved with $\nu_t = C_\nu \frac{k^2}{\varepsilon}$. The kinetic energy k and the dissipation ε are solutions of

$$\begin{aligned} \partial_t k &= -\left(\boldsymbol{u}\cdot\nabla\right)k + \nabla\cdot\left(\left(\nu+\nu_t\right)\nabla k\right) + \nu_t\left|\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T\right|^2 - \varepsilon & (11)\\ \partial_t\varepsilon &= -\left(\boldsymbol{u}\cdot\nabla\right)\varepsilon + \nabla\cdot\left(\left(\nu + \frac{\nu_t}{\sigma_\varepsilon}\right)\nabla\varepsilon\right) + C_1\frac{\varepsilon}{k}\nu_t\left|\nabla\boldsymbol{u}+\nabla\boldsymbol{u}^T\right|^2 - C_2\frac{\varepsilon^2}{k} & (12)\end{aligned}$$

with standard model constants $C_\nu = 0.09$, $C_1 = 1.44$, $C_2 = 1.92$, $\sigma_\varepsilon = 1.3$.

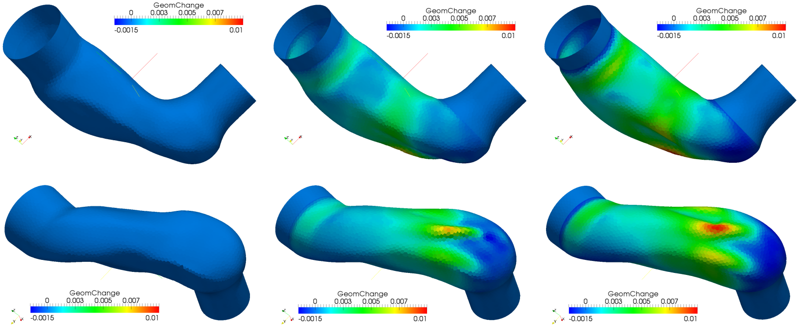
Shape optimization after 20 iterations:

- Left: negative shape gradient.
- Middle: part of the shape gradient related to achieve uniform outflow and minimizing the total pressure loss.
- Right: part of the shape gradient related to the geometrical constraints.



Shape optimization with geometrical constraints for Re=200.000

Geometry with the change of geometry coloured by the distance values to the initial geometry at iteration 0, 20 70.



Geometry after 70 iterations and distance values to the design space (in meter). The optimal geometry is at most 0.2mm outside of the design space.

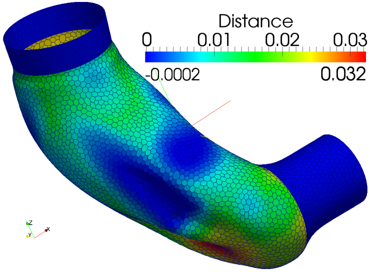


Figure 5: Left: distance values. Right: distance values outside of the design space.

Laplace-Beltrami smoothing

Equation on the surface Γ:

$$
\begin{aligned}
-\varepsilon\Delta_\Gamma w + w &= -g_{\mathcal{J}_{12}} \quad \text{auf} \quad \Gamma, && (13)\\
w &= 0 \quad \text{auf} \quad \partial\Gamma. && (14)
\end{aligned}
$$

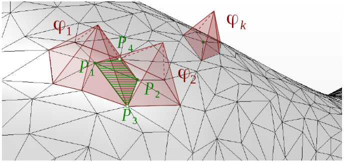
Benefits of the Laplace-Beltrami usage:

- Higher regularity of each grid movement.
- Keeping the property of a descent direction.
- Preconditioning gradient method.

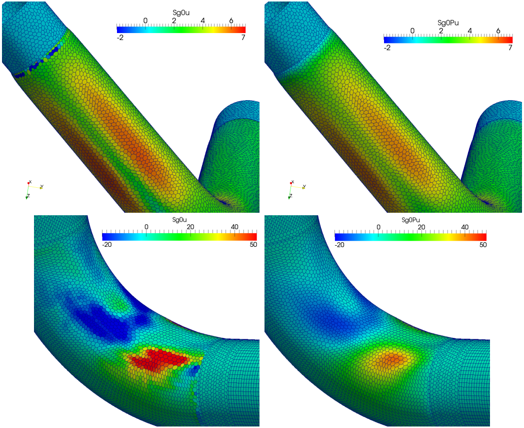
Notes on the numerical realiszation:

- Usage of a triangulated surface mesh - grid management in OpenFOAM.
- Discretization with finite elemets 3D tent function.
- Efficient storage of sparse matrix and usage of iterative solver.

Linear basis functions φ_j on a triangulated surface with common support $supp\,(\varphi_1\varphi_2) \neq 0$.



Laplace-Beltrami smoothing: numerical results



$$
\begin{aligned}
-\varepsilon \Delta_\Gamma w + w &= -g_{\mathcal{J}_{12}} && \text{auf } \Gamma, \\
w &= 0 && \text{auf } \partial\Gamma.
\end{aligned}
$$

Figure 6: Left: without LB-smoothing, middle: using LB-smoothing.

Shape optimization tested on other geometries

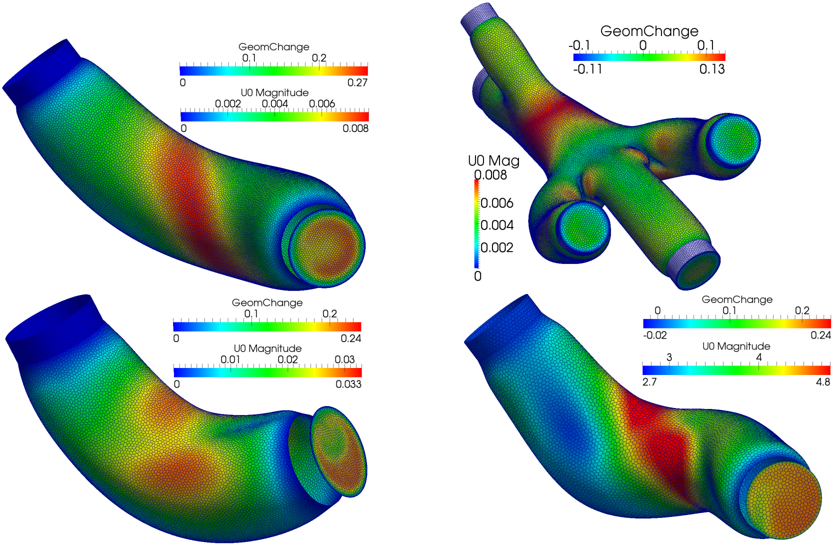


Figure 7: Final geometries: upper: Re = 200, Re = 400;
lower: Re = 1000, Re = 200 000.

Program

- Navier-Stokes system w/ turbulence model
- multi-criteria optimization
- continuous adjoint-based optimization solver w/ turbulence model
- preconditioning, MOR, parallelization
- design / construction space constraint
- flexible application context
- many advanced features (smoothing, mesh quality, remeshing)
- industrial apps + prototyping