# Adjoint thermo optimization

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Institute of Scientific Computing/move-csc

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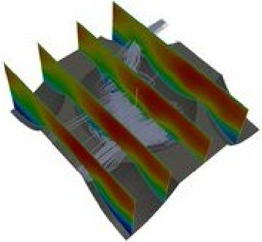


# Optimal shape design

## Motivation

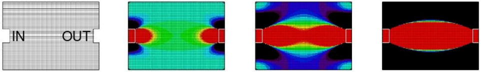
- Find the optimal design, i.e.
  - shape
  - volume
    (surface mesh/volume mesh)

  which minimizes/maximizes a certain cost functional, e.g.
  - drag
  - noise
  - pressure loss
  - strain
  - weight
  - swirl

# Different optimization tasks

## Topology optimization

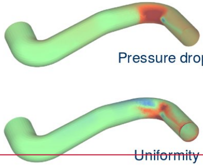
- Volume optimization – starting point **maximal design space**
- Design variable $\alpha_i$ (porosity/virtual sand)

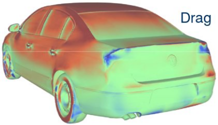



Borrvall, Petterson: *Topology optimization of fluids in Stokes flow*, Num.Meth.Fluids. 41, 2003

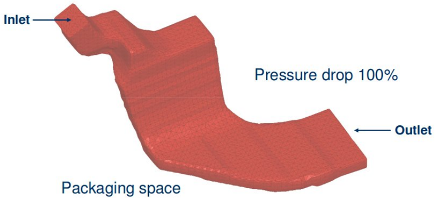
## Shape optimization

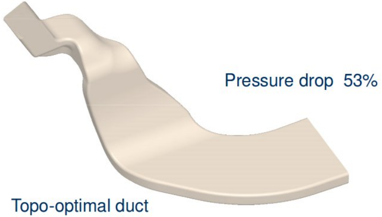
- Surface optimization
- starting point **topology optimization**
- Design variable $\beta_i$ (surface normal displacement)



# Example | Duct optimization

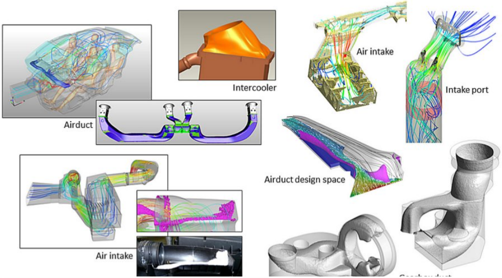


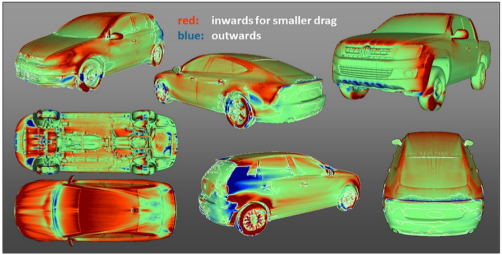




T. T. Robinson, C. G. Armstrong, H. S. Chua, C. Othmer, Th. G.
*Optimizing Parameterized CAD Geometries Using Sensitivities Based on Adjoint Functions*
Computer-Aided Design and Applications 9(3):253-268, 2012.

# Examples | Topology & shape optimization

Othmer et al.
(2006 - today)
VW Research



# References

## General approach stems from control theory

### Introduction into PDEs

- Lions (1971) *Optimal Control of Systems Governed by PDEs*
- Pironneau (1984) *Optimal shape design for elliptic systems*

### Introduction into CFD

- Jameson (1988) *Aerodynamic design via control theory*
- Giles (1997) *Design optimisation for complex geometries*
- Löhner (2003) *An adjoint-based design methodology for CFD optimization problems*

### Topology optimization for CFD

- Borrvall/Petersson (2003) *Topology optimization of fluids in Stokes flows*
- Othmer/Grahs (2005) *Approaches to fluid dynamic optimization in the car development process*
- Othmer (2006-today) *Surface & topo optimization in industrial context*
- Othmer (2008) *A continuous adjoint formulation for the computation of topological and surface sensitivities of ducted flows*, Int. J. Numer. Methods Fluids 58.

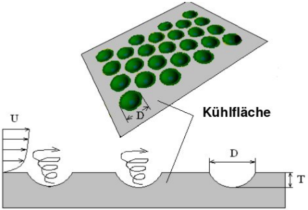
# Adjoint heat shape optimization

Apply the shape optimization process
(**adjoint approach**) to heat depended problems

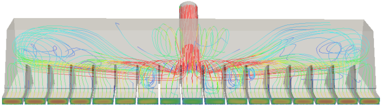
- **Tasks**
  - Augment governing equations (*Navier-Stokes*) with heat/temperature
  - Derive adjoint system
  - Choose desired optimization goal (*cost function*)
  - Derive boundary conditions w.r.t. cost function
  - Solve primal-adjoint system
  - Update surface (*normal displacement*)
    by means of *sensitivity information* from primal-adjoint system

# Applications

- Heat transfer on dimpled surfaces




- Uniformity at HVAC outlets



- ...

Joined work with *Johan Turnow, Uni Rostock*

# Formulation

- Let $I$ be a specific cost function
- $\Omega \subset \mathbb{R}^N$ an admissible domain with boundary $\Gamma$
- Typically, the form has to satisfy a set of given constraints $\mathcal{R} = 0$ mostly defined as PDEs with state variables $U$.
- The form is parametrized by of set of design variables $\beta$
- We can formulate the problem by

$$\min_{\beta} / \max I(\mathbf{s}, \alpha) \quad \text{subject to} \quad \mathbf{r}(\mathbf{s}, \beta) = 0 \text{ on } \Omega$$

# Sensitivity

- We look for the sensitivity of the cost function wrt. the design variables, i.e.

$$\frac{dI}{d\beta} = \frac{\partial I}{\partial \mathbf{s}}\frac{d\mathbf{s}}{d\beta} + \frac{\partial I}{\partial \beta} \quad \text{with constraint} \quad \frac{\partial \mathbf{r}}{\partial \mathbf{s}}\frac{d\mathbf{s}}{d\beta} + \frac{\partial \mathbf{r}}{\partial \beta} = 0$$

- By defining

$$\mathbf{g}^T := \frac{\partial I}{\partial \mathbf{s}}, \quad \mathbf{u} := \frac{\partial \mathbf{s}}{\partial \beta}, \quad \mathbf{A} := \frac{\partial \mathbf{r}}{\partial \mathbf{s}}, \quad \mathbf{f} := -\frac{\partial \mathbf{r}}{\partial \beta}$$

we can convert this in standard form

$$\frac{dI}{d\beta} = \mathbf{g}^T\mathbf{u} + \frac{\partial I}{\partial \beta} \quad \text{subjected to} \quad \mathbf{A}\mathbf{u} = \mathbf{f}$$

- One can evaluate $\mathbf{g}^T\mathbf{u}$ by solving $\mathbf{A}\mathbf{u} = \mathbf{f}$

# Shifting to the dual problem

## Problem

- For multiple design variable $\beta_i$ (f.i. *surface nodes*)
  each has different $\mathbf{f} := -\frac{\partial \mathbf{r}}{\partial \beta}$

  $\Rightarrow$ As many primal solution $\mathbf{u}$ as design variables required

## Remedy

- Shift to the dual or adjoint system $\mathbf{A}^\star \mathbf{v} = \mathbf{g}$
- Solve once for $\mathbf{v}$ and can evaluate

$$\mathbf{g}^T \mathbf{u} \equiv \mathbf{v}^T \mathbf{f}$$

This holds since we have

$$\mathbf{v}^T \mathbf{f} = \mathbf{v}^T \mathbf{A} \mathbf{u} = (\mathbf{A}^\star \mathbf{v})^T \mathbf{u} = \mathbf{g}^T \mathbf{u}$$

# Alternative Lagrange viewpoint

- We introduce Lagrange function/multipliers and transform into an unconstrained optimization problem:

$$L(\mathbf{s}, \beta) \quad = \quad I(\mathbf{s}, \beta) - \lambda^T \mathbf{r}(\mathbf{s}, \beta)$$

- Considering general variation $\delta\mathbf{s}$ and $\delta\beta$ gives

$$\delta L \quad = \quad \left( \frac{\partial I}{\partial \mathbf{s}} - \lambda^T \frac{\partial \mathbf{r}}{\partial \mathbf{s}} \right) \delta\mathbf{s} + \left( \frac{\partial I}{\partial \beta} - \lambda^T \frac{\partial \mathbf{r}}{\partial \beta} \right) \delta\beta$$

- If $\lambda^T$ is chosen to satisfy the adjoint equation

$$\frac{\partial I}{\partial \mathbf{s}} - \lambda^T \frac{\partial \mathbf{r}}{\partial \mathbf{s}} = 0 \quad \Rightarrow \quad \left( \frac{\partial \mathbf{r}}{\partial \mathbf{s}} \right)^T \lambda = \left( \frac{\partial I}{\partial \mathbf{s}} \right)^T$$

we obtain

$$\delta L \quad = \quad \left( \frac{\partial I}{\partial \beta} - \lambda^T \frac{\partial \mathbf{r}}{\partial \beta} \right) \delta\beta$$

# Governing equations

We start from the incompressible Navier-Stokes equations:

$$\begin{aligned} \partial_t(\rho \mathbf{u}) + (\mathbf{u}\cdot\nabla)\mathbf{u} &= -\nabla p + \nabla\cdot[2\nu D(\mathbf{u})] \\ \partial_t \rho + \nabla\cdot\mathbf{u} &= 0 \end{aligned}$$

with

- $p$ pressure, $\mathbf{u} = (u_1, \ldots, u_3)^T$ velocity, $T$ Temperature
- $D(\mathbf{u}) = \frac{1}{2}[\nabla\mathbf{u} + (\nabla\mathbf{u})^T]$ stress tensor
- $\nu$ kinematic viscosity

We equip the system with an thermal diffusion equation, i.e.

$$\frac{\partial T}{\partial t} + (\mathbf{u}\cdot\nabla)T = \nabla(\alpha\cdot\nabla T)$$

with $\alpha$ thermal diffusivity.

# Residual form of the N.-S. system

- We are interested in a steady-state solution,
  $\Rightarrow$ omit the time-derivatives

- Rewrite the system in residual form, i.e.

$$\mathbf{r}(\mathbf{s}) = \begin{pmatrix} (r_1, r_2, r_3)^T \\ r_4 \\ r_5 \end{pmatrix} = \begin{pmatrix} (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p - \nabla \cdot [2\nu D(\mathbf{u})] \\ -\nabla \cdot \mathbf{u} \\ (\mathbf{u} \cdot \nabla) T - \nabla(\alpha \cdot \nabla T) \end{pmatrix}$$

with state vector $\mathbf{s} = (\mathbf{u}, p, T)^T$

# Deriving the adjoint system

**Starting point**: vanishing variation of the Lagrange function:

$$\begin{aligned}
\delta_{\mathbf{s}} L &= \sum_i \left( \int_\Omega \frac{\partial I_\Omega}{\partial s_i} \delta s_i \,\mathrm{d}\Omega + \int_\Gamma \frac{\partial I_\Gamma}{\partial s_i} \delta s_i \,\mathrm{d}\Gamma \right) + \sum_{i,j} \int_\Omega \hat{s}_i \frac{\partial r_j}{\partial s_i} \delta s_i \,\mathrm{d}\Omega \\
&= \int_\Omega \frac{\partial I_\Omega}{\partial \mathbf{u}} \delta \mathbf{u} \,\mathrm{d}\Omega + \int_\Gamma \frac{\partial I_\Gamma}{\partial \mathbf{u}} \delta \mathbf{u} \,\mathrm{d}\Gamma + \int_\Omega \hat{s} \cdot \delta_{\mathbf{u}} \mathbf{r} \,\mathrm{d}\Omega \\
&\quad + \int_\Omega \frac{\partial I_\Omega}{\partial p} \delta p \,\mathrm{d}\Omega + \int_\Gamma \frac{\partial I_\Gamma}{\partial p} \delta p \,\mathrm{d}\Gamma + \int_\Omega \hat{s} \cdot \delta_p \mathbf{r} \,\mathrm{d}\Omega \\
&\quad + \int_\Omega \frac{\partial I_\Omega}{\partial T} \delta T \,\mathrm{d}\Omega + \int_\Gamma \frac{\partial I_\Gamma}{\partial T} \delta T \,\mathrm{d}\Gamma + \int_\Omega \hat{s} \cdot \delta_T \mathbf{r} \,\mathrm{d}\Omega \equiv 0.
\end{aligned}$$

with $\hat{\mathbf{s}} = (\hat{\mathbf{u}}, \hat{p}, \hat{T})^T$ adjoint state variables (Lagrange multiplier)

# Variation of the residual form

The variation of the residual form with respect to the flow field is

$$
\begin{aligned}
\delta_{\mathbf{s}}\mathbf{r} &= \delta_{\mathbf{u}}\mathbf{r} + \delta_p\mathbf{r} + \delta_T\mathbf{r} \\
&= \begin{pmatrix} (\delta\mathbf{u}\cdot\nabla)\mathbf{u} + (\mathbf{u}\cdot\nabla)\delta\mathbf{u} - \nabla\cdot[2\nu D(\mathbf{u})] \\ -\nabla\cdot\delta\mathbf{u} \\ +(\delta\mathbf{u}\cdot\nabla)T \end{pmatrix} \\
&+ \begin{pmatrix} \nabla\delta p \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} \mathbf{0} \\ 0 \\ (\mathbf{u}\cdot\nabla)\delta T - \nabla\cdot(\alpha\nabla\delta T) \end{pmatrix}
\end{aligned}
$$

# Variation of the residual form

After several basic transformation

$$
\begin{aligned}
\delta_{\mathbf{s}} L \;=\; & \int\limits_{\Omega} \begin{pmatrix} \delta \mathbf{u} \\ \delta p \\ \delta T \end{pmatrix} \cdot \begin{pmatrix} -\nabla \hat{\mathbf{u}} \cdot \mathbf{u} - (\mathbf{u} \cdot \nabla) \hat{\mathbf{u}} - \nabla \cdot (2\nu \mathbf{D}(\hat{\mathbf{u}})) + \nabla \hat{p} - T \nabla \hat{T} & + \\ -\nabla \cdot \delta \mathbf{u} & + \\ (\delta \mathbf{u} \cdot \nabla) T & + \end{pmatrix} \\
+ & \int\limits_{\Gamma} \begin{pmatrix} \delta \mathbf{u} \\ \delta p \\ \delta T \end{pmatrix} \cdot \begin{pmatrix} \mathbf{n}(\hat{\mathbf{u}} \cdot \mathbf{u} + \hat{\mathbf{u}}(\mathbf{u} \cdot \mathbf{n}) + 2\nu \mathbf{n} \cdot \mathbf{D}(\hat{\mathbf{u}}) + T \hat{T} \mathbf{n} - \hat{p} \mathbf{n} & + \frac{\partial I_\Gamma}{\partial \mathbf{u}} \\ \hat{\mathbf{u}} \cdot \mathbf{n} & + \frac{\partial I_\Gamma}{\partial p} \\ \nu \mathbf{n} \cdot \nabla \hat{T} + \hat{T}(\mathbf{u} \cdot \mathbf{n}) & + \frac{\partial I_\Gamma}{\partial T} \end{pmatrix} \\
+ & \int\limits_{\Gamma} \begin{pmatrix} \mathbf{u} \\ p \\ T \end{pmatrix} \cdot \begin{pmatrix} -2\nu \mathbf{n} \cdot \mathbf{D}(\delta \mathbf{u}) \\ 0 \\ -\nu \mathbf{n} \cdot (\delta T) \end{pmatrix} \mathrm{d}\Gamma \\
= & \int\limits_{\Omega} \delta \mathbf{s} \cdot \left( \hat{\mathbf{r}} + \frac{\partial I}{\partial_{\mathbf{s}}} \right) \mathrm{d}\Omega + \int\limits_{\Gamma} \delta \mathbf{s} \cdot \hat{\mathbf{b}}_{c_1} \, \mathrm{d}\Gamma + \int\limits_{\Gamma} \mathbf{s} \cdot \hat{\mathbf{b}}_{c_2} \, \mathrm{d}\Gamma
\end{aligned}
$$

# Adjoint system

The corresponding inhomogeneous adjoint system
(Time-independent incompressible adjoint N.-S. with heat diffusion)
to the optimization problem is $\hat{\mathbf{r}} = \frac{\partial I}{\partial_{\mathbf{s}}}$ i.e.

$$\begin{aligned} \mathbf{D}(\hat{\mathbf{u}})\mathbf{u} + \nabla \cdot (2\nu \mathbf{D}(\hat{\mathbf{u}})) + \nabla \hat{p} - T \nabla \hat{T} &= \frac{\partial I_\Omega}{\partial \mathbf{u}} \\ \nabla \cdot \hat{\mathbf{u}} &= \frac{\partial I_\Omega}{\partial p} \\ \mathbf{u} \cdot \nabla \hat{T} + \nabla \cdot (\nu \nabla \hat{T}) &= \frac{\partial I_\Omega}{\partial T} \end{aligned}$$

# Adjoint Boundary conditions

For the boundary integrals we have to fulfil the following expression:

$$
\begin{aligned}
0 &\equiv \delta \mathbf{s} \cdot \hat{\mathbf{b}}_{c_1} + \mathbf{s} \cdot \hat{\mathbf{b}}_{c_2} \\
&= \begin{pmatrix} \delta \mathbf{u} \\ \delta p \\ \delta T \end{pmatrix} \cdot \begin{pmatrix} \mathbf{n}(\hat{\mathbf{u}} \cdot \mathbf{u} + \hat{\mathbf{u}}(\mathbf{u} \cdot \mathbf{n}) + 2\nu \mathbf{n} \cdot \mathbf{D}(\hat{\mathbf{u}}) + T\hat{T}\mathbf{n} - \hat{p}\mathbf{n} + \frac{\partial I}{\partial \mathbf{u}} \\ \hat{\mathbf{u}} \cdot \mathbf{n} \qquad + \frac{\partial I}{\partial p} \\ \nu \mathbf{n} \cdot \nabla \hat{T} + \hat{T}(\mathbf{u} \cdot \mathbf{n}) \qquad + \frac{\partial I}{\partial T} \end{pmatrix} \\
&+ \begin{pmatrix} \mathbf{u} \\ p \\ T \end{pmatrix} \cdot \begin{pmatrix} -2\nu \mathbf{n} \cdot \mathbf{D}(\delta \mathbf{u}) \\ 0 \\ -\nu \mathbf{n} \cdot (\delta T) \end{pmatrix}, \qquad \forall \delta \mathbf{s}, \mathbf{s}.
\end{aligned}
$$

Thus, BCs depend on objective function

# Objective functions

- Heat conduction on the wall

$$I_{hc} = \frac{1}{2} \int_{wall} \left( \frac{\partial T}{\partial \mathbf{n}} \right)^2 \, \mathrm{d}\,\Gamma$$

- Uniformity (outlet)

$$I_u = \frac{1}{2} \int_{wall} \left( T - \frac{A_{inlet}}{A_{outlet}} T_{inlet} \right)^2 \, \mathrm{d}\,\Gamma$$

Depending on the

- objective function
- primal boundary conditions

the adjoint boundary conditions changes.

I.e. for each objective function own boundary conditions

# Implementation in OpenFOAM

## Base solver

- `simpleFoam`

## Adjoint solver (for minimizing pressure loss).

- `adjointShapeOptimizationFoam`
- OpenFOAM 4.0 release

## based on

C. Othmer, E. de Villiers, H.G. Weller
*Implementation of a continuous adjoint for topology optimization of ducted flows*, 18th AIAA Computational Fluid Dynamics Conference Miami, Florida, AIAA-2007-3947

# Extensions (carried our so far)

- primal/adjoint heat diffusion, i.e.

```
fvScalarMatrix TaEqn
( fvm::div(-phi, Ta) == fvm::laplacian(nuEff, Ta));
```

- derivation of the BCs according to the chosen cost function
- implementation of the BCs in OpenFOAM:

```
adjointOutletTemperatureHeatflux
adjointOutletPressureHeatflux
adjointOutletVelocityHeatflux
adjointWallTemperatureHeatflux
adjointOutletTemperatureUniformity
...
```

- further improvements (e.g. stabilization of adjoint convection)
- derivation/implementation of the sensitivity vector field

# Mesh deformation

**Mesh deformation**

1. Smoothing sensitivity vector field
2. Mapping on the mesh/surface
3. Mesh deformation
   (Mesh motion solver in OpenFOAM)

**Test case**

- Dimpled surface
- Optimization due to different/combined cost functions

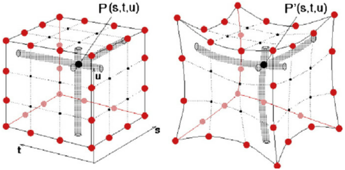
**Report** (in progress)

Th. Grahs, J. Turnow *Adjoint-based heat transfer optimization for dimpled surfaces*, Informatikberichte, Institute of Scientific Computing, TU Braunschweig. (hopefully finished before semester starts...)

# Next steps

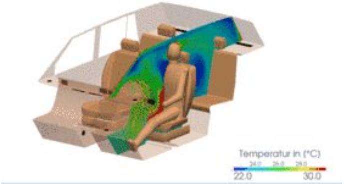
## Comparison of morphing strategies

- Mesh motion solver in OpenFOAM
- ANSA (commercial tool)
- Free Form Deformation (FFD) techniques




## Further application

- HVAC
- Thermal management
- Thermal comfort




## Methodology

- Adjoint thermal wall functions
- Combined topology&surface optimization (Immersed boundary