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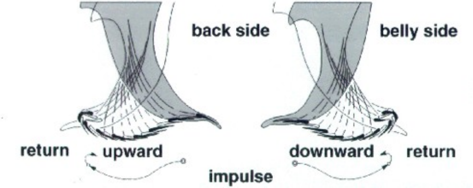
Numerical Optimization in Engineering Applications

Contents

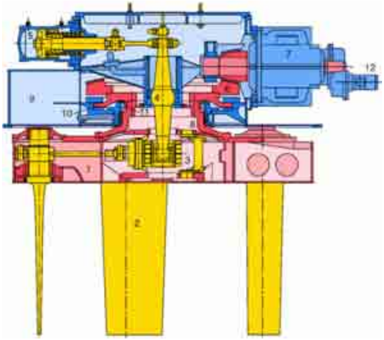
Voith-Schneider-Propeller

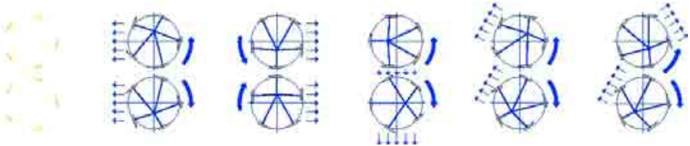
- introduced 1926 by the austrian engineer E. Schneider
- developed, produced and improved by J.M. Voith, Heidenheim
- Steering and propulsion in one unit
- Cooperation with: D. Jürgens, M. Palm (Voith), S. Singer



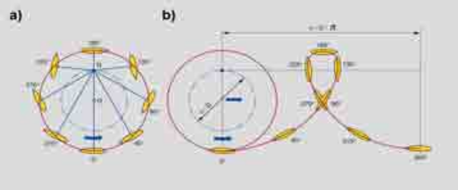
VSP

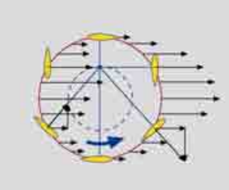




VSP - 2 -

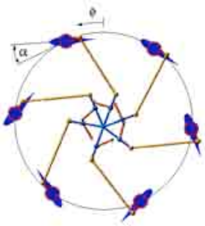
- allows thrust in any direction (360°)
- mostly used in ships with special purposes

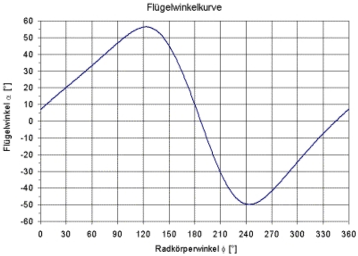




Blade steering curve (bsc)

- important control parameter (Hydromechanics)
- defines orientation of the blades during the revolution of the propeller





1st Task

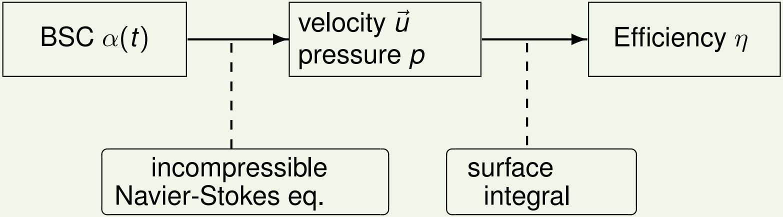
Determine a BSC such that

$$\textbf{Efficiency} = \frac{\textbf{Propulsion}}{\textbf{Energy}} \qquad \text{is optimized!}$$

- So far done only by experiments

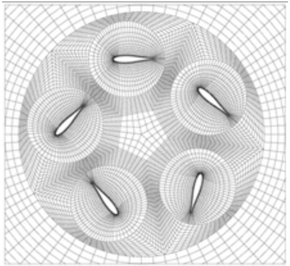
Optimization of the bsc

Target: f : BSC $\mapsto$ Efficiency



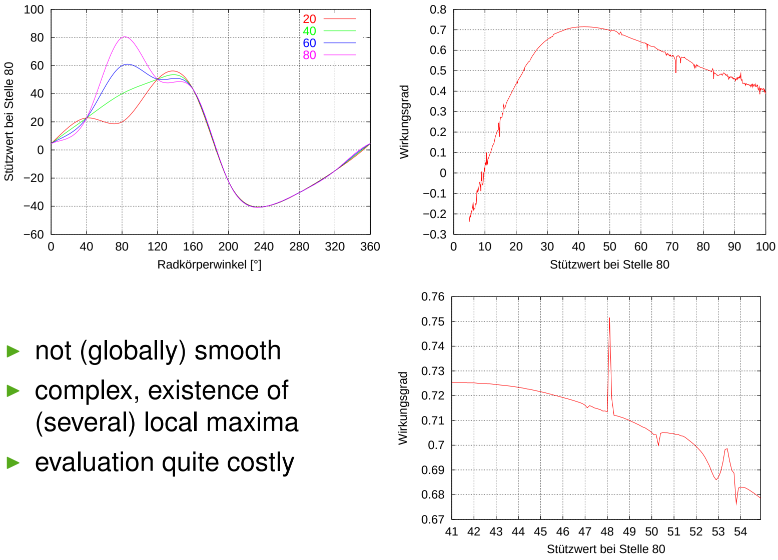
- periodic state is required (needs typically 5-10 rotations)
- time stepping: 1 degree (of propeller rotation)

Numerical Simulation of Navier-Stokes equations



- discretization with $\sim$ 3.5 Mio. cells
- 2 nested rotations
- turbulence model: RANSE
- Used so far:
  - vortex lattice, in house
  - 3D-Finite Volumes (COMET, commercial)
  - open foam
- cpu-time on parallel-cluster (48 nodes): about 3d

Properties of the target functional $f : \alpha \mapsto \eta$



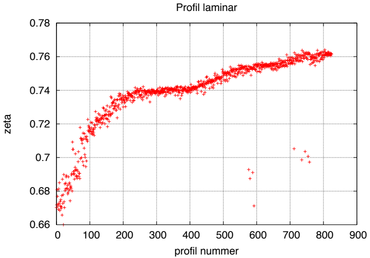
- not (globally) smooth
- complex, existence of (several) local maxima
- evaluation quite costly

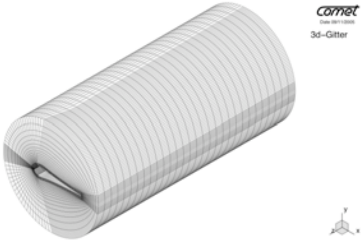
Numerical optimization — First results

- Gradient-based schemes are ruled out
- direct methods: Hooke-Jeeves, Simplex (Nelder, Mead)
- global search: „tunneling“

- Results: enormous improvement of efficiency
- validation by experiments/reality
- used in new generation propellers
- Ref: ZAMM **87**, no. 10 (2007), 698-710.

Shape optimization (MS10)

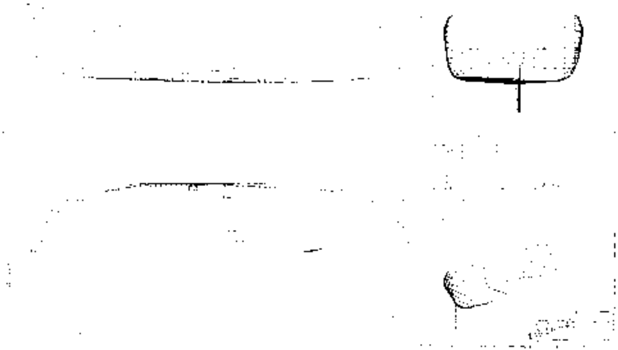




- R. Deininger
- re-meshing required in each step
- many iterations due to direct method

- Result: further improvement of efficiency
- validation by experiments/reality

A new challenge

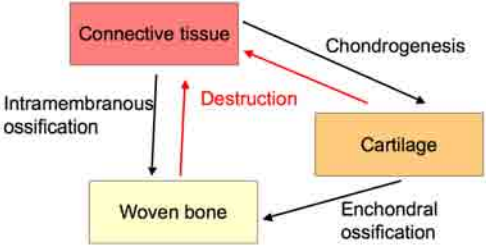


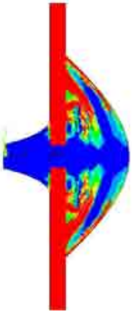
- optimize shape of ship hull **and** propeller
- coupling of flow around ship
- M. Hopfensitz, J.C. Matutat (BMWi)

Fracture Healing: A Medical Problem

(L. Claes, U. Simon, D. Nolte)

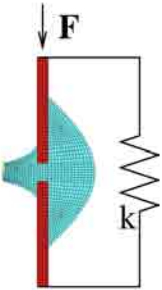
- Goals:
  - Replace intramedular nail by external fixator
  - Minimize healing time
- Around a fracture gap a callus is build
- Reduction of strains by fixation
- Tissue differentiation inside the callus

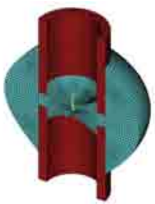




Fracture Healing: Numerical Simulation in 2D/3D

- state: of concentrations of
  - bone
  - cartilage
  - connective tissue
  - vascularity
- 2D model: axial symmetrical geometry
- 3D model: general load case
- **Optimization:**
  minimize healing time!
- FE-model (ANSYS)





Simulation Results (2D) in two-week steps

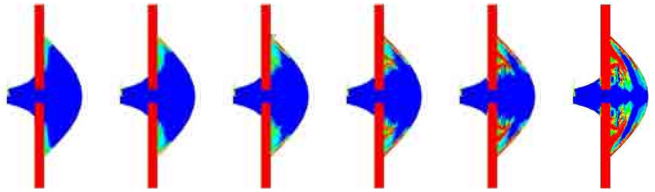


Figure: Bone concentrations with fixator stiffness of $145\frac{N}{mm}$ (*linear*)

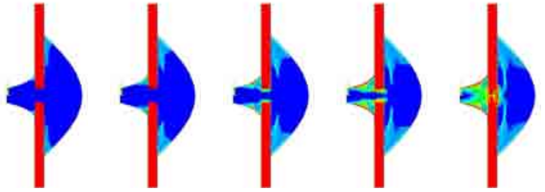
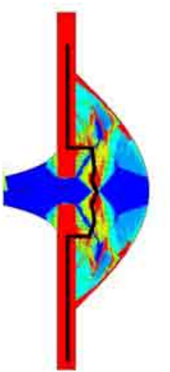


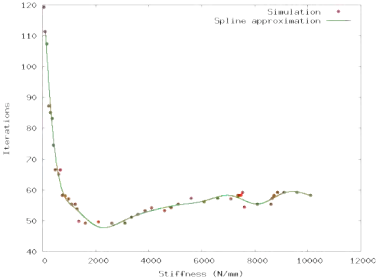
Figure: Bone concentrations with fixator stiffness of $1300\frac{N}{mm}$ (*linear*)

Definition and computation of healing

- Definition of a healing:
  bony connection of bone parts
- Computation by path search algorithm
- Healing time: first bridging of bone parts



Optimization of Fracture Fixator



Smoothing and optimization:

- function values w.r.t. discrete times (days, weeks)
- Least-squares spline approximations
- Minimization of the approximations

Results:

- Interval of possible optimal fixator configurations
- Drastic reduction of healing time

ZEISS
HAKA
Bundesministerium für Bildung und Forschung
ZSW
uzwr
ulmer zentrum für wissenschaftliches rechnen
VOITH
Engineered reliability.
Baden-Württemberg
MINISTERIUM FÜR WISSENSCHAFT, FORSCHUNG UND KUNST
Deutsche Forschungsgemeinschaft
DFG
PROF. DR.-ING. HELMUT KRAMER
DIPL.-ING. FRIEDHELM ALBRECHT
Ingenieurgesellschaft mbH & Co. KG

Situation in our applications

- quite promising results so far
- used in ‘real-world’ framework
- slow convergence / large range of solutions of optimization due to
  - use of direct method
  - random influences
  - discrete data
- moreover: complex high-dimensional simulations required
- new challenges:
  - realtime
  - coupling of shape optimization and optimal control

Possible way-outs

1. Automatic Differentiation (AD) and Gradient-based methods
2. Reduced Basis Methods (RBM)
3. Optimization for parameter-dependent problems

1. AD (Automatic Differentiation) - MS75, 84: Wed

- also known as algorithmic differentiation
- R. Leidenberger, CD-adapco (Peric)

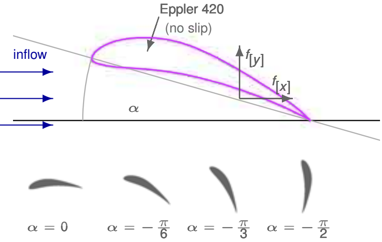
```
dimension x(10)
y = 1.0
do i = 1,n
 if (x(i) .gt. 0.0) then
  y = x(i) * y * y
 endif
enddo
```

(a)

```
dimension x(10)
```

```
dimension x(10)
dimension dy(10), dx(10,10)
do j=1,10
 dx(i,i) = 1.0
enddo
  do j = 1, 10
 dy(j) = 0.0
enddo
```

A 2D problem



Configuration

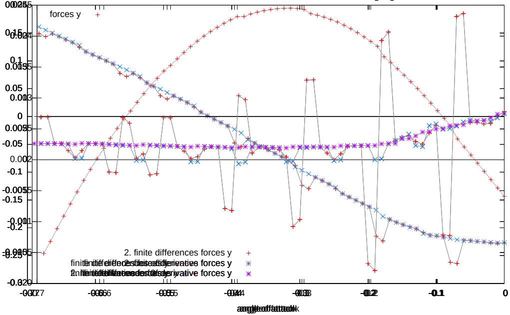
- Solver: caffa
  Computer Aided Fluid Flow Analysis
  (Ferziger & Peric)
- Angle of attact α
- Surface forces: $f(\alpha) = \big(f_{[x]}(\alpha), f_{[y]}(\alpha)\big)^T$

optimization problem

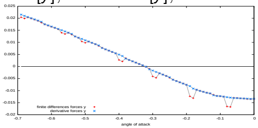
- $\max\limits_{\alpha \in (0, \alpha_{max})} f_{[y]}(\alpha)$
- Known: $f_{[y]}(\alpha)$ is concave for $\alpha \in (0, \alpha_{max})$
- $\alpha^* = \arg\left\{ \max\limits_{\alpha \in (0, \alpha_{max})} f_{[y]}(\alpha) \right\} \iff f'_{[y]}(\alpha^*) = 0$ (Euler-Lagrange equation)
- Newton iteration: $\Phi_{f_{[y]}}(\alpha_k) = \alpha_{k-1} - \dfrac{f'_{[y]}(\alpha_{k-1})}{f''_{[y]}(\alpha_{k-1})}$

Regularization

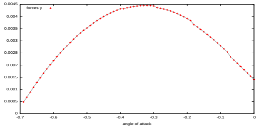
…puted by caffa)



$f'_{[y],FD}(\alpha)$ & $f'_{[y],AD}(\alpha)$



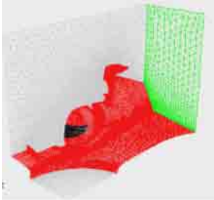
forces: $f_{[y]}(\alpha)$

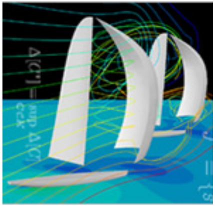


Results

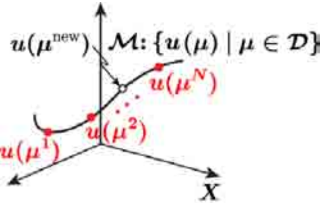
- AD successful in 2D- and 3D-applications
- regularization increases from $f'_{[y]}(\alpha)$ to $f''_{[y]}(\alpha)$ and from 2D to 3D
- (almost) quadratic convergence of Newton iteration

2. Reduced Basis Methods (RBM) – CP12, MS106,119,127,141 Wed-Fri

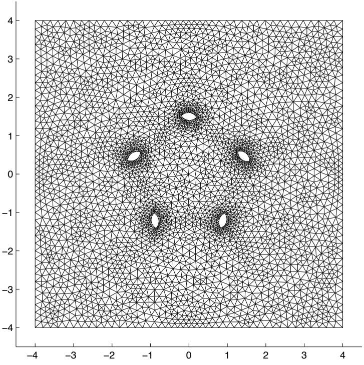




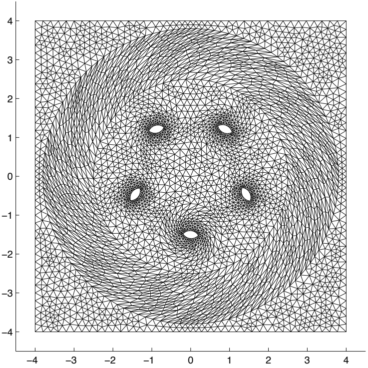
- C. Canuto, T. Tonn (SINUM 2009), F. Iacono
- offline-online procedure (Maday, Patera, Rozza, Grepl, ...)
- **offline:**
  - several parameter studies plus evaluation
  - determine few (global) basis functions (modes, snapshots, ...)
  - POD, Karhunen-Loeve, PCA, ...
- **online:**
  - solve small (dense) system for new parameters
- parameters here:
  - BSC, shape of the propeller,
  - shape of the ship, bone ...
- snapshots here: different BSCs, fixator stiffness



Transformation to reference situation



reference domain $\hat{\Omega}$



after transformation

- Realization of rotation by transformation of the domain/grid
- Reduction to a reference configuration

Influence of the parameter

- Parameter BSC enters into transformation to the reference domain
- Change of variables in the integrals

$$\begin{aligned} a(u, v; \mu) &= \int_{\Omega_\mu} \nabla u(x) \cdot \nabla v(x)\, dx \\ &= \int_{\hat{\Omega}} \nabla \hat{u}(\hat{x}) \cdot \nabla \hat{v}(\hat{x})\, \underline{T}(\mu; \hat{x})\, d\hat{x} \end{aligned}$$

- Bilinear form is parameter dependent (not separable):

$$a(u, v; \mu) \neq \ell(\mu)\, \tilde{a}(u, v)$$

- flow domain is not convex
  - No H^2-regularity!
  - Thus: $f \in L_2(\Omega) \not\Rightarrow u \in H^2(\Omega)$
  - $u \notin H^1(\partial\Omega)$
  - Derivatives are not in $L_2(\Omega)$, but only in $H^{-1/2}(\Omega)$

Primal problem

(Extension of K. Veroy, A.T. Patera; 2005), SINUM 2009):

Primal problem

$$\begin{cases} \text{For } \mu \in \mathcal{D} \subset \mathbb{R}^p \text{ determine } u(\mu) \in X_\mathcal{N}, \text{ s.t. } \forall v \in X_\mathcal{N}: \\ g(u(\mu), v; h(\mu)) := a(u(\mu), v; h_a(\mu)) + b(u(\mu), u(\mu), v; h_b(\mu)) - f(v) = 0, \end{cases}$$

where $h = (h_a, h_b)$ (non-affine)

- $\Omega \subset \mathbb{R}^n$, $X_\mathcal{N} \subset H^1(\Omega)$, $\dim(X_\mathcal{N}) = \mathcal{N}$ (FE-space, „large“)
- $a(w, v; h_a)$ linear in $w, v \in X_\mathcal{N}$ and $h_a \in L^\infty(\Omega)$;
- $b(w, z, v; h_b)$ linear in $w, z, v \in X_\mathcal{N}$ and $h_b \in L^\infty(\Omega)$;

Existence and uniqueness

Let dg be the Frèchet derivative of g:

$$\beta(z;h) := \inf_{w\in X_\mathcal{N}} \sup_{v\in X_\mathcal{N}} \frac{dg(w,v;h)[z]}{\|w\|_{X_\mathcal{N}}\,\|v\|_{X_\mathcal{N}}}$$ **Inf-sup-parameter**

$$\gamma(z;h) := \sup_{w\in X_\mathcal{N}} \sup_{v\in X_\mathcal{N}} \frac{dg(w,v;h)[z]}{\|w\|_{X_\mathcal{N}}\,\|v\|_{X_\mathcal{N}}}$$ **continuity constant**

Assumption (continuity, inf-sup)

1. *unif. inf-sup:* $\exists \beta_0 > 0$, *s.t.* $\forall \mu \in \mathcal{D}$: $\beta(u(\mu); h(\mu)) \geq \beta_0$.
2. *unif. continuity:* $\forall \mu \in \mathcal{D}$ *exist* $0 \leq \rho_a, \rho_b < \infty$, *s.d.* $\forall w, z, v \in X_\mathcal{N}$:

$$|a(w,v;h_a)| \leq \rho_a \|w\|_{X_\mathcal{N}} \|v\|_{X_\mathcal{N}} \|h_a\|_{L^\infty(\Omega)},$$
$$|b(w,z,v;h_b)| \leq \rho_b \|w\|_{X_\mathcal{N}} \|z\|_{X_\mathcal{N}} \|v\|_{X_\mathcal{N}} \|h_b\|_{L^\infty(\Omega)}.$$

- Note: Might not be realistic for all $\mu \in \mathcal{D}$!
- But can be verified a-posteriori!

Primal RBM problem

For $1 \leq N \leq N^{\max}$ („small"), let

- $S^N := \{\mu_n \in \mathcal{D}, 1 \leq n \leq N\}$ space of **parameter samples**
- $W^N := \text{span}\{\Xi_n := u(\mu_n), 1 \leq n \leq N\}$ corresponding **Lagrange space**

Primal RBM problem

$$\begin{cases} \text{For } \mu \in \mathcal{D} \text{ determine } \widehat{u}(\mu) \in W^N: \\ g(\widehat{u}(\mu), v; \widehat{h}(\mu)) = 0 \qquad \forall v \in W^N \end{cases}$$

- solution by Newton
- (online-)complexity independent of $\mathcal{N} \gg N$

Dual problem

Consider error functional $\widehat{s}_1(\mu) := \ell\left(\widehat{u}(\mu)\right)$ via:

Dual problem

$$\begin{cases} \text{For } \mu \in \mathcal{D} \text{ determine } \psi(\mu) \in X_{\mathcal{N}}, \text{ s.d. } \forall v \in X_{\mathcal{N}}: \\ dg\left(v, \psi(\mu); \widehat{u}(\mu) + \frac{1}{2} e(\mu); h(\mu)\right) = -\ell(v), \end{cases}$$

where $e(\mu) := u(\mu) - \widehat{u}(\mu)$.

$\rightsquigarrow$ This is a **linear** problem.

Dual RBM problem:

- **(Online-)complexity** $\sim$ one Newton iteration

Optimal selection of snapshots

Goal: „optimal“ adaptive selection of snapshots

- Choose sample set $\Xi \subset \mathcal{D}$ (small, but representative)
- Initial set $S^1 := \{\mu_1\}$
- Tolerance $\varepsilon > 0$.

For $N = 1, 2, \ldots$

1. compute

$$\mu^* := \arg\max_{\mu\in\Xi} \Delta(\mu)$$

2. if $\Delta(\mu^*) > \varepsilon$, update $S^{N+1} := S^N \cup \{\mu^*\}$ and continue
3. stop

where $\Delta(\mu)$ is an **easily computable**, **reliable a-posteriori** error estimator

Brezzi-Rapaz-Raviart (RBB)-Theory

Define a „**proximity-indicator**“ (a-posteriori):

$$\tau(\mu) \quad := \quad 4\rho_b(\mu)\big(\widehat{\beta}(\mu)\big)^{-2}\big(R(\mu) + E(\mu)\big),$$

- where

$$R(v;\mu) \quad := \quad g\left(\widehat{u}(\mu), v; \widehat{h}(\mu)\right), \qquad R(\mu) \quad := \quad \|R(\cdot;\mu)\|_{X'_{\mathcal{N}}},$$
$$E(v;\mu) \quad := \quad g\left(\widehat{u}(\mu), v; h(\mu) - \widehat{h}(\mu)\right), \qquad E(\mu) \quad := \quad \|E(\cdot;\mu)\|_{X'_{\mathcal{N}}},$$

Define an „**inf-sup indicator**“ (a-posteriori):

$$0 < \widehat{\beta}(\mu) \leq \beta(\widehat{u}(\mu); h(\mu))$$

for all $\mu \in \mathcal{D}$.

Well-posedness and a-posteriori estimator

Proposition (Well-posedness with proximity-indicator)

For $\tau(\mu) \leq \frac{1}{2}$ we have $\beta(u(\mu); h(\mu)) \geq \widehat{\beta}(\mu)/\sqrt{2} > 0$.
Primal and dual problem are well-posed.

Proposition (A-posteriorierror estimator for the primal problem)

For $\tau(\mu) < 1$ ex. a unique $u(\mu)$ with

1. $u(\mu) \in \mathcal{B}\left(\widehat{u}(\mu), \widehat{\beta}(\mu)\,(2\rho_b(\mu))^{-1}\right)$,
   where $\mathcal{B}(z, r) := \{v \in X_{\mathcal{N}} : \|v - z\|_{X_{\mathcal{N}}} < r\}$,
2. $\|u(\mu) - \widehat{u}(\mu)\|_{X_{\mathcal{N}}} \leq \Delta(\mu) := \widehat{\beta}(\mu)\,(2\rho_b(\mu))^{-1}\left(1 - \sqrt{1 - \tau(\mu)}\right)$.

Proof: Using **Banach fix point theorem** w.r.t. $H^{\mu} : X_{\mathcal{N}} \to X_{\mathcal{N}}$ defined by

$$dg(H^{\mu} w, v; h(\mu))[\widehat{u}(\mu)] = dg(w, v; h(\mu))[\widehat{u}(\mu)] - g(w, v; h(\mu)), \;\; v \in X_{\mathcal{N}}.$$

Similar results also for:

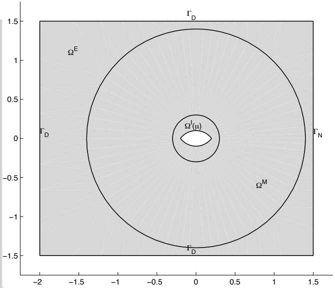
- dual problem

Numerical Results

Model problem (1 blade)

Fo $\mu \in \mathcal{D} := [0, \frac{\pi}{2}]$ solve

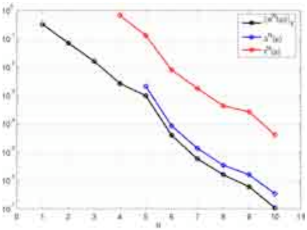
$$\begin{cases} -a\Delta u + (\underline{b} \cdot \nabla u)\, u + cu^2 = 0\,, & \text{in } \Omega(\mu), \\ u = 0\,, & \text{on } \partial B(\mu), \\ u = g\,, & \text{on } \Gamma_D, \\ \frac{\partial u}{\partial n} = 0\,, & \text{on } \Gamma_N. \end{cases}$$



Here: $a = 0.1$, $\underline{b} = (0.5, 0.5)^T$ and $c = 0$

Primal Problem

N	$\|e^N(\mu)\|_{X_\mathcal{N}}$	$\Delta^N(\mu)$	$\eta^N(\mu)$	$\tau^N(\mu)$
2	7.02e-02	NaN	NaN	Inf
4	2.60e-03	NaN	NaN	6.61e-01
6	3.91e-05	8.32e-05	2.34e+00	7.85e-03
8	1.60e-06	3.43e-06	2.04e+00	4.25e-04
10	1.08e-07	3.40e-07	5.03e+00	4.02e-05

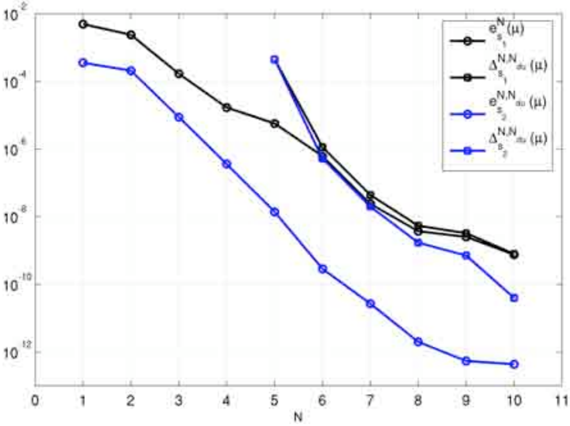


- $e^N(\mu) := u(\mu) - \widehat{u}^N(\mu)$: error
- $\Delta^N(\mu)$: error estimator
- $\eta^N(\mu) := \Delta^N(\mu) / \|e^N(\mu)\|_{X_\mathcal{N}}$: efficiency
- $\tau^N(\mu)$: proximity-indicator

Error functional

- $s(\mu) := \ell(\hat{u}(\mu))$ where

$$\ell(v) := \int_{\partial B} \frac{\partial v}{\partial n} \, dx$$



speed up

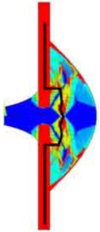
Error functional:

	$N=2$	$N=4$	$N=6$	$N=8$	$N=10$
$\widetilde{N}=0$	385	364	346	328	311
$\widetilde{N}=1$	351	287	261	244	228
$\widetilde{N}=2$	349	285	258	240	224
$\widetilde{N}=3$	349	284	257	240	224
$\widetilde{N}=4$	349	284	257	240	223
$\widetilde{N}=5$	348	284	257	239	223

Matlab 6.5 with *Femlab 2.3* on *AMD Opteron Processor 252* with 2.6 GHz

Summary

- complex, real-world optimization problems
- offer several (also academic) challenging questions
- Scientific Computing has been established as a new tool (Südwestmetall award, Price Cooperation Science-Economy 2005 & 2009)



- Automatic Differentiation ($\rightsquigarrow$ MS)
  - efficient, stable computation of derivatives
  - allows use of Gradient method
  - and computation of sensitivities
- Reduced Basis Methods ($\rightsquigarrow$ MS)
  - offer efficient solvers for high-dimensional problems
  - a-posteriori error analysis (nonlinear problems)
- Interdisciplinary cooperation $\rightsquigarrow$ CSE

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