# From Simulation to Optimization: Discrete Adjoint Equations

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CHEMNITZ UNIVERSITY OF TECHNOLOGY 175 Years

# Overview

1. Motivation
2. Sensitivity analysis
3. Examples

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Modelling and Simulation of scientific/engineering problems

- modelling
- PDE or ODE
- numerical approximation/simulation
- predictions, analysis
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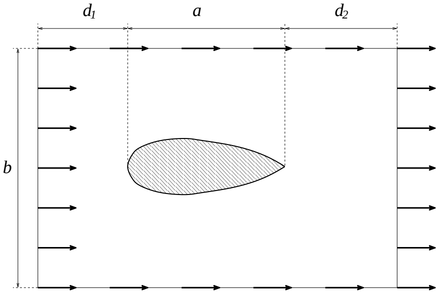
- An object is moving with $v = 1$ in a channel of viscous fluid.
- Goal: find shape such that drag $\rightarrow$ min.
- constraint: $a = const$, $V \geq const.$, symmetric



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# Assumptions

- number of parameters to be optimised $\gg 1$
- simulation expensive compared to post-processing
- Let $J$ be a scalar valued function

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# Naive way 1: Finite Difference

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$$0 = R(\underline{u}(s), s)$$

solve $R(\underline{u}, s) = 0$, evaluate $J_0 := \widetilde{J}(\underline{u}, s)$
for $i = 1, \ldots, \dim(s)$
  perturb $i$-th parameter in $s$ by $h > 0$, $\tilde{s} = s + h$
  solve $R(\underline{\tilde{u}}, \tilde{s}) = 0$, evaluate $J_i := \widetilde{J}(\underline{\tilde{u}}, \tilde{s})$
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- Stationary heat equation

$$-\Delta u = f \qquad \text{in } \Omega$$
$$u = 0 \qquad \text{on } \partial\Omega$$

- Finite Element or Finite Difference Discretisation

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- e.g. forward Euler

$$\begin{aligned} \dot{u} &= f(u, t, s) && \forall t \in [a, b], \\ u(a) &= u_a(s) \end{aligned}$$

$$\begin{aligned} \underline{u}_0 &= u_a(s) \\ \underline{u}_i &= \underline{u}_{i-1} + \tau f(\underline{u}_{i-1}, t_{i-1}, s) && \forall i = 1, \dots, n \end{aligned}$$

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Adjoint discrete ODE:

$$\begin{aligned} \frac{\partial R}{\partial \underline{u}}^T \Psi &= \frac{\partial J}{\partial \underline{u}} \\ \Rightarrow \Psi_n &= \frac{\partial J}{\partial \underline{u}_n} \\ \Psi_i &= \Psi_{i+1} + \tau \frac{\partial f(\underline{u}_{i+1}, t_{i+1}, s)}{\partial u} \Psi_{i+1} + \frac{\partial J}{\partial \underline{u}_i} \quad \forall i = n-1, \ldots, 0 \end{aligned}$$

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Compare:

Discrete ODE (forward in time)

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$$m := \dim(J), \quad k := \dim(s)$$

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| $\mathcal{O}(k)$ LS | $\mathcal{O}(m)$ LS | $\mathcal{O}(m)$ PDE |
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| fwd adaptive | fwd adaptive | fwd+adj adaptive |
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| simplest | simple | more difficult (e.g. BC) |

Difficulties:

- A priori effort.
- Re-use of code.
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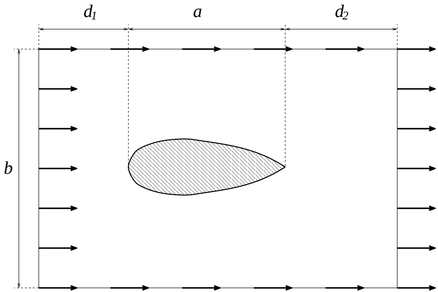

# Example 3: Shape optimisation
## Navier Stokes, drag minimisation

- Fluid dynamics: stationary Navier-Stokes Equations

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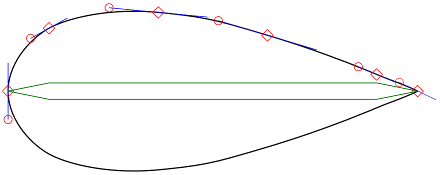

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- Only required for one matrix-vector product $-\Psi^T \frac{\partial R}{\partial s}$.
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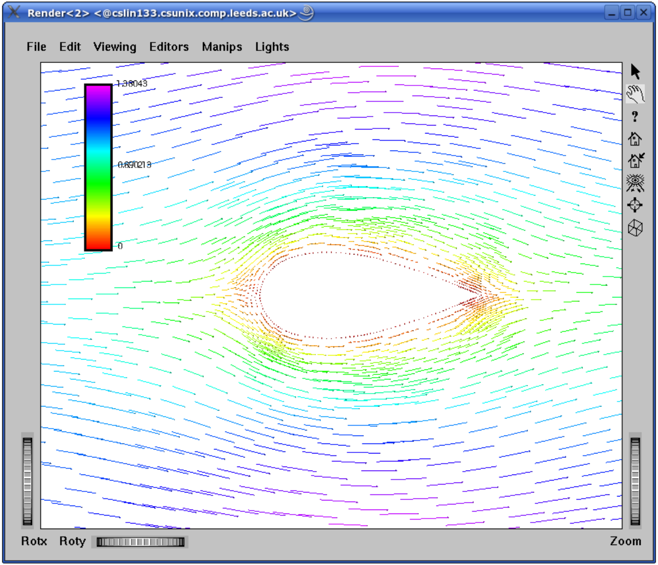
  [S./Jimack 2008]

# Evaluation of required partial derivatives

- Non-trivial part is $-\Psi^T \frac{\partial R}{\partial s}$, $s$ are nodal coordinates.
- Jacobian $\frac{\partial R}{\partial s}$ is sparse.
  But needs not be build as a whole.
- Only required for one matrix-vector product $-\Psi^T \frac{\partial R}{\partial s}$.
  $\Rightarrow$ Cheaper to evaluate only locally and sum up local contributions to $-\Psi^T \frac{\partial R}{\partial s}$ (assembly).
- Local contributions:
  by hand, algorithmic differentiation, or even finite differences [S./Jimack 2008]

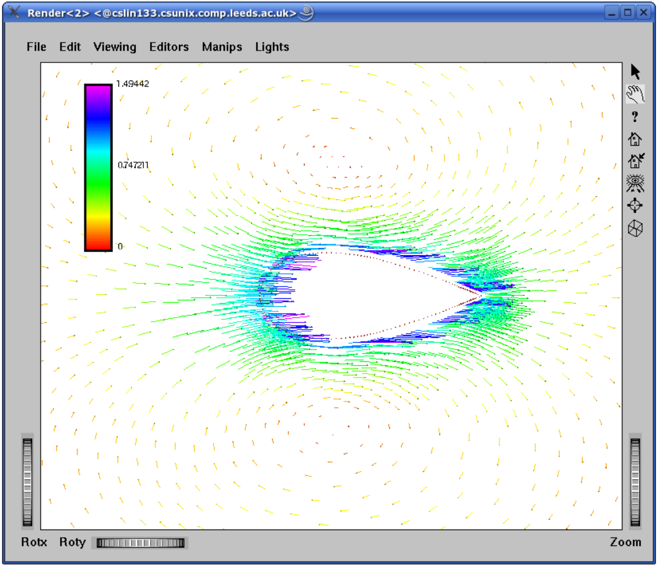
solution: velocities



# Example 3: Shape optimisation

Navier Stokes, drag minimisation, $Re = 10$

adjoint: velocities



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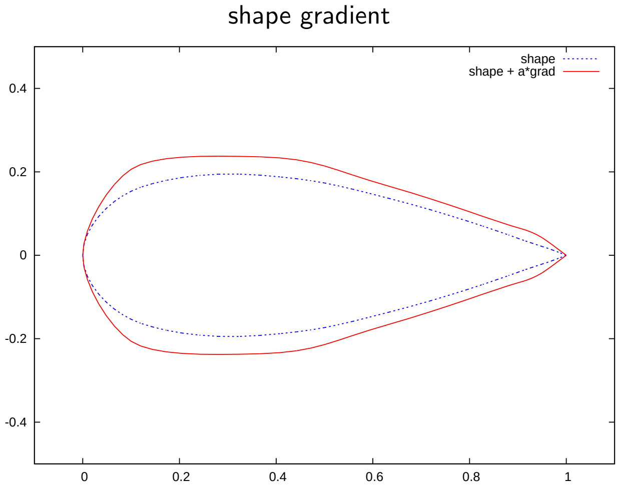

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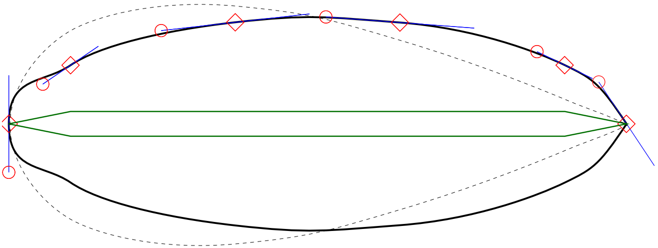
Navier Stokes, drag minimisation, $Re = 10$

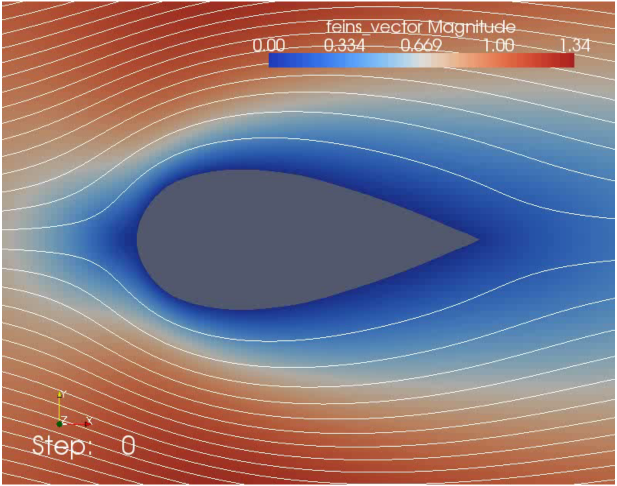



$f_0 = 1.4056 \qquad f_* = 1.3714 \qquad \Rightarrow 2.4\%$ reduced

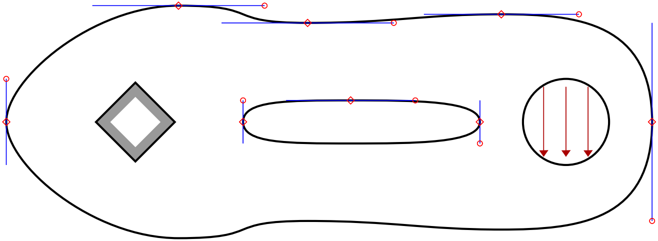
- 10 parameters for optimisation
- 18 SQP steps
- 69 function evaluations
- $\sim$ 145,000 DOFs in each nonlinear equation system,
  $J(s)$ : 9:20 min, adjoint 6:10 min

optimisation movie

$$f_0 = 1.4056 \qquad f_* = 1.3714$$



sketch of pedal crank problem:

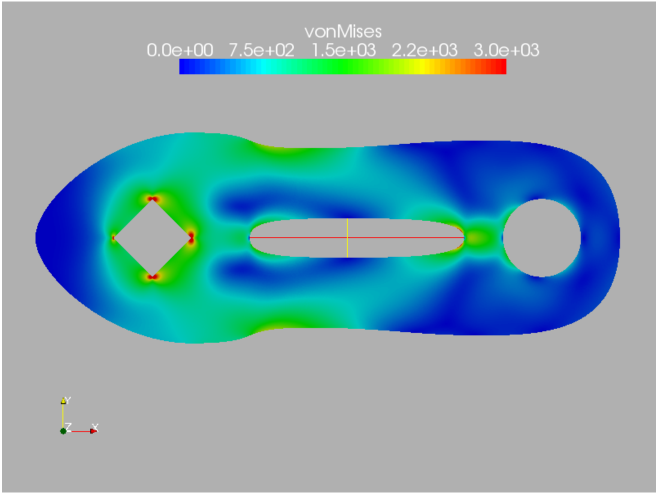


24 free parameters

performance functional: deformation energy

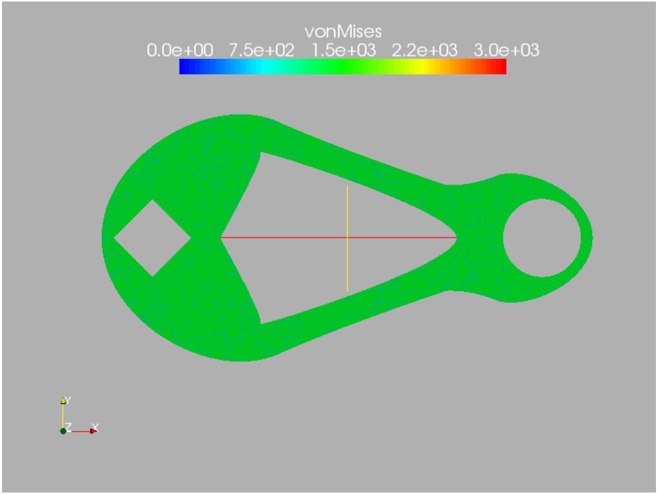
$$I(\mathcal{F}) := \frac{1}{2} a(u, u) - b(u) \quad + \alpha \int_{\Omega} 1 \, d\Omega$$

initial design



# Example 3: Shape optimisation
## Linear elasticity (with Andreas Günnel)

optimal shape: $I(\mathcal{F})$ $\alpha = 10$



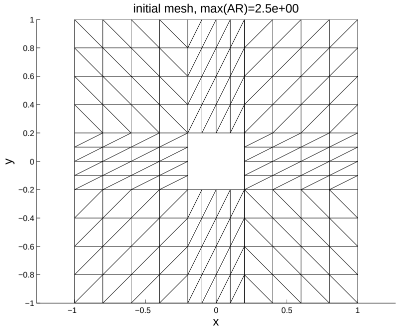
Singularly perturbed reaction diffusion problem

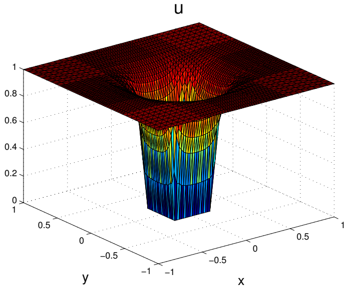
$$\begin{aligned} -\varepsilon^2 \Delta u + u &= 1 && \text{in } \Omega \\ u &= 0 && \text{on } \Gamma_D \\ \frac{\partial u}{\partial n} &= 0 && \text{on } \Gamma_N \end{aligned}$$

$$J := \sum_{T \in \mathcal{T}} J_{e,T}^2 \quad \text{local DWR error estimate}$$

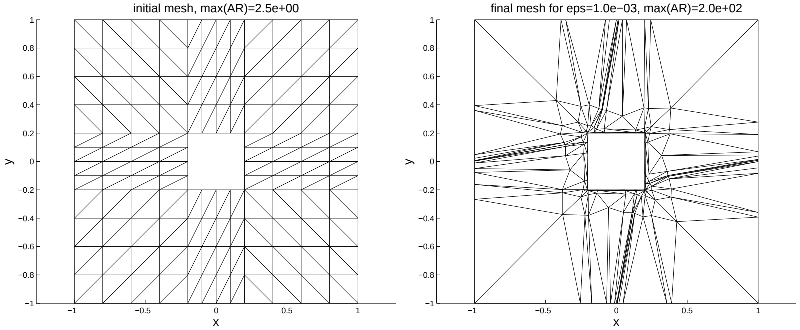
# Example 4: Mesh optimisation

Domain, Solution



Meshes, $\varepsilon = 10^{-3}$
initial and optimised coarse mesh
256 DOFS for optimisation



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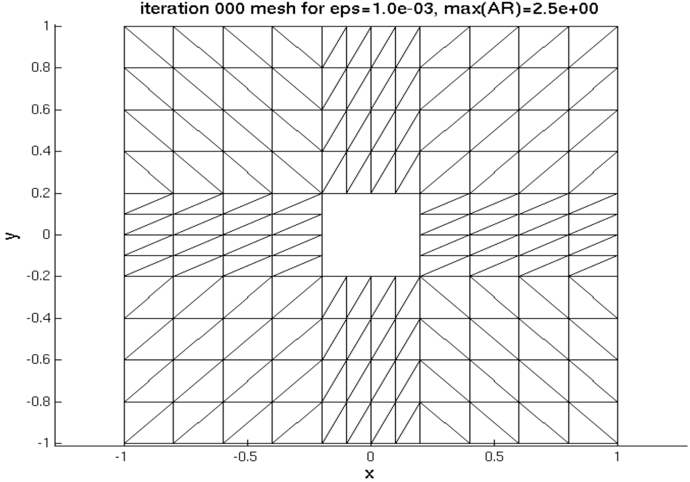
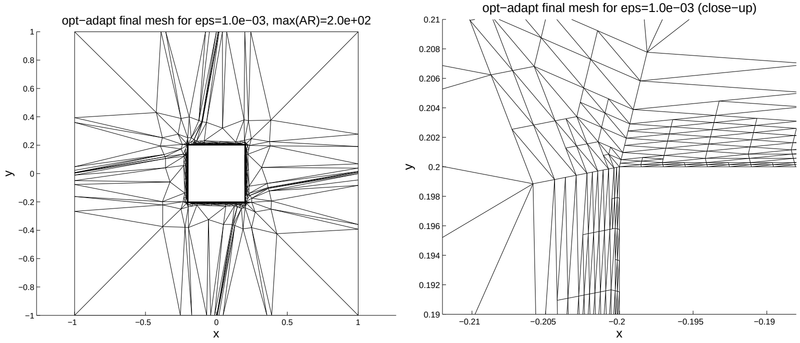
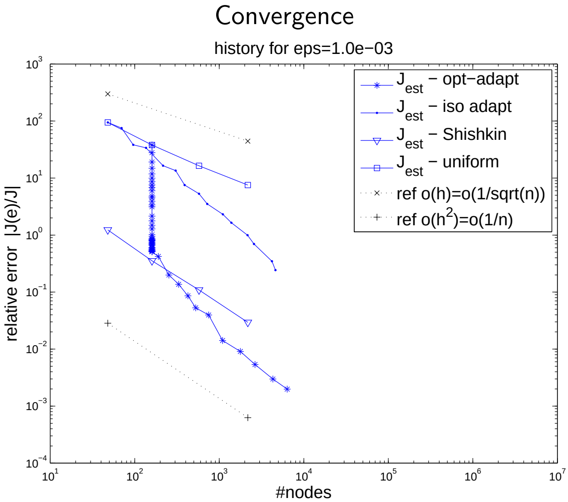
Meshes, $\varepsilon = 10^{-3}$



Meshes, $\varepsilon = 10^{-3}$

`opt-adapt`




Convergence
history for eps=1.0e−03
relative error |J(e)/J|
#nodes
J_est − opt−adapt
J_est − iso adapt
J_est − Shishkin
J_est − uniform
ref o(h)=o(1/sqrt(n))
ref o(h^2)=o(1/n)

# Conclusions

- Discrete-Adjoint-Technique gives a relatively simple way to extend an existing simulation code to include sensitivity analysis, and thus to allow optimisation.
  - Advantages: simple, reuse of code.
  - Disadvantages: optimisation of the discretised problem, rather than approximation of the optimal solution of the continuous problem.
- Technique very general, can be applied in very different settings [S., PhD Thesis 2006]

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Thank you!

Congratulations Peter!

# Hope you to see you in Chemnitz now and then.