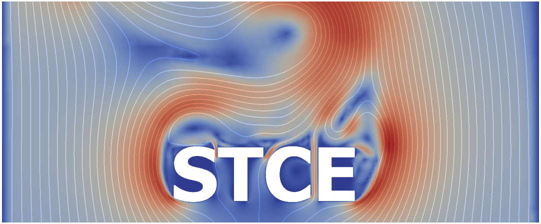


An Introduction to Discrete Adjoint Optimization with OpenFOAM

OpenFOAM Workshop 2019

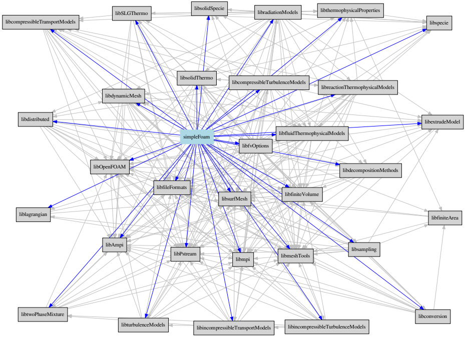
Dr. Markus Towara, feat. Andreas Pesch (RUB)

Duisburg, July 23th 2019

- this file: `https://stce.rwth-aachen.de/files/ofw19_slides.pdf`
- handout: `https://stce.rwth-aachen.de/files/ofw19_handout.pdf`
- Only need one of the following:
- Binaries: `https://stce.rwth-aachen.de/files/ofw19_binary.tar.gz`
- Docker image: `https://stce.rwth-aachen.de/files/ofw19_docker.tar.gz`
- VM: `https://stce.rwth-aachen.de/files/ofw19_vm.tar.gz`

OpenFOAM Softwarepackage

- Open-Source CFD software package (GPLv3)
- Finite volume discretization on 3D unstructured meshes
- Cell centered physical quantities (mostly)
- Highly complex C++ code, heavily relying on inheritance and templates
- Code: $\sim$ 1M LOC, 9k files
- Minimal external dependencies
- Parallelization using MPI

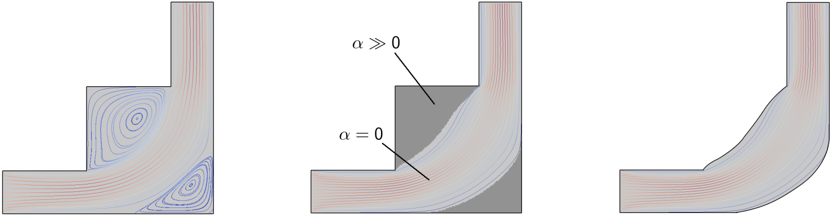


- Augment NS momentum equations by source term $\mathbf{u}\alpha$: [1, 2]

$$(\mathbf{u} \otimes \boldsymbol{\nabla})\,\mathbf{u} = \nu \boldsymbol{\nabla}^2 \mathbf{u} - \frac{1}{\rho}\boldsymbol{\nabla} p - \alpha \mathbf{u}$$

- Parameter α allows to penalize cells / regions of the geometry to redirect flow
- Penalty term can be interpreted as porosity, according to Darcy's law [3]

$$\frac{\Delta p}{\Delta x} = -\left(\frac{\mu}{\kappa}\right)\mathbf{u}$$



Initial design space | Optimized penalty field | Re-Parametrization

- Define cost function $\mathcal{J}$, e.g. total pressure loss between inlet and outlet:

$$\mathcal{J} = -\int_\Gamma \left(p + \frac{1}{2}\|\mathbf{u}\|^2\right) \mathbf{u} \cdot \mathbf{n} \,\mathrm{d}\Gamma$$

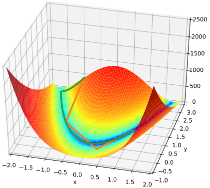
- Calculate sensitivity of the cost function w.r.t. parameters α_i

$$\frac{\mathrm{d}\mathcal{J}}{\mathrm{d}\alpha_i} = ???$$

- Calculate an updated porosity field α^{n+1}, e.g. using gradient descent:

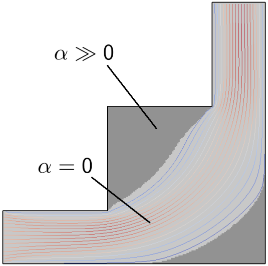
$$\alpha_i^{n+1} = \alpha_i^n - \lambda \cdot \frac{\mathrm{d}\mathcal{J}^n}{\mathrm{d}\alpha_i^n}, \quad \text{with constraints} \quad 0 \le \alpha_i \le \alpha_{\max}$$

- Loop until α converged...



Efficient optimization methods need gradients!

- Number of inputs $p = n$ to be optimized might be in the millions
- Calculating the gradient with finite differences extremely expensive
- Number of outputs usually $1 \leq m \ll n$
- Adjoint method allows to calculate the gradient with only m additional (augmented) function evaluations

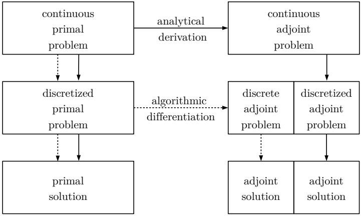


Continuous method:

- *Differentiate first, discretize later*
- Derive adjoint equations analytically
- Implement, discretize, and solve adjoint equations along primal

\+ Fast, physically interpretable

– Hard to derive, can be inconsistent to primal



Discrete method:

- *Discretize first, differentiate later*
- Use implementation to get the derivatives (Algorithmic Differentiation)

\+ Flexible, derivation automatic, sensitivities consistent to implementation

– Memory intensive, generally slower than continuous

- Consider multivariate function f mapping vector $\boldsymbol{x}$ to a scalar y:

$$f(\boldsymbol{x}) : \mathbb{R}^n \to \mathbb{R}$$

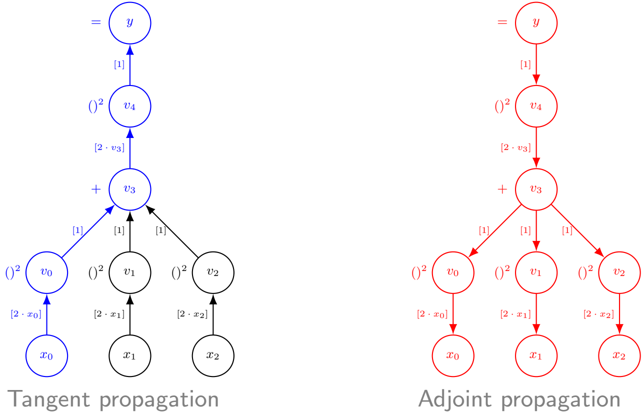
First Order Tangent Model	First Order Adjoint Model
$\dot{f}(\mathbf{x}, \dot{\mathbf{x}}) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \times \mathbb{R}$	$\bar{f}(\mathbf{x}, \bar{y}) : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R} \times \mathbb{R}^n$
$y = f(\boldsymbol{x})$	$y = f(\boldsymbol{x})$
$\dot{y} = \boldsymbol{\nabla} f(\boldsymbol{x}) \cdot \dot{\boldsymbol{x}}$	$\bar{\boldsymbol{x}} = \bar{\boldsymbol{x}} + \boldsymbol{\nabla} f(\boldsymbol{x})^T \cdot \bar{y}$

- Adjoint model is the obvious choice for high dimensional optimization problems

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^p} f(\boldsymbol{x}, \boldsymbol{\alpha}) \quad f(\boldsymbol{x}, \boldsymbol{\alpha}) : \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^m \quad \text{with} \quad p \gg m$$

- Second and higher derivatives can be obtained by nesting models

$$f(\mathbf{x}) = \left(x_0^2 + x_1^2 + x_2^2\right)^2 \qquad \underbrace{\nabla f(\mathbf{x})}_{\in \mathbf{R}^n} \equiv \frac{\partial y}{\partial \mathbf{x}} = \begin{pmatrix} (2x_0)\cdot(1)\cdot(2\cdot(x_0^2+x_1^2+x_2^2)) \\ (2x_1)\cdot(1)\cdot(2\cdot(x_0^2+x_1^2+x_2^2)) \\ (2x_2)\cdot(1)\cdot(2\cdot(x_0^2+x_1^2+x_2^2)) \end{pmatrix}$$



- Need to differentiate basic operation like $+, -, \sin, \exp, \ldots$
- Partial derivatives will be assembled using chain rule
- In C++ can be achieved by utilizing operator overloading, i.e. replacing intrinsic operations by custom ones
- Different tools available, e.g. `dco/c++`, ADOL-C, CoDiPack [4, 5, 6]
- Need to change datatypes of floating point values to custom datatpye

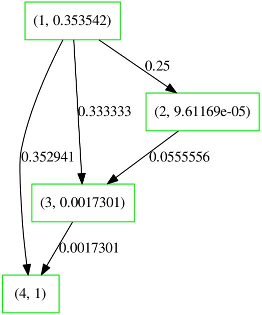


Figure: Internal `dco/c++` tape structure

OpenFOAM Adjoint Mode with dco/c++

- Idea: use central OpenFOAM typedef to replace all floating point values by custom AD data type [7]
- Should take care of bulk of AD work
- Minor manual adjustments needed, which accumulate over a large codebase

in `src/OpenFOAM/primitives/Scalar/doubleScalar/doubleScalar.h` replace:

```
namespace Foam{
  typedef double doubleScalar;
  ...
}
```

with:

```
#include "dco.hpp"
namespace Foam{
  typedef dco::ga1s<double>::type doubleScalar;
  ...
}
```

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namespace Foam{
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with:

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#include "dco.hpp"
namespace Foam{
  typedef dco::gt1s<double>::type doubleScalar;
  ...
}
```

Tangent vector mode can be implemented analogously (e.g. `dco::gt1v<double,16>::type`).

Features of Discrete Adjoint OpenFOAM

Groundworks:

- Typedef approach allows to differentiate the whole simulation code (Black-Box)
- For practical applications not feasible, further optimizations are needed
- A partial lists of features and methods enbabled by them are listed below

Algorithmic optimizations:

- Checkpointing [8]
- Reverse accumulation and Piggy-backing [9, 10]
- Symbolic differentiation of embedded linear solvers (SDLS) [11, 12]
- Adjoints of MPI parallelism by Adjoint-MPI [13, 12]

Case studies: [14]

- Topology optimization
- Parametric optimization
- Shape optimization

Currently working on CHT, see talk tomorrow.

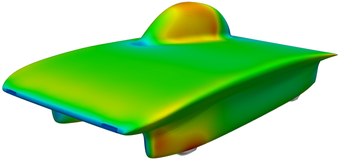

Figure: Shape sensitivity of Sonnenwagen w.r.t. (viscous) drag [15]

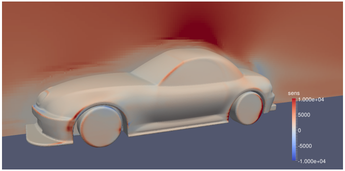

Figure: Shape sensitivity of touring car body [17]

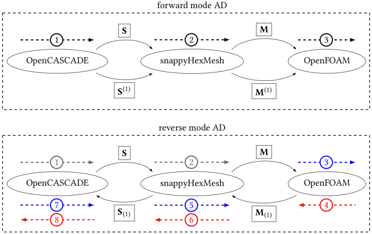

Figure: Differentiation of CAD toolchain [16]

- `wget https://stce.rwth-aachen.de/files/ofw19_docker.tar.gz`
- `tar -xzf ofw19_docker.tar.gz`
- import docker image and create container: `./create.sh`
- run and attach to container: `./run.sh`
- contents of `tutorial_data` will become the home directory of the docker container
- (discrete adjoint) OpenFOAM (v1812) installed in `/opt/discreteAdjointOpenFOAM-plus`

- Inspect environment with `env`
- Discrete Adjoint specific:
  - `DOF_COMPILER=Gcc`
  - `DOF_AD_OPTION=A1S`
  - `DOF_COMPILE_OPTION=Opt`
- Other `DOF_AD_OPTIONS` could be (not compiled in docker image):
  - `Passive` passive mode (double)
  - `A1S` adjoint mode
  - `T1S` tangent mode
  - `T2A1S` tangent over adjoint mode (2nd order)

- First we look at the implementation of a black box solver
- starting with `simpleFoam`
- due to memory demand not very practical, but a good starting point for other solvers
- you can follow along in `$OFW_DATA/adjointSimpleFoam/adjointSimpleFoam.C`

```
int main(int argc, char *argv[])
{
    #include "createFields.H"

    simpleControl simple(mesh);
    // run until end time reached / converged
    while (simple.loop())
    {
        // Pressure-velocity SIMPLE corrector
        #include "UEqn.H"
        #include "pEqn.H"

        turbulence->correct();
        runTime.write();
    }
    return 0;
}
```

Calculation of the Residual in OpenFOAM

Momentum Equation:

$$\nabla \cdot (\phi, \mathbf{U}) - \nabla \cdot (\nu \nabla \mathbf{U}) + \alpha \mathbf{U} = -\nabla \mathbf{p}$$

with mass flux through faces $\phi = \rho A \mathbf{U} \cdot \mathbf{n}$

`UEqn.H`:

```
fvVectorMatrix UEqn
(
    fvm::div(phi, U)
  - fvm::laplacian(nu, U)
  + fvm::Sp(alpha, U)
  ==
    fvOptions(U)
);
fvOptions.constrain(UEqn);
UEqn.relax();
fvVectorMatrix UEqnFull(UEqn == -fvc::grad(p));
```

Example Adjoint Solver, start with simpleFoam


```
int main(int argc, char *argv[]){
    ADmode::global_tape = ADmode::tape_t::create();
    ADmode::global_tape->register_variable(alpha[i],n);

    while (simple.loop()){
        #include "UEqn.H"
        #include "pEqn.H"
        turbulence->correct();
    }

    scalar J = 0;
    forAll(costFunctionPatches(),patchI)
        J += calcCost(patchI);

    dco::derivative(J) = 1.0;
    ADmode::global_tape->interpret_adjoint();

    // get adjoints, scale with cell volume, write to sens
    forAll(alpha,i){
        sens[i] = dco::derivative(alpha[i])/mesh.V()[i];
    }
}
```

```
int main(int argc, char *argv[]){
    ADmode::global_tape = ADmode::tape_t::create();
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```

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    while (simple.loop()){
        #include "UEqn.H"
        #include "pEqn.H"
        turbulence->correct();
    }

    scalar J = 0;
    forAll(costFunctionPatches(),patchI)
        J += calcCost(patchI);

    dco::derivative(J) = 1.0;
    ADmode::global_tape->interpret_adjoint();

    // get adjoints, scale with cell volume, write to sens
    forAll(alpha,i){
        sens[i] = dco::derivative(alpha[i])/mesh.V()[i];
    }
}
```

- Symbolically differentiating Linear Solvers leaves GAP in Tape, needs to be filled during interpretation[1]
- The adjoint projections $\bar{A}$ and $\bar{\mathbf{b}}$ can be obtained by solving the additional equation system[2]:

$$A^T \cdot \bar{\mathbf{b}} = \bar{\mathbf{x}} \quad \Rightarrow \bar{\mathbf{b}}$$

- $\bar{A}$ can be obtained by calculating the outer product of $-\bar{\mathbf{b}}$ and $\mathbf{x}^T$:

$$\bar{A} = -\bar{\mathbf{b}} \cdot \mathbf{x}^T$$

[1] U. Naumann et al.: *Algorithmic Differentiation of Numerical Methods: First-Order Tangents and Adjoints for Solvers of Systems of Nonlinear Equations*, ACM TOMS, Vol. 41

[2] M. B. Giles: *Collected Matrix Derivative Results for Forward and Reverse Mode Algorithmic Differentiation*

```
SDLS yes;

solvers{
  "(.*)" {
    solver          smoothSolver;
    smoother        symGaussSeidel;
    tolerance       1e-05;
    relTol          0;
    SDLS            $SDLS;
  }
  "(p|pReverse|Phi)" {
    solver          GAMG;
    tolerance       1e-06;
    relTol          0;
    smoother        DIC;
    SDLS            $SDLS;
  }
}

SIMPLE {
  nNonOrthogonalCorrectors 0;
  consistent        yes;
  costFunctionPatches (inlet outlet);
  costFunction "pressureLoss";
}
```

Checkpointing

- Trade memory demand for run time
- Only adjoin one time step at a time, then restore primal from an earlier time step and recalculate, record and adjoin next iteration step.
- Online Checkpointing using `Revolve` or `Equidistant`
- `cd $OFW_DATA/adjointSimpleCheckpointingFoam`
- `cd pitzDaily`
- inspect `system/checkpointingDict`

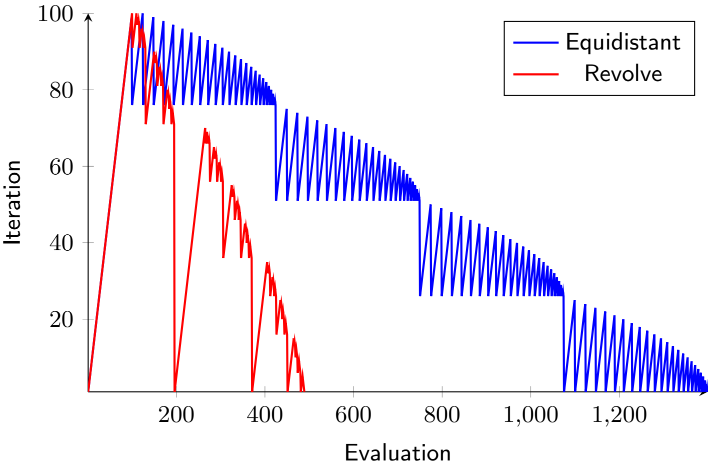
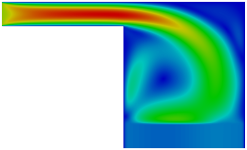
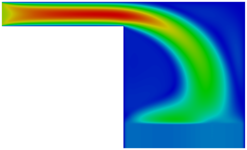


Figure: Revolve and equidistant for 100 iteration steps and 4 checkpoints.

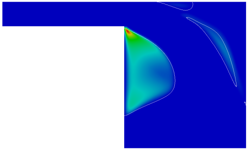
- For steady state cases one can utilize reverse accumulation or piggy backing
- Recording of single iteration step is repeatedly adjoined, forming a fixed point iteration yielding the correct adjoints
- Comparable to continuous adjoint, where adjoints are propagated forward alongside the primal
- Solver: `$OFW_DATA/piggyOptSimpleFoam`
- Case: `$OFW_DATA/piggyOptSimpleFoam/filter_case` with porosity at outlet, reconstructed from first Othmer paper [2].



Initial flow field



Optimized flow field



Topology penalty field

Lets implement our own cost function

- Solver: `$OFW_DATA/flowUniformity`
- Case: `$OFW_DATA/flowUniformity/flow_uniformity_case`
- Combination of flow uniformity and pressure loss function

```
scalar Jp = CostFunction(mesh).eval();
Foam::wordList outlets(2);
outlets[0]="outlet0";
outlets[1]="outlet1";

std::vector<scalar> meanMagU(outlets.size(),0.0);
forAll(outlets,cI)
{
  label patchI = mesh.boundaryMesh().findPatchID(outlets[cI] );
  fvPatch& patch = mesh.boundary()[patchI];
  meanMagU[cI] = gAverage(phi.boundaryField()[patchI]/patch.magSf());
}
scalar Jv = pow(meanMagU[0]-meanMagU[1],scalar(2.0));

scalar J = Jp + 0.0002 * Jv;
dco::derivative(J) = 1.0;
```

Result

- Secondary design goal pressure loss necessary
- else big sponge is a feasible solution

Initial flow field

Optimized flow field

Topology penalty field

- more sophisticated optimization methods should be explored
- multiple objectives can be evaluated with same tape (adjoint vector mode or sequential)
- can also use external optimizers, e.g. ceres, pyOpt

Discrete adjoint workflow:

- Use individual mesh point locations $\mathbf{P}$ as parameters
- Interpolate adjoint sensitivities $\bar{\mathbf{P}}$ of points to boundary face centers $\Rightarrow \bar{\mathbf{P}}_F$
- Take scalar product with face normal $\mathbf{n}_F$, divide by face area A_F: $s = \frac{\bar{\mathbf{P}}_F \cdot \mathbf{n}_F}{A_F}$

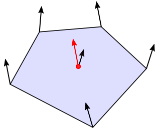


Figure: Point to face midpoint interpolation of sensitivity vectors

Continuous adjoint workflow:

- Calculate adjoint velocities $\mathbf{v}$ and pressure q using continuous adjoint NS[3]
- Surface sensitivity: $\frac{\partial \mathcal{J}}{\partial \beta} = -A\nu(\mathbf{n} \cdot \nabla)\mathbf{u}_t \cdot (\mathbf{n} \cdot \nabla)\mathbf{v}_t$

[3] calculated using OpenFOAM `adjointShapeOptimization` (sic!) solver modified to obtain shape adjoints according to [2]

- Consider laminar flow past cylinder at $Re = 2$ and $Re = 20$
- *Structured* non-orthogonal 2D mesh
- Compare discrete and adjoint sensitivities w.r.t. surface drag, obtained by the significantly different approaches outlined before

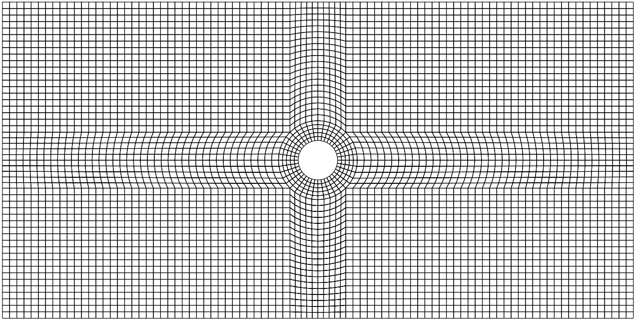
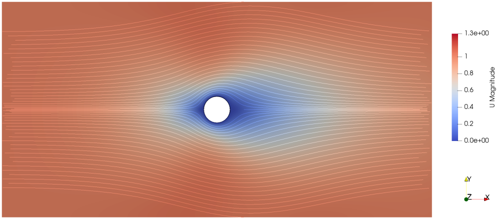
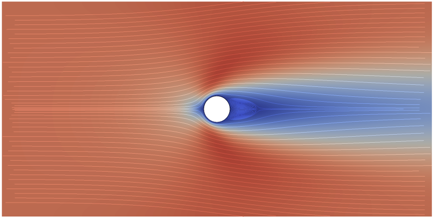


Figure: Structured non-cartesian mesh around cylinder

Re=2



Re=20



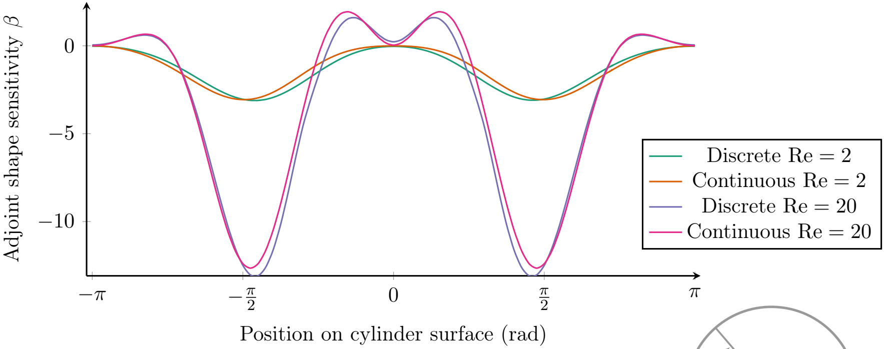
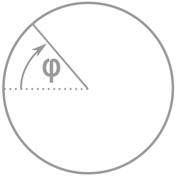


Figure: Surface sensitivity over angle



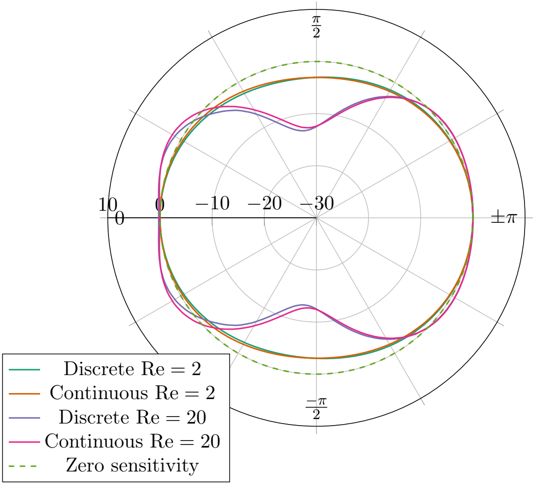
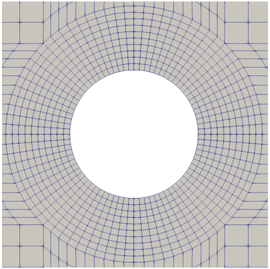
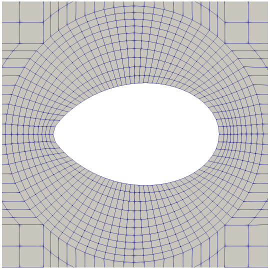


Figure: Surface sensitivity on cylinder surface in polar coordinates

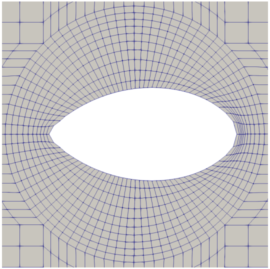
- Case: `$OFW_DATA/piggyShapeSimpleFoam/cylinderMirror`
- based on standard OpenFOAM tutorial case `cylinder`
- remove mirror plane by `mirrorMesh`
- `adjointMoveMesh` moves mesh points
- `adjointShapeOptimizationFoam` calculates sensitivities (with or without volume constraint).



Initial mesh



Optimization step 100



Optimization step 200

Thats all folks!

- Questions? `towara@stce.rwth-aachen.de`
- Full source access available `stce.rwth-aachen.de/foam`
- v1906 merge to appear soon

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