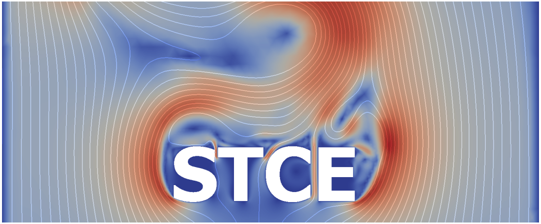

Discrete OpenFOAM

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Outline

OpenFOAM Introduction

From OpenFOAM 1.7 to 2.3

Features of discrete adjoint OpenFOAM

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Features of discrete adjoint OpenFOAM

OpenFOAM

- **Open F**ield **O**peration and **M**anipulation
- Open-Source (GPLv3) CFD solver
- developed by OpenCFD Ltd., currently at version 2.3.x
- includes tools for meshing, pre-, post-processing
- rising adoption in industry and academia due to lack of licence costs $\rightarrow$ well suited for parallel architectures

CFD Basics

- In our applications usually some form of Navier Stokes equation
- Navier Stokes equations for incompressible steady flow:

$$\mathbf{v} \cdot \nabla \mathbf{v} = \nu \nabla^2 \mathbf{v} - \frac{1}{\rho} \nabla p \qquad \text{momentum conservation}$$

$$\nabla \cdot \mathbf{v} = 0 \qquad \text{mass conservation}$$

- Or in three Dimensions:

$$v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} = -\frac{\partial p'}{\partial x} + \nu \left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2} \right)$$

$$v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} = -\frac{\partial p'}{\partial y} + \nu \left(\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2} \right)$$

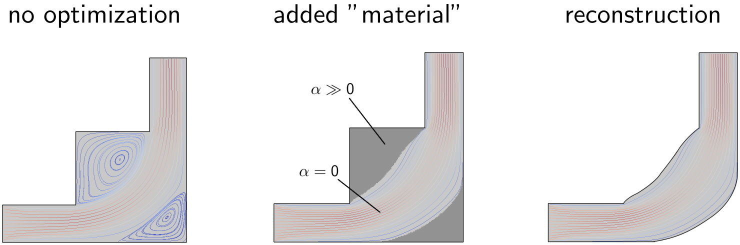
$$v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} = -\frac{\partial p'}{\partial z} + \nu \left(\frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

(Decoupled) Solution of the partial differential equations (SIMPLE-Algorithm):

- discretize / linearize momentum conservation equations
- solve momentum equations for velocity v, assume pressure p as known
- obtained velocity field fulfills momentum equation but not mass conservation equation as the pressure field was guessed and not correct
- discretize mass conservation equation
- use mass conservation equation to correct pressure field
- use new pressure field to correct velocity field
- Loop...

Topology Optimization



Add penalty term α to Navier-Stokes equation[1] :

$$(\mathbf{v} \cdot \nabla)\,\mathbf{v} = \nu \nabla^2 \mathbf{v} - \nabla p - \alpha \mathbf{v}$$

[1] C. Othmer: *A continuous adjoint formulation for the computation of topological and surface sensitivities of ducted flows.* Intern. J. f. Num. Meth. in Fluids. p. 861–877, 2008.

How to find appropriate α

- Define Cost Function J, e.g. total pressure loss between inlet and outlet:

$$J = \int_\Gamma p + \frac{1}{2} v_n^2 \; d\Gamma$$

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

$$\frac{\partial J}{\partial \alpha_i} = ???$$

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

$$\alpha_i^{n+1} = \alpha_i^n - \lambda \cdot \frac{\partial J^n}{\partial \alpha_i^n}, \quad \text{while insuring} \quad 0 < \alpha_i < \alpha_{max}$$

- Loop until α converged...

How to get derivatives?

- we coupled our operator-overloading tool `dco/c++` with OpenFOAM
- allows us to compute (arbitrary) first order derivatives in adjoint mode
- process descriped in [2]

[2] A Discrete Adjoint Model for OpenFOAM Proceedings of the International Conference on Computational Science, ICCS 2013

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Features of discrete adjoint OpenFOAM

- Started work on discrete OpenFOAM in late 2011
- up until now discrete adjoint OpenFOAM was using legacy version 1.7 of OpenFOAM (ca. 2010)
- at this time source was provided as tarball
- many newer cases are incompatible / need adjusting to run with OpenFOAM 1.7
- introduced support for OpenFOAM 2.3.x (2014) from scratch, working on official Git-Repo from Git-Hub
- merge for future releases of OpenFOAM should hopefully be way easier

OpenFOAM a1s mode

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

```
namespace Foam
{

  typedef double doubleScalar;
  ...

}
```

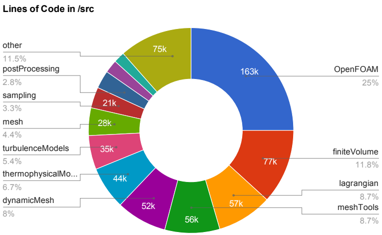
with:

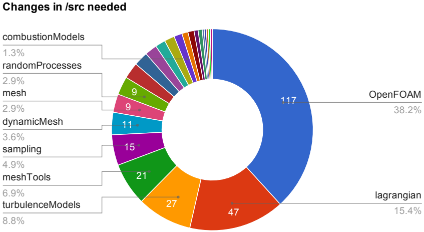
```
#include "dco.hpp"
namespace Foam
{

  typedef dco::a1s::type doubleScalar;
  ...

}
```

in Reality

- some changes have to be made in the OpenFOAM code:
  - unions don't support active datatypes
  - some casts are missing and have to be done by hand
    - i.e. `int i = 2.5` is fine, `int i = dco::a1s::type(2.5)` is not
  - some function macros (pow,max,min) have to be adapted
  - some templates have to be instantiated by hand (i.e. for double)

OpenFOAM LOC Analysis





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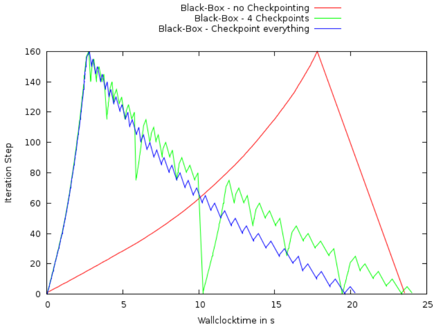
discrete Adjoint solvers

- incompressible steady flow
  - based on `simpleFOAM`
  - checkpointing support
  - optimization with steepest descent
  - reverse accumulation work in progress
- incompressible unsteady flow
  - based on `pisoFOAM`
  - checkpointing support
  - optimization with steepest descent (unsteady cost function, steady solution)
- compressible steady flow with coupled heat transfer
  - based on `chtMultiRegionSimpleFOAM`
  - Work in progress

Checkpointing Interface

- supports revolve (offline) and equidistant checkpointing
- if checkpoint size $\ll$ tape size both shemes perform similar

First Results



- Black-Box approach severely bound by memory bandwith! (Need to allocate around 20 GB)
- By doing Checkpointing we can actually get faster...

How to improve?

- Knowledge and Profiling reveals that most of calculation time and tape memory is spent in (iterative) linear solvers
- Analytical insight allows us to treat the adjoints of linear solvers analytically

Lemma

For a Linear Equation Sytem $Ax = b$ *we can calculate the adjoints for A and b by:* [3]

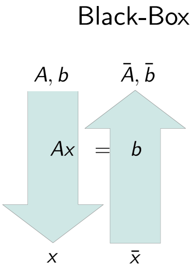
$\bar{b} = A^{-T}\bar{x} \rightarrow A^T\bar{b} = \bar{x}$

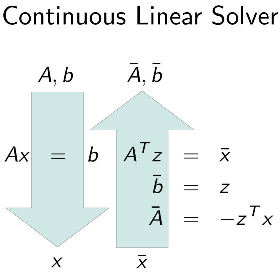
$\bar{A} = -\bar{b} \cdot x^T$

- This gives us an additional Linear Equation System which we have to solve during the gathering of the adjoints

[3] M. Giles, Collected Matrix Derivative Results for Forward and Reverse Mode Algorithmic Differentiation, *Advances in Automatic Differentiation 2008*

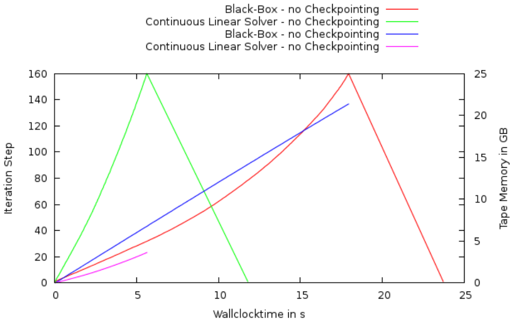
Treatment of Linear Solvers





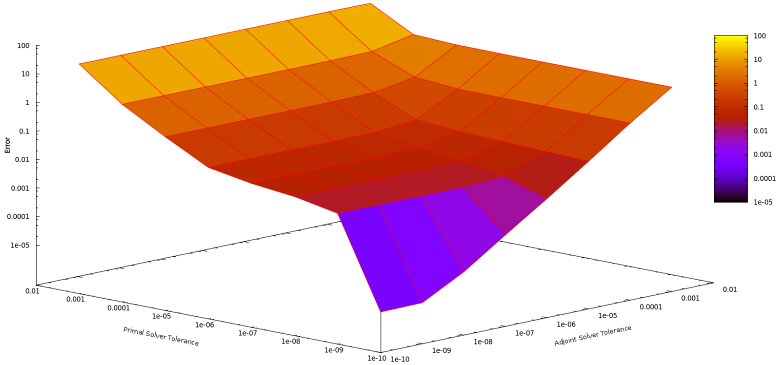
- when we encounter an linear solver during the augmented forward run we can stop taping
- when we encounter the gap in the tape during the interpretation we have to fill in the gap by hand
- have to remember A and x!

Results



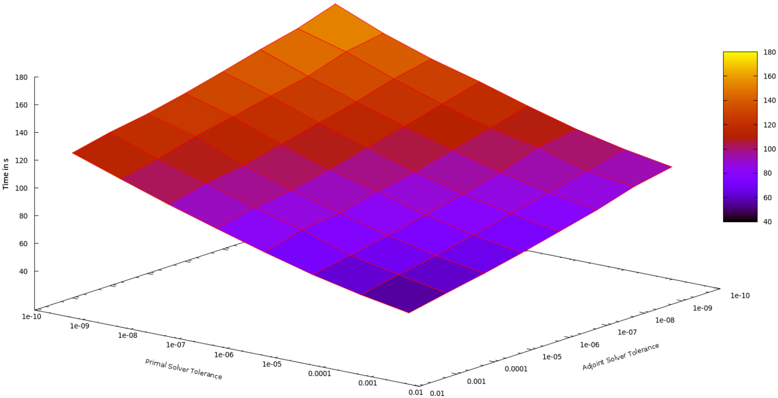
- we are seeing a nice improvement in both runtime and memory usage

Error



Error
100
10
1
0.1
0.01
0.001
0.0001
1e-05
0.01
0.001
0.0001
1e-05
1e-06
1e-07
1e-08
1e-09
1e-10
Primal Solver Tolerance
1e-10
1e-09
1e-08
1e-07
1e-06
1e-05
0.0001
0.001
0.01
Adjoint Solver Tolerance

Runtime



Time in s
180
160
140
120
100
80
60
40
1e-10
1e-09
1e-08
1e-07
1e-06
1e-05
0.0001
0.001
0.01
Primal Solver Tolerance
Adjoint Solver Tolerance

Summary and Outlook

- Black-Box discrete adjoint methods: Stringent memory requirements, not so fast.
- Improvements via Checkpointing and Linear solver treatment.
- further improvements possible for steady cases through reverse accumulation (implemented $\rightarrow$ EuroAD)
- parallelisation with (A)MPI still to be done

Thank you!
Questions?