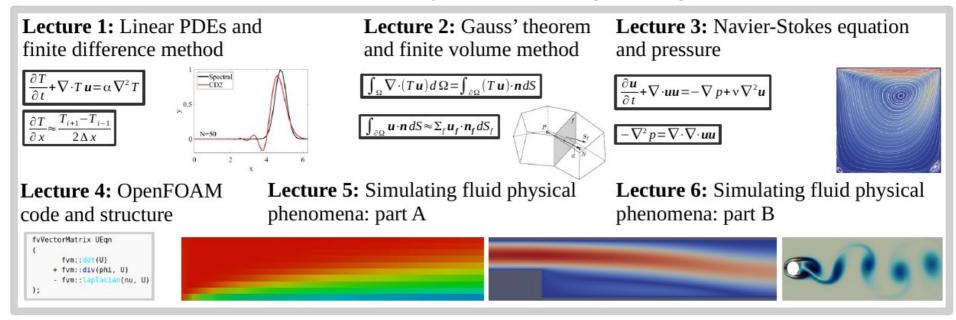


EEN-E2001 Computational Fluid Dynamics

Lecture 3*: OpenFOAM code and structure

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January 30th 2023 Aalto University, School of Engineering



^{*}Lectures 3 and 4 had to be swapped this year

OpenFOAM

Part 1

How to do simulations?

Part 2

How do solvers work?

Part 1

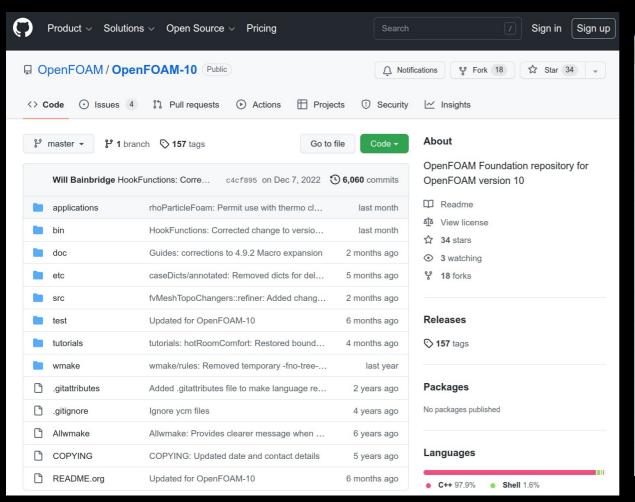
How to do simulations?

Terminology

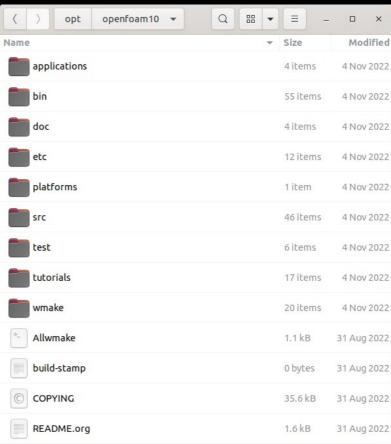
Solver	Executable application designed to solve a specific problem in fluid or continuum mechanics (scalarTransportFoam , icoFoam ,)
Utility	Executable application, designed to perform tasks that involve data manipulation (blockMesh, postProcess, foamListTimes,)
Library	Precompiled C++ libraries that are dynamically linked to the solvers and utilities. There are separate libraries containing e.g. turbulence models, post-processing functions, etc.
Case folder	Folder containing OpenFOAM dictionaries, describing particular problem (case)
Dictionary	A file/entity that contains data entries in the format understandable by OpenFOAM (0/U , system/controlDict ,)
Function objects	Tools to ease workflow configurations and enhance workflows by producing additional user-requested data

OpenFOAM 10 – open-source CFD library

github.com/OpenFOAM/OpenFOAM-10



/opt/openfoam10/



OpenFOAM

Pre-processing

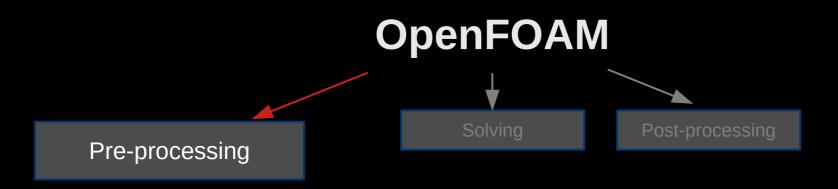
Solving

Post-processing

- 1. Choose solver
- 2. Set up case dictionaries
- 3. Generate mesh
- 4. (optional) Adding extra terms and constraints
- 5. (optional) Set up function objects

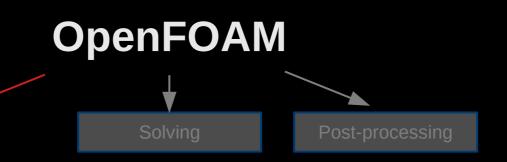
- 1. Running solvers
- 2. Run-time controls

- 1. Post-processing and sampling
- 2. Visualization



1. Choosing solver

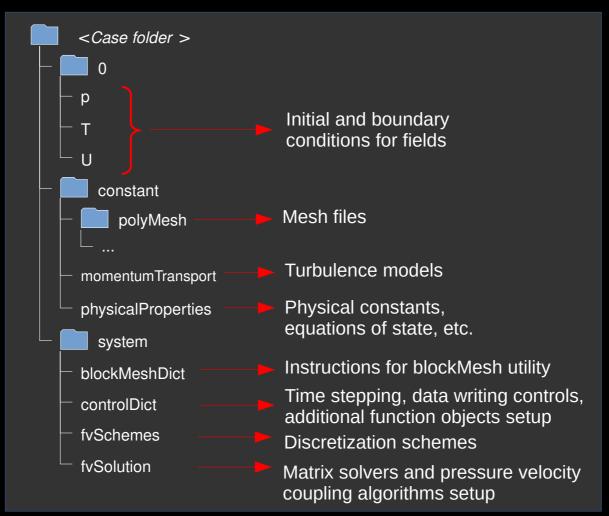
Example list of solvers				
scalarTransportFoam	Convection-diffusion of a passive scalar			
icoFoam	Simplified PISO solver for incompressible , laminar flow of Newtonian fluids			
simpleFoam	Incompressible fluid flow solver, using SIMPLE algorithm. Used for steady-state flows			
pisoFoam	Incompressible fluid flow solver, using PISO algorithm. Used for transient flows			
pimpleFoam	Incompressible fluid flow solver, using PIMPLE algorithm. Used for transient flows			
rhoPimpleFoam	Compressible fluid flow solver, using PIMPLE algorithm			
buoyantPimpleFoam	Compressible fluid flow solver with buoyancy modeling, using PIMPLE algorithm			
reactingFoam	Compressible reacting fluid flow solver with chemistry reactions, using PIMPLE algorithm			
interFoam	Two incompressible fluids flow solver using "volume of fluid" model, using PIMPLE algorithm			
interPhaseChangeFoam	Two incompressible fluids flow solvers using "volume of fluid" model with phase-change, using PIMPLE algorithm			
multiphaseEulerFoam	System of any number of compressible fluid phases flow solver, using PIMPLE algorithm			



Pre-processing

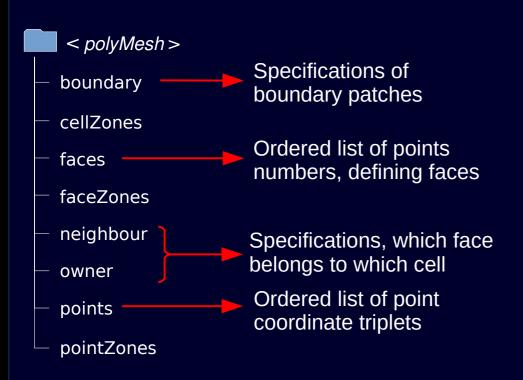
2. Setting up case dictionaries

Usually starts with copying tutorial case

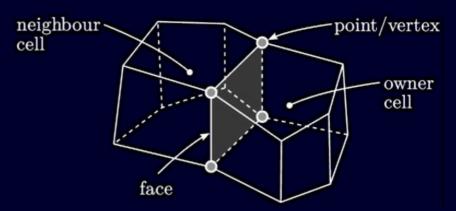


OpenFOAM Solving Post-processing

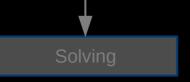
3. Mesh generation



Main mesh generation utilities				
blockMesh	for simple structured meshes			
snappyHexMesh	for meshing complex geometries (using stl, obj, vtk,)			
starToFoam fluentMeshToFoam gmshToFoam 	import 3rd party mesh formats			



OpenFOAM



Post-processing

Pre-processing

4. Adding extra terms and constraints constant/fvModels

system/fvConstraints

```
limitp
{
   type   limitPressure;

   min     0.8e5;
   max     1.2e5;
}
```

Commands to list available options:

```
scalarTransportFoam -listFvModels
scalarTransportFoam -listFvConstraints
```

Command to show info and find usage examples:

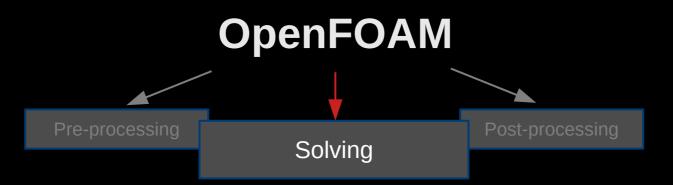
```
foamInfo -a heatSource
foamInfo -a limitPressure
```

https://github.com/OpenFOAM/OpenFOAM-10/tree/master/src/fvModels https://github.com/OpenFOAM/OpenFOAM-10/tree/master/src/fvConstraints

5. Set up function objects system/controlDict

scalarTransportFoam -listFunctionObjects
FoamInfo -a probes

https://doc.cfd.direct/openfoam/user-guide-v10/post-processing-cli



1. Running solver

a) On a single core

scalarTransportFoam

b) On multiple cores (requires system/decomposeParDict)

decomposePar mpirun -np 4 scalarTransportFoam -parallel reconstructPar

c) On supercomputing cluster: using schedulers

2. Run-time controls

If you set in system/controlDict:

runTimeModifiable true;

You can modify entries in dictionaries during runtime.

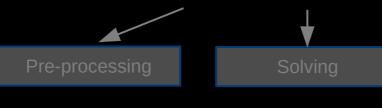
E.g. adjust tolerances, change write times, change time step etc.

You can also track residuals of your simulation using foamMonitor utility.

You can stop the simulation and write the fields immediately by setting in *system/controlDict*:

stopAt writeNow;

OpenFOAM



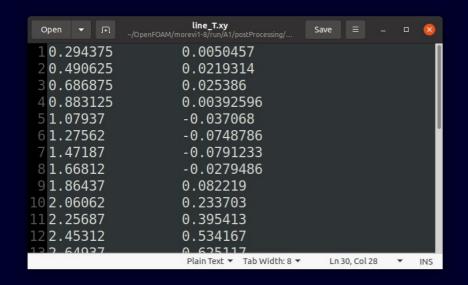
Post-processing

1. Post-processing and sampling

Utility postProcess can execute functionObjects after simulation is finished.

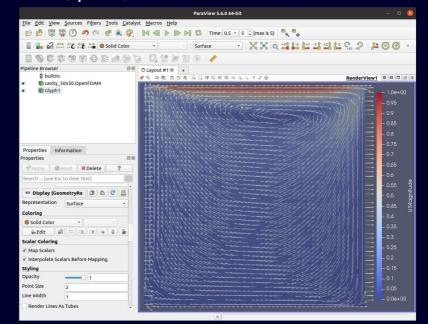
E.g. sample data over a line (requires file system/singleGraph):

postProcess -func singleGraph



2. Visualization

Use paraFoam to visualize fields, make videos, renders, plots, etc.



Or export the data to 3rd part format, e.g. VTK:

foamToVTK

Part 2

How do solvers work?

Main question:

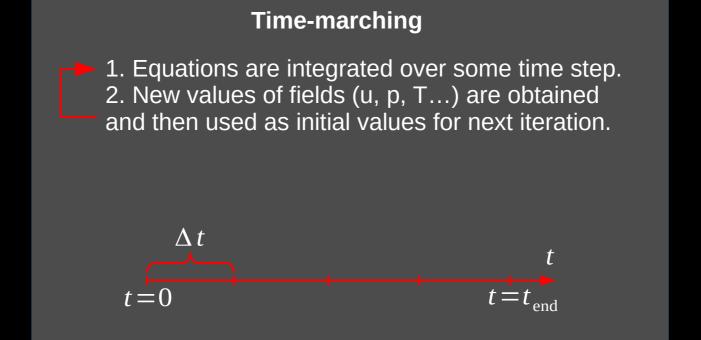
How does OpenFOAM solver proceed from one time step to the next one?

```
Time = 0.96

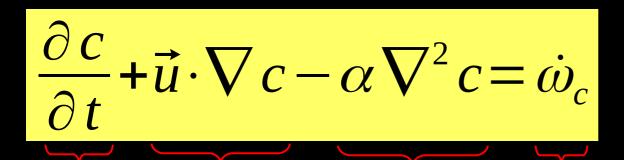
smoothSolver: Solving for T, Initial residual = 0.0190827, Final residual = 2.62384e-06, No Iterations 2
Time = 0.965

smoothSolver: Solving for T, Initial residual = 0.0190088, Final residual = 2.47331e-06, No Iterations 2
Time = 0.97
```

Matrix equation solver logs. But where does the matrix come from?



Scalar transport equation

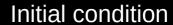


Temporal derivative

Convection

Diffusion

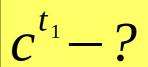
Source



$$c(t=t_0)=c^{t_0}$$

Time step

$$\Delta t = t_1 - t_0$$

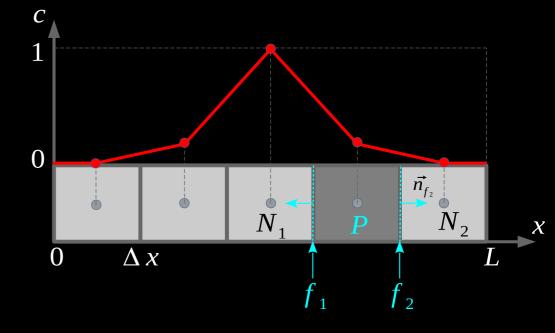


N – number of cells

$$\begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{22} & \cdots & a_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{vmatrix} \cdot \begin{vmatrix} c_{1}^{t_{1}} \\ c_{2}^{t_{1}} \\ \vdots \\ c_{N}^{t_{1}} \end{vmatrix} = \begin{vmatrix} b_{1} \\ b_{2} \\ \vdots \\ b_{N} \end{vmatrix}$$

1d convection of a Gaussian Goal: calculate field c after Δt u = const > 0, $t_1 = t_0 + \Delta t$, **5 cells**

$$\frac{\partial c}{\partial t} + \nabla \cdot (\vec{u}c) = 0$$
Integrate over cell P

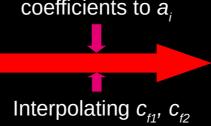


$$\frac{1}{V_{p}} \int_{V_{p}} \nabla \cdot (\vec{u}c) dV = \frac{1}{V_{p}} \int_{A_{p}} (\vec{u}c) \vec{n} dA_{p} \approx \frac{1}{V_{p}} \sum_{f} (\vec{u}_{f}c_{f}) \cdot \vec{n}_{f} A_{f} = \frac{u_{f_{2}}c_{f_{2}} - u_{f_{1}}c_{f_{1}}}{\Delta x} = u \frac{c_{f_{2}} - c_{f_{1}}}{\Delta x}$$
Gauss theorem Finite number of faces 1d uniform wellocity

Implicit Euler temporal discretization:

$$\frac{c_P^{t_1} - c_P^{t_0}}{\Delta t} + u \frac{c_{f_2}^{t_1} - c_{f_1}^{t_1}}{\Delta x} = 0$$

Putting constant coefficients to a_i



 $a_{P}c_{P}^{t_{1}}+\sum_{N_{i}}a_{N_{i}}c_{N_{i}}^{t_{1}}=b_{P}$

 $c_{f_1} = \frac{c_{N_1} + c_P}{2}$

upwind

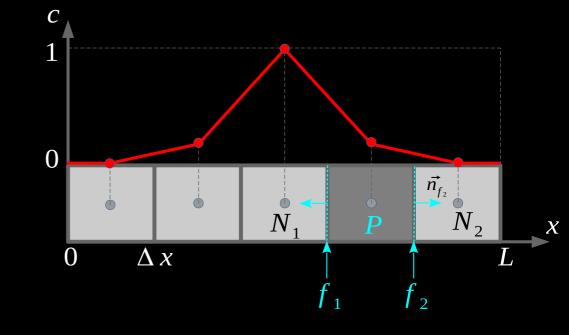
$$c_{f_1} = c_p$$

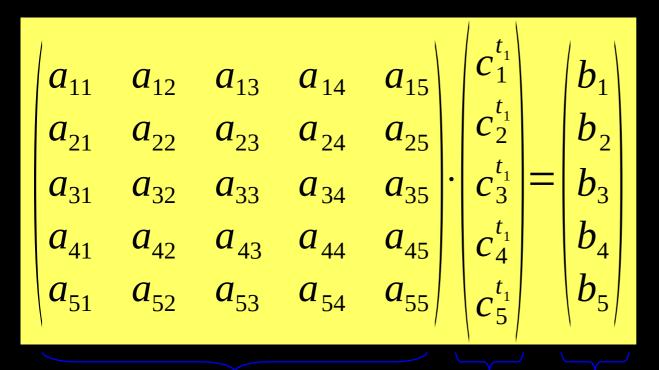
We have 1 equation for each of 5 cells. Total:

- 5 equations
- 5 unknowns

$$a_{P}c_{P}^{t_{1}}+\sum_{N_{i}}a_{N_{i}}c_{N_{i}}^{t_{1}}=b$$

Diagonal Components ("owner") Off-diagonal Components ("neighbor")





 $A\vec{c^{t_1}} = \vec{b}$

Use some matrix solver to obtain field c at time t_i

Known coefficient matrix

Field vector Known vector to be solved of explicit terms

scalarTransportFoam source code

Located in *applications/solvers/basic/scalarTransportFoam/*

```
Info<< "\nCalculating scalar transport\n" << endl;</pre>
#include "CourantNo.H"
while (simple.loop(runTime))
    Info<< "Time = " << runTime.userTimeName() << nl << endl:</pre>
    fvModels.correct();
    while (simple.correctNonOrthogonal())
        fvScalarMatrix TEqn
             fvm::ddt(T)
          + fvm::div(phi, T)
           fvm::laplacian(DT, T)
             fvModels.source(T)
        );
        TEgn.relax();
        fvConstraints.constrain(TEgn);
        TEqn.solve();
        fvConstraints.constrain(T);
    runTime.write();
Info<< "End\n" << endl;</pre>
```

Loop over time steps, as defined in system/controlDict

$$\frac{\partial c}{\partial t} + \vec{u} \cdot \nabla c - \alpha \nabla^2 c = \dot{\omega}_c$$

Matrix equation is constructed here

$$A\vec{c^{t_1}} = \vec{b}$$

Call matrix solver, defined in system/fvSolution

Write data, if current time step fits writeTime defined in system/controlDict

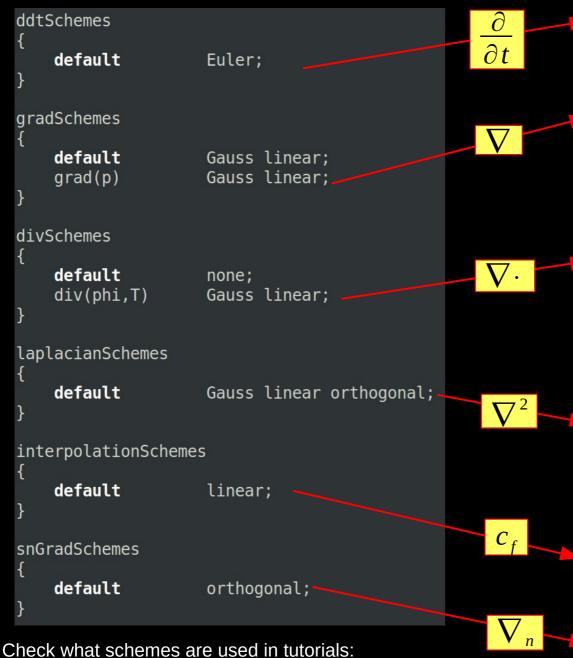
```
Time = 0.96

smoothSolver: Solving for T, Initial residual = 0.0190827, Final residual = 2.62384e-06, No Iterations 2
Time = 0.965

smoothSolver: Solving for T, Initial residual = 0.0190088, Final residual = 2.47331e-06, No Iterations 2
Time = 0.97
```

Discretization schemes

Located in *system/fvSchemes*



Temporal discretization schemes: Euler (1st ord.), backward (2nd ord.), ...

In the most cases, linear works perfectly well here. In our applications we discretize pressure gradient here.

div(phi,...) are the most important schemes usually! Here we discretize convection term. upwind (1st ord.), linear (2nd ord.), limitedLinear, Gamma and vanLeer are probably the most common choices

The keyword "linear" refers to interpolation scheme, where linear is usually enough. The second keyword in surface normal gradient scheme, which usually is either orthogonal or corrected (for meshes with orthogonality)

Cell to face interpolations of values. Used in the interpolation of velocity to face centers for the calculation of flux

Component of gradient normal to a cell face

Check what schemes are used in tatorials.

foamSearch -c \$FOAM_TUTORIALS fvSchemes "divSchemes/div(phi,U)"

Flux limiting schemes

$$c_{f_1} = c_{f_1}^{low} - \phi(r_{N_1})(c_{f_1}^{low} - c_{f_1}^{high})$$

$$c_{f_2} = c_{f_2}^{low} - \phi(r_P)(c_{f_2}^{low} - c_{f_2}^{high})$$

 $C_{f_1}^{low}$

- low resolution flux (upwind)

 $C_{f_1}^{high}$

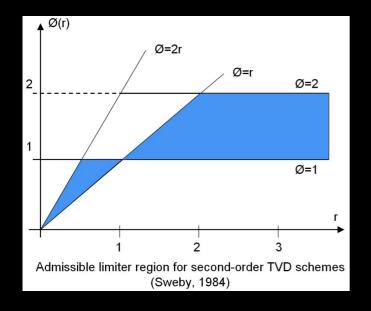
- high resolution flux (linear)

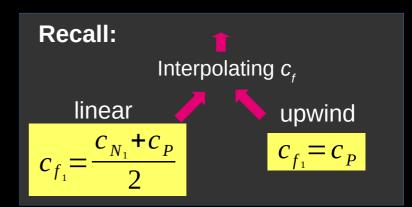
 $\phi(r_P)$

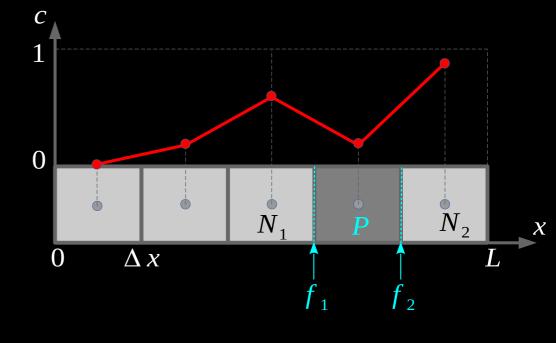
- flux limiter function

$$r_{P} = \frac{c_{P} - c_{N_{1}}}{c_{N_{2}} - c_{P}}$$

ratio of successive gradients

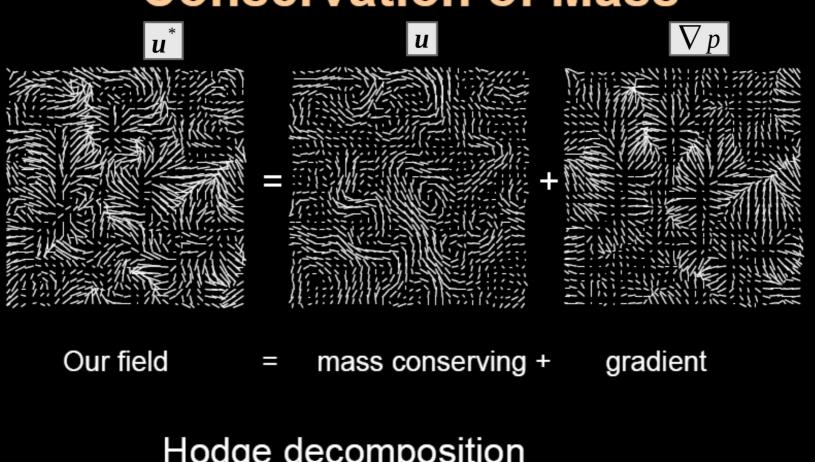






Vector fields can be divided into two parts via "Helmholtz-Hodge" decomposition

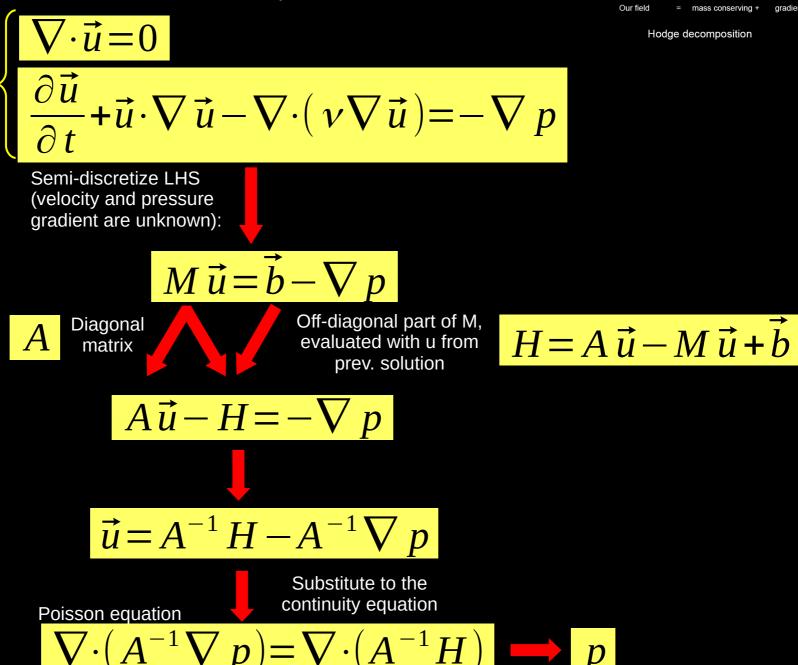
Conservation of Mass



Hodge decomposition

Pressure-velocity coupling algorithms

Start with Navier-Stokes equations:



Conservation of Mass

Hodge decomposition

Simplified solution scheme

Initial guess

1. Momentum predictor

Solve the momentum equation for the velocity field. This velocity field does not satisfy the continuity equation.

$$M\vec{u} = -\nabla p$$



2. Explicit part evaluation

Use the velocity to calculate explicit part H

$$H = A\vec{u} - M\vec{u} + \vec{b}$$



3. Pressure-corrector

Solve the Poisson equation for the pressure field.

$$\nabla \cdot (A^{-1} \nabla p) = \nabla \cdot (A^{-1} H)$$



4. Explicit velocity calculation

Use the pressure field to calculate new velocity field, satisfying the continuity equation. Pressure field is not corrected anymore

$$\vec{u} = A^{-1} H - A^{-1} \nabla p$$

ner corrector (PISO loop)

non-orthogonal

OpenFOAM code (icoFoam)

```
fvVectorMatrix UEqn
   (
        fvm::ddt(U)
    + fvm::div(phi, U)
    - fvm::laplacian(nu, U)
);

if (simple.momentumPredictor())
{
    solve(UEqn == -fvc::grad(p));
    fvOptions.correct(U);
}
```

```
volScalarField rAU(1.0/UEqn.A());
volVectorField HbyA(constrainHbyA(rAU*UEqn.H(), U, p));
surfaceScalarField phiHbyA
(
    "phiHbyA",
    fvc::flux(HbyA)
    + fvc::interpolate(rAU)*fvc::ddtCorr(U, phi)
);
```

```
U = HbyA - rAU*fvc::grad(p);
```

Pressure-velocity coupling algorithms

Parameters are located in system/fvSolution

```
PIMPLE
{
    momentumPredictor no;
    nOuterCorrectors 1;
    nCorrectors 2;
    nNonOrthogonalCorrectors 0;
}
```

momentumPredictor	switch controlling the momentum predictor. Can be set to "off" for some flows, including low Reynolds number and multiphase.		
nOuterCorrectors	sets the number of outer correctors, number of loops over the entire system of equations within on time step, representing the total number of times the system is solved; must be ≥ 1 and is typically set to 1, replicating the PISO algorithm. If you experience pressure fluctuations, increasing this number can help.		
nCorrectors	sets the number of inner correctors, i.e. times the algorithm solves the pressure equation and momentum corrector in each step; typically set to 2 or 3.		
nNonOrthogonalCorrectors	specifies repeated solutions of the pressure equation, used to update the explicit non-orthogonal correction; typically set to 0 for orthogonal meshes and ≥ 1 for meshes with non-orthogonality		

Further reading:

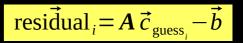
SIMPLE: https://openfoamwiki.net/index.php/The_SIMPLE_algorithm_in_OpenFOAM

PISO: https://openfoamwiki.net/index.php/OpenFOAM_guide/The_PISO_algorithm_in_OpenFOAM_PIMPLE: https://openfoamwiki.net/index.php/OpenFOAM_guide/The_PIMPLE_algorithm_in_OpenFOAM_

Matrix solver setup

Located in system/fvSolution





```
relTol_i = \frac{residual_i}{residual_0}
```

```
solvers
        solver
                        PCG:
                                              Usually:
        preconditioner
                        DIC:
                                              • PCG with DIC preconditioner
        tolerance
                        1e-06;

    GAMG with GaussSeidel smoother

        relTol
                        0.05;
    pFinal
                                              Tolerance for the final inner corrector step.
        $p;
                                              Usually tolerance is tightened here and
        relTol
                        0;
                                              relTol=0
        solver
                        smoothSolver;
                                                Solver selection here depends on your
                        symGaussSeidel;
        smoother
                                                grid parameters, which determines the
        tolerance
                        1e-05;
                                                filling of your matrix.
        relTol
                        0;
                                                PBiCGStab with DILU preconditioner is
                                                quite robust
```

```
Time = 0.295

smoothSolver: Solving for Ux, Initial residual = 0.00336414, Final residual = 4.87212e-06, No Iterations 2 smoothSolver: Solving for Uy, Initial residual = 0.00395571, Final residual = 6.13208e-06, No Iterations 2 DICPCG: Solving for p, Initial residual = 0.00198918, Final residual = 9.51425e-05, No Iterations 27 time step continuity errors: sum local = 1.56381e-08, global = 5.72285e-20, cumulative = 2.48268e-20 DICPCG: Solving for p, Initial residual = 0.00061602, Final residual = 9.64995e-07, No Iterations 65 time step continuity errors: sum local = 1.49115e-10, global = 2.02111e-20, cumulative = 4.50379e-20 ExecutionTime = 0.31 s ClockTime = 1 s
```

Further reading

User guide:

Online: https://doc.cfd.direct/openfoam/user-guide-v10/index

Offline: /opt/openfoam10/doc/Guides/OpenFOAMUserGuide-A4.pdf

Programmers Guide:

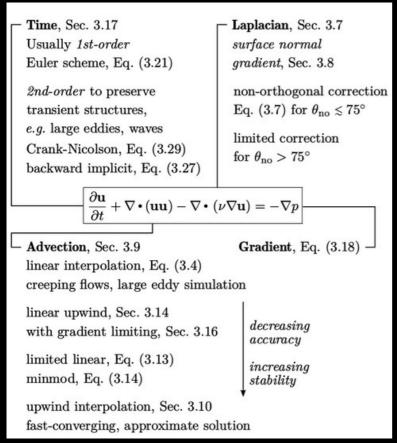
https://sourceforge.net/projects/openfoam/files/v2112/ProgrammersGuide.pdf/download

CFD textbook by authors of OpenFOAM (free web version):

https://doc.cfd.direct/notes/cfd-general-principles/

User guide Tutorial relevant to HW2

Textbook



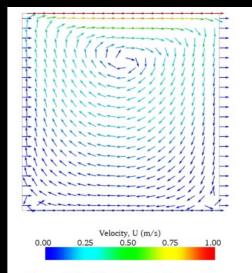


Figure 2.8: Velocities in the cavity case.

Programmer's guide

Operation	Comment	Mathematical Description	Description in OpenFOAM
Addition		a + b	a + b
Subtraction		a - b	a - b
Scalar multiplication		sa	s * a
Scalar division		\mathbf{a}/s	a / s
Outer product	$\operatorname{rank} \mathbf{a}, \mathbf{b} >= 1$	ab	a * b
Inner product	$rank \mathbf{a}, \mathbf{b} >= 1$	a·b	a & b