



OpenFOAM Fundamentals

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OpenFOAM Parallel Performance Engineering Workshop



Agenda



Time TBC

Daresbury Laboratory, Keckwick Lane, WA4 4AI



Table of Content

- What is OpenFOAM?
- OpenFOAM Structure
- Numerics of OpenFOAM
 - Finite Volume Method
 - Time Discretisation
 - Pressure Velocity Coupling
 - Volume of Fluid



What is OpenFOAM?

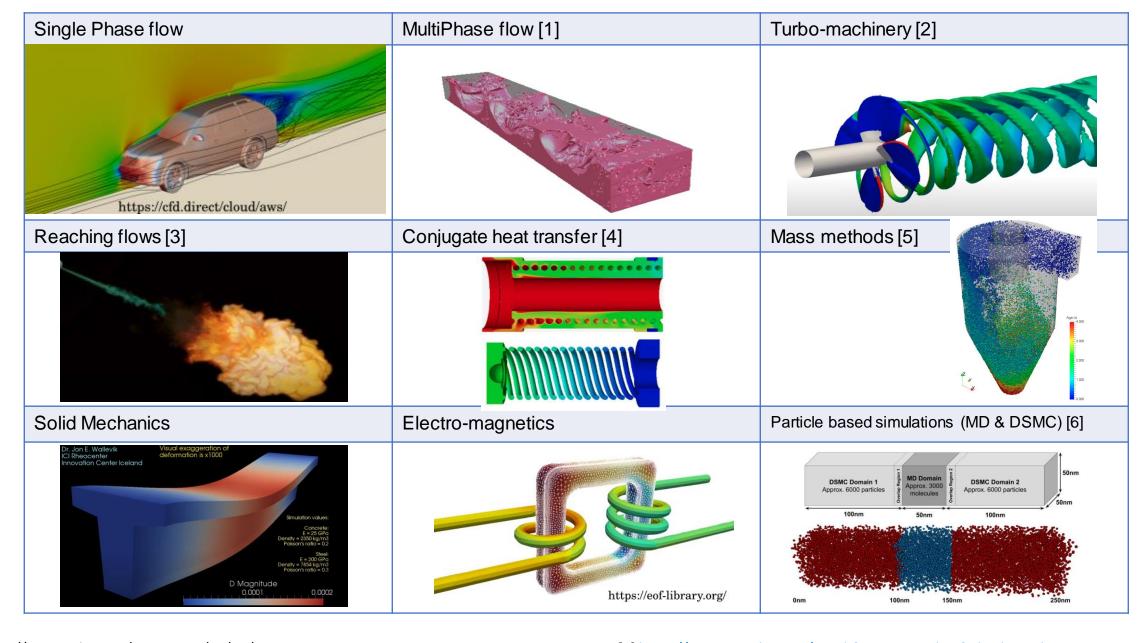




What is OpenFOAM

- FOAM stands for "Field Operation and Manipulation"
- It is a library of tools written in C++ with high utilisation of Object Oriented Programming
- There are different versions:
 - OpenFOAM ESI (OpenFOAM-v20xx) (<u>www.openfoam.com</u>)
 - OpenFOAM foundation(OpenFOAM x) (<u>www.openfoam.org</u>)
 - OpenFOAM Extend (https://github.com/Unofficial-Extend-Project-Mirror)
- The core solvers are similar
- Switching between solvers is easy, giving the capabilities are available in both versions.
- There are some differences
 - ESI has more solvers and utilities (overset method, interIsoFoam)
 - ESI do more frequent releases
 - Foundation has a more generalized implementation
 - Some solvers gives different results

```
\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \bullet \phi \mathbf{U} - \nabla \bullet \mu \nabla \mathbf{U} = -\nabla p solve ( \text{fvm::ddt(rho, U)} \\ + \text{fvm::div(phi, U)} \\ - \text{fvm::laplacian(mu, U)} \\ == \\ - \text{fvc::grad(p)} );
```



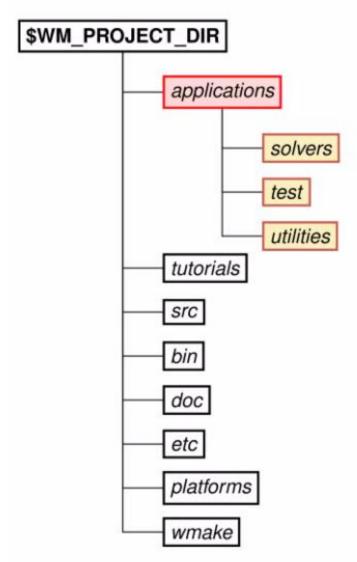
- [1] https://www.mdpi.com/2076-3417/12/17/8481
- [3]https://ecn.sandia.gov/diesel-spray-combustion/target-condition/spray-ab/
- [5] https://www.foamacademy.com/wp-content/uploads/2016/11/GOFUN2017_ParticleSimulations_slides.pdf
- [6] https://www.sciencedirect.com/science/article/pii/S0045793020302966

- [2] https://www.youtube.com/watch?v=9eNYtOQlixY&ab_channel=EngineerDo
- [4] https://www.sciencedirect.com/science/article/pii/S1359431117349840









1. applications:

alias: app = 'cd \$FOAM_APP'.

This directory contains the source files of all the executables created using the C++ libraries. It contains the following directories:

1.1 solvers:

alias: *sol* = 'cd \$FOAM_SOLVERS'.

Source code to solve a particular continuum mechanics problem.

1.2 test:

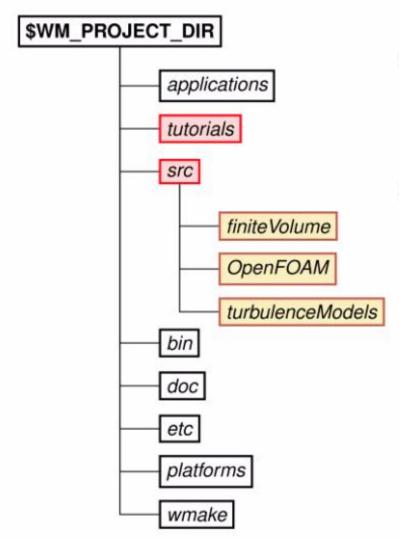
Sample codes to help understand the usage of OpenFOAM libraries.

1.3 Utilities:

alias: util = 'cd \$FOAM_UTILITIES'.

Source code to perform pre- and post-processing tasks involving data manipulation and algebraic manipulations.

Source: https://www.slideshare.net/pengding2/introdcution-to-openfoamworking-with-free-



2. tutorials:

alias: *tut* = 'cd \$FOAM_TUTORIALS'.

Contains tutorials that demonstrate the usage of all solvers and most of the utilities.

3. src:

alias: src = 'cd \$FOAM_SRC'.

It contains several subdirectories which include the source code for all libraries. The important folders are:

3.1 finiteVolume:

alias: foamfv = 'cd \$FOAM_SRC/finiteVolume'.
Includes classes for finite volume space/time discretisation, boundary conditions etc.

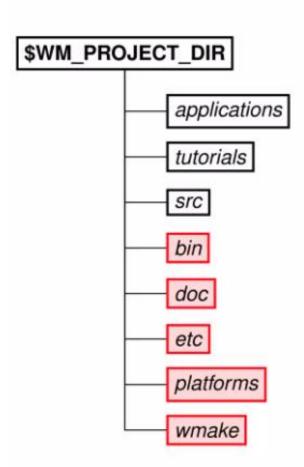
3.2 OpenFOAM:

This core library includes important definitions.

3.3 turbulenceModels:

Contains libraries for turbulence models.

Source: https://www.slideshare.net/pengding2/introdcution-to-openfoamworking-with-free-software



4. bin:

This directory contains shell scripts such as paraFoam, foamLog etc.

doc:

It contains all the documentation relevant to the version of OpenFOAM including:

- 5.1 User and Programmer's guides
- 5.2 Doxygen generated documentation
- 5.3 OpenFOAM coding style guide

6. etc:

It contains global OpenFOAM dictionaries and setup files.

7. platforms:

The binaries generated during the compilation of the applications and the dynamic libraries are stored here.

8. wmake:

Compiler settings are included in this directory including optimisation flags. It also contains *wmake*, a special make command which understands the **OpenFOAM** file structure.

Source: https://www.slideshare.net/pengding2/introdcution-to-openfoamworking-with-free-software

OpenFOAM Case Structure

Basic OpenFOAM case

\$FOAM_TUTORIALS/multiphase/interFoam/RAS/damBreak/damBreak

- This is not a comprehensive list of case files!
- Some files can be placed at different directory, i.g. blockMesh

damBreak **Time Directories** alpha.water Contains the field values epsilon and boundary nut conditions of specific nuTilda time p_rgh **Constant directory** constant Contains the physical properties and the boundary mesh information faces neighbour PolyMesh sub-directory owner Contains mesh info points transportProperties turbulenceProperties **System directory** blockMeshDict Mainly for defining the controlDict

decomposeParDict

fvSchemes fvSolution

setFieldsDict

numerical schemes and

their parameters.



Numerics of OpenFOAM



Governing Equation

General conservation equation

$$\underbrace{\frac{\partial \rho \phi}{\partial t}}_{\text{Convection}} = -\underbrace{\nabla \cdot \rho \mathbf{u} \phi}_{\text{Convection}} + \underbrace{\nabla \cdot (D \nabla \phi)}_{\text{Diffusion}} + \underbrace{S_{\phi}}_{\text{Source term}}$$

Momentum conservation equation

$$\frac{\partial \rho \mathbf{u}}{\partial t} = -\nabla \cdot \rho \mathbf{u} \mathbf{u} + \nabla \cdot (\rho \nu \nabla \mathbf{u}) + -\nabla p + S$$

Mass Conservation Equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \rho \mathbf{u}$$

Finite Volume Method

- The domain is discretized into small cells, and the values of the cell is the integral of the function inside the cell.
- Insure flux conservation, and can be used for complex geometry and mesh refinement.





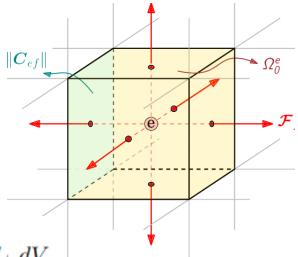
$$\int_{V} \frac{\partial \rho \phi}{\partial t} . dV = -\int_{V} \nabla \cdot \rho \mathbf{u} \phi . dV + \int_{V} \nabla \cdot (D \nabla \phi) . dV + \int_{V} S_{\phi} . dV$$

Gauss's divergence theorem:

$$\int_{V} \nabla \cdot \mathbf{a} dV = \int_{S} \mathbf{a} dS$$

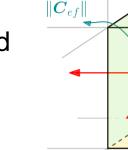
• Then the conservation equation cab be expressed as:

$$\int_{V} \frac{\partial \rho \phi}{\partial t} dV = -\int_{S} \rho \mathbf{u} \phi dS + \int_{S} (D \nabla \phi) dS + \int_{V} S_{\phi} dV$$



Finite Volume Method

- The domain is discretized into small cells, and the values of the cell is the integral of the function inside the cell.
- Insure flux conservation, and can be used for complex geometry and mesh refinement.



- OF uses cell-centered finite volume method.
- Integral form of the conservation equation:

$$\int_{V} \frac{\partial \rho \phi}{\partial t} . dV = + \int_{V} \nabla \cdot \rho \mathbf{u} \phi . dV + \int_{V} \nabla \cdot (D \nabla \phi) . dV + \int_{V} S_{\phi} . dV$$

Gauss's divergence theorem:

$$\int_{V} \nabla \cdot \mathbf{a} dV = \int_{S} \mathbf{a} dS$$

Then the conservation equation cab be expressed as:

$$\int_{V} \frac{\partial \rho \phi}{\partial t} dV = -\int_{S} \rho \mathbf{u} \phi dS + \int_{S} (D\nabla \phi) dS + \int_{V} S_{\phi} dV$$

Finite Volume Method: Time Derivative

$$\int_{V} \frac{\partial \rho \phi}{\partial t} dV = \frac{\partial}{\partial t} \int_{V} \rho \phi dV$$

• In Second order discretisation we assume that ϕ changes linearly in

space:

$$\phi(\mathbf{x}) = \phi_p + (\mathbf{x} - \mathbf{x}_p) \cdot \nabla \phi$$

• The volume integration of ϕ

$$\int_{V} \phi(\mathbf{x}) dV = \int_{V} \phi_{p} dV + \int_{V} (\mathbf{x} - \mathbf{x}_{p}) \cdot \nabla \phi_{p} dV$$

• Note: $\int_V (\mathbf{x} - \mathbf{x}_p) \cdot \nabla \phi_p dV = 0$ as $\mathbf{x}p$ in the center of the cell and $\nabla \phi_p$ is constant

$$\int_{V} \phi(\mathbf{x}) dV = \phi_p V$$

$$\int_{V} \frac{\partial \rho \phi}{\partial t} dV = \frac{\partial}{\partial t} \int_{V} \rho \phi dV \to \frac{\partial}{\partial t} (\rho_{p \phi p}) V$$

Finite Volume Method: Convection Term

$$\int_{V} \nabla \cdot \rho \mathbf{u} \phi \, dV = \int_{S} \rho \mathbf{u} \phi \, dS = \sum_{i} S(\rho \mathbf{u} \phi)_{f} = \sum_{i} F \phi_{f}$$

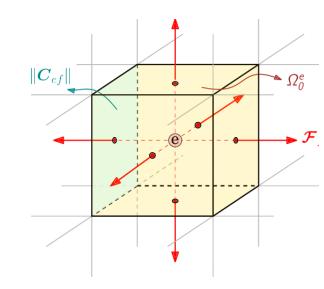
- Where *F* is the flux, and *i* is the iterator over the cell,
- and **S** is surface area of the face
- Central Differencing (CD)

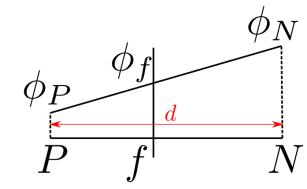
$$\phi_f = \alpha \phi_P + (1 - \alpha)\phi_N$$
$$\alpha = \frac{\overline{fN}}{d}$$

- Second order, unbounded, causes unphysical oscillations
- Upwind differencing (UD)

$$\phi_f = \begin{cases} \phi_P & , F \ge 0. \\ \phi_N & , F < 0. \end{cases}$$

First order, bounded faces



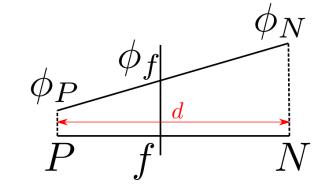


Finite Volume Method: Diffusion Term

$$\int_{V} \nabla \cdot (D\nabla\phi) dV = \int_{S} D\nabla\phi dS = \sum_{i} S \cdot (D\nabla\phi)_{f}$$

$$(\nabla\phi)_{f} = \begin{cases}
\frac{\phi_{N} - \phi_{p}}{d}, & \text{For orthogonal grid.} \\
\alpha(\nabla\phi)_{P} + (1 - \alpha)(\nabla\phi)_{N}, & \text{For non-orthogonal grid.}
\end{cases}$$

$$(\nabla \phi)_f = \begin{cases} \frac{\phi_N - \phi_p}{d}, & \text{For orthogonal grid.} \\ \alpha(\nabla \phi)_P + (1 - \alpha)(\nabla \phi)_N, & \text{For non-orthogonal grid.} \end{cases}$$



 Both are second-order accurate but differ in boundness and suitability for non-orthogonal meshes

$$S \cdot (\nabla \phi)_f = \underbrace{\Delta \cdot (\nabla \phi)_f}_{\text{orthogonal contribution}} + \underbrace{\kappa \cdot (\nabla \phi)_f}_{\text{non-orthogonal contribution}}$$

$$S = \Delta + \kappa$$

$$\Delta = \begin{cases} \frac{d \cdot S}{d \cdot d} d & \text{Minimum correction approach.} \\ \frac{d}{|d|} |S| & \text{Orthogonal correction approach.} \\ \frac{d}{d \cdot S} |S|^2 & \text{Over-relaxed approach.} \end{cases}$$

Finite Volume Method: Usage in OF

• The gradient and divergance schemes are defined in \$case/system/fvSchemes

• There are different limiter, gradient and interpolations schemes.

https://www.openfoam.com/documentation/guides/v2112/doc/guide-schemes-gradient.html https://www.openfoam.com/documentation/guides/v2112/doc/guide-schemes-divergence-example.html



Numerics of OpenFOAM Time discretisation



Time Integration for Transient Flows

$$\int_{t}^{t+\Delta t} \left(\frac{\partial \rho \phi}{\partial t}\right)_{P} V_{P} dt = \int_{t}^{t+\Delta t} \left[-\sum_{f} F \phi_{f} + \sum_{f} DS \cdot (\nabla \phi)_{f} + S_{\phi} V_{P} \right] dt$$

- Backward time scheme
- Euler implicit time scheme
- Crank-Nicolson time scheme

• https://www.openfoam.com/documentation/guides/v2112/doc/guide-schemes-time.html

Time Integration: Explicit

$$\int_{t}^{t+\Delta t} \left(\frac{\partial \rho \phi}{\partial t}\right)_{P} V_{P} dt = \int_{t}^{t+\Delta t} \left[-\sum_{f} F \phi_{f} + \sum_{f} DS \cdot (\nabla \phi)_{f} + S_{\phi} V_{P} \right] dt$$
$$\left(\frac{\partial \rho \phi}{\partial t}\right)_{P} = \left(\frac{\rho^{n} \phi^{n} - \rho^{o} \phi^{o}}{dt}\right)_{P}$$

- The super script 'n' and 'o', refers to values at new time 't+dt' and the previous time 't'.
- For clarity drop the density, i.e. consider incompressible flow

$$\left(\frac{\partial \phi}{\partial t}\right)_P = \left(\frac{\phi^n - \phi^o}{dt}\right)_P$$

All the values are taken from the old time step

$$\phi_P^n = \phi_P^o + \frac{\Delta t}{V_P} \left[-\sum_f F^o \phi_f^o + \sum_f D^o S \cdot (\nabla \phi)_f^o + S_\phi^o V_P \right]$$

• First order, limited by the Courant number

$$Co = \frac{\mathbf{u}_f \cdot d}{\Delta t}$$

Time Integration: Euler Implicit

$$\int_{t}^{t+\Delta t} \left(\frac{\partial \rho \phi}{\partial t}\right)_{P} V_{P} dt = \int_{t}^{t+\Delta t} \left[-\sum_{f} F \phi_{f} + \sum_{f} DS \cdot (\nabla \phi)_{f} + S_{\phi} V_{P} \right] dt$$
$$\left(\frac{\partial \phi}{\partial t}\right)_{P} = \left(\frac{\phi^{n} - \phi^{o}}{dt}\right)_{P}$$

All the values are expressed in terms of the new time step

$$\phi_f = \alpha \phi_P^n + (1 - \alpha) \phi_N^n$$
$$S \cdot (\nabla \phi)_f = \Delta \cdot \frac{\phi_N^n - \phi_P^n}{d} + \kappa \cdot (\nabla \phi)_f^n$$

The resulted equation in matrix form is

$$a_P \phi_P^n + \sum_N a_N \phi_N^n = R_P$$

First order, Stable even for Co>1, Bounded

Time Integration: Backward Differencing

$$\int_{t}^{t+\Delta t} \left(\frac{\partial \rho \phi}{\partial t}\right)_{P} V_{P} dt = \int_{t}^{t+\Delta t} \left[-\sum_{f} F \phi_{f} + \sum_{f} DS \cdot (\nabla \phi)_{f} + S_{\phi} V_{P} \right] dt$$

All the values on the RHS are expressed in terms of the new time step

$$\left(\frac{\partial \phi}{\partial t}\right)_{P} = \left(\frac{\phi^{n} - \phi^{o}}{dt}\right)_{P} \qquad \frac{\partial \phi}{\partial t} = \frac{1.5\phi^{n} - 2\phi^{o} + 0.5\phi^{oo}}{\Delta t}$$

- Need to solve a system of algebraic equations
- Properties: Implicit, Second order, Boundedness not guaranteed, Conditionally stable

Time Integration: Crank-Nicholson

$$\int_{t}^{t+\Delta t} \left(\frac{\partial \rho \phi}{\partial t}\right)_{P} V_{P} dt = \int_{t}^{t+\Delta t} \left[-\sum_{f} F \phi_{f} + \sum_{f} DS \cdot (\nabla \phi)_{f} + S_{\phi} V_{P} \right] dt$$
$$\left(\frac{\partial \phi}{\partial t}\right)_{P} = \left(\frac{\phi^{n} - \phi^{o}}{dt}\right)_{P}$$

All the values are expressed in terms of the new and the old time steps

$$\int_{t}^{t+\Delta t} \phi dt = 0.5(\phi^{n} + \phi^{o})\Delta t$$

$$\frac{\phi_P^n - \phi_P^o}{\Delta t} V_P = \frac{1}{2} \left[-\sum_f F^n \phi_f^n + \sum_f D^n S \cdot (\nabla \phi)_f^n + S_\phi^n V_P \right]$$
$$+ \frac{1}{2} \left[-\sum_f F^o \phi_f^o + \sum_f D^o S \cdot (\nabla \phi)_f^o + S_\phi^o V_P \right]$$

- Need to solve a system of algebraic equations
- Properties: Second order, Bounded

Time Integration: Usage

• The Time integration schemes are defined in \$case/system/fvSchemes

- Schemes list names
 - Euler: transient, first order implicit, bounded.
 - backward: transient, second order implicit, potentially unbounded.
 - CrankNicolson: transient, second order implicit, bounded.

$$\Psi = \begin{cases} 1 & \text{Corresponds to pure Crank-Nicolson} \\ 0 & \text{Corresponds to pure pure Euler} \end{cases}$$

 https://www.openfoam.com/documentation/guides/v2112/doc/guide-schemes-timeexample.html



Numerics of OpenFOAM Pressure Velocity Coupling



Pressure-Velocity Coupling

$$a_P U_P + \sum_N a_N U_N = R_P$$
 , or $MU = R$

With 'N' being the eight

$$R = -\nabla p + S(U)$$

$$a_P U_P = -\nabla p + S(U_P) - \sum_N a_N U_N$$

$$a_P U_P = -\nabla p + H_N \quad , \text{ or } \quad AU = H - \nabla p$$

• *A* is a diagonal matrix

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

• Substitute in the continuity equation $\nabla \cdot \mathbf{u} = 0$

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

Pressure velocity Coupling

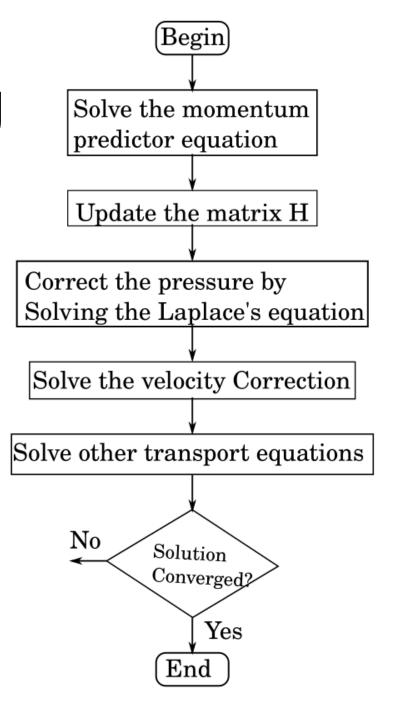
Summary of the equation to be solved:

$$MU = -\nabla p - S(U)$$
 Momentum predictor

$$H = AU - MU$$

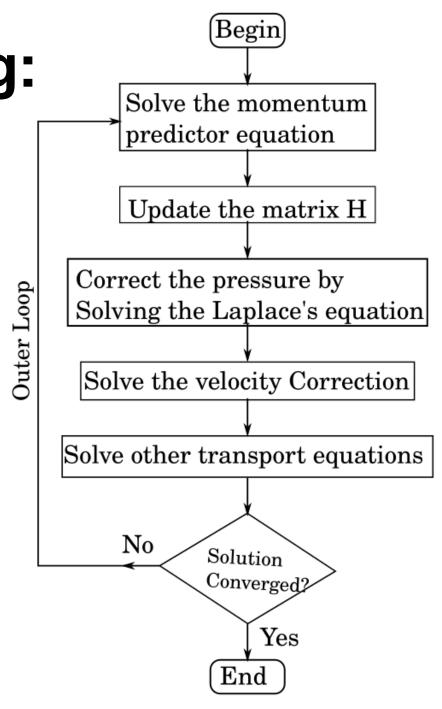
$$\nabla \cdot A^{-1} \nabla p = \nabla \cdot (A^{-1}H)$$
 Laplace's equation of the pressure

$$U = A^{-1}H - A^{-1}\nabla p$$
 Velocity Corrector



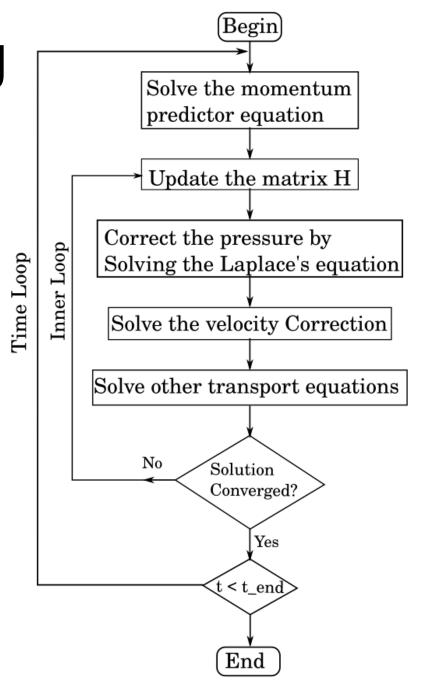
Pressure velocity Coupling: SIMPLE

- Semi-Implicit-Method-Of-Pressure-Linked-Equations.
- Used for Steady State simulations, but needs under-relaxation.
- Stable for large Co.
- https://www.openfoam.com/documentatio n/guides/v2112/doc/guide-applicationssolvers-simple.html



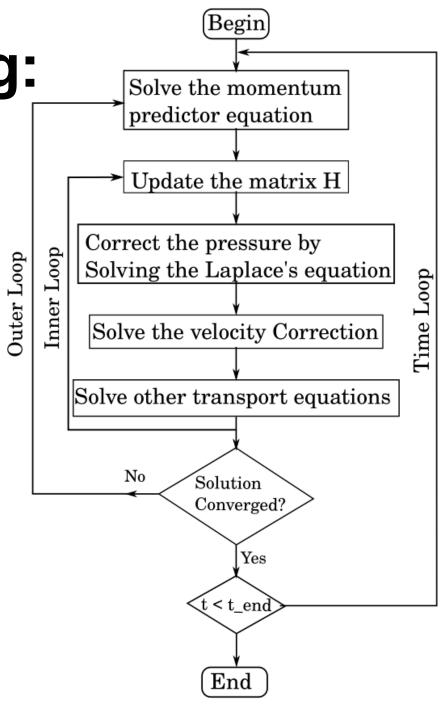
Pressure velocity Coupling PISO

- Pressure Implicit with Splitting of Operators
- Unsteady simulation
- The momentum equation is solved once each time step
- The correction is repeated via the inner loop till convergence in each time step
- Issa, Raad I. "Solution of the implicitly discretised fluid flow equations by operator-splitting." Journal of computational physics 62.1 (1986): 40-65.



Pressure velocity Coupling: PIMPLE

- Compines SIMPLE and PISO alogrithms
- Unsteady simulation
- The momentum equation can be solved multiple times time step (outer loop)
- The correction is repeated via the inner loop
- Allowes large Co



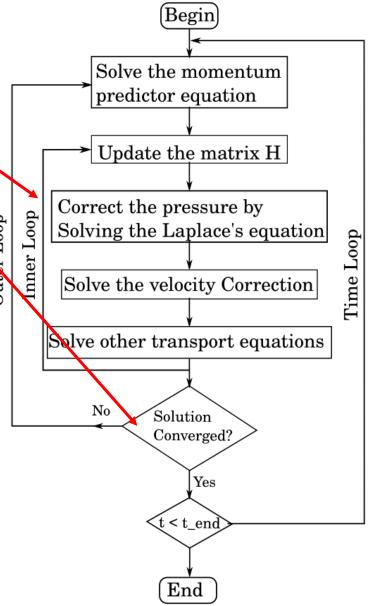
Pressure velocity Coupling:

Usage

- Defined in \$case/system/fvSolution
- https://openfoamwiki.net/index.php/OpenFOAM g uide/The PIMPLE algorithm in OpenFOAM
- Monitor the residuals
 - foamLog <logFile>
 - In \$case/system/controlDict, add residuals function

```
functions
    residuals
                                solverInfo;
            type
                                (utilityFunctionObjects);
           writeResidualFields true;
                                writeTime;
           writeControl
                                (" *"); // (U, P)
            fields
                  Get the
                                          Get the
                 residuals for
                                          residuals for
                 all the
                                          specific fields
                 available
```

```
nCorrectors.
   nOuterCorrectors
                        50:
   residualControl
                tolerance 1e-5;
                relTol
                            0;
                tolerance 5e-4:
                relTol
relaxationFactors
   fields
               0.3:
       pFinal
   equations
        "U|k|epsilon"
        "(U|k|epsilon)Final"
```





Numerics of OpenFOAM Volume of Fluid

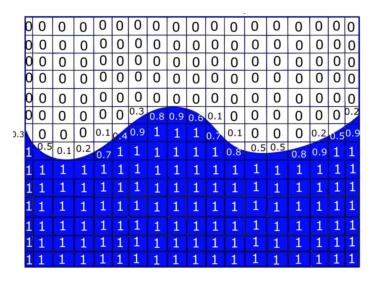




Volume of Fluid (VOF)

- Interface capturing methods use a fixed grid
- Uses a labelling function for each cell having value [0 1]

$$\alpha = \frac{V_1}{V} = \begin{cases} 1 & \text{Fluid 1} \\ 0 < \alpha < 1 & \text{Interface Cells} \\ 0 & \text{Fluid 2} \end{cases}$$



Assume that the local properties changes linearly with the volume fraction

$$\rho = \alpha \rho_1 + (1 - \alpha)\rho_2$$

$$\mu = \alpha \mu_1 + (1 - \alpha)\mu_2$$

- The governing equations can be used with no change
 - Note: Source term to account for the surface tension can be added

Volume of Fluid (VOF)

- There are two categories[1]:
 - Algebraic Method schemes are typically much simpler to implement, more efficient and are not restricted to structured meshes but not as accurate.
 - **Geometric methods** involving an explicit reconstruction of the interface from the volume fraction data. They usually involve complex geometric operation making their implementation cumbersome.
- OpenFOAM ESI (V1706 and later) has these two methods built-in
 - Algebraic Method using MULES scheme
 - Geometric Method using isoAdvector
- Note: isoAdvector is available as Third party solver for other versions of OpenFOAM
 - https://github.com/isoAdvector

Volume of Fluid (VOF): Algebraic Method

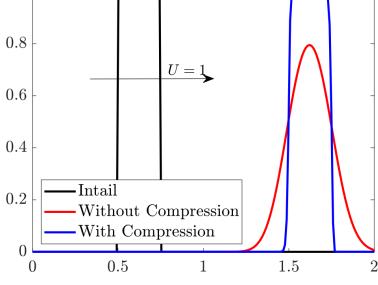
• To track the interface, a transport equation of the volume fraction is needed

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = 0$$

- The diffusion is high leading to surface smearing
- To reduce surface smearing, a compression term is added:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\mathbf{u}\phi) + \nabla \cdot (U_C \quad \alpha(1-\alpha)) = 0$$

$$U_C = C_{\alpha} |\mathbf{u}| \frac{\nabla \alpha}{|\nabla \alpha|}$$



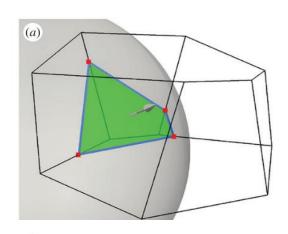
- Where C_{α} is user specific, 0 for no compression or 1 for strong compression
- Note: The actuale implementation in OF uses two schemes
 - Upwind differencing away from the interface (reduce the computational effor)
 - High order scheme at the interface

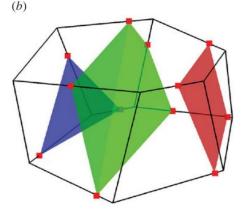
Volume of Fluid (VOF): isoAdvector Method

Geometric method

- Reconstruct the surface of the interface using the isosurface concept of the volume fraction
- Model the motion of the constructed surface

- Olsson, E.: A description of isoAdvector a numerical method for improved surface sharpness in two-phase flows. In Proceedings of CFD with OpenSource Software, 2017,
- Roenby J, Bredmose H, Jasak H. A computational method for sharp interface advection. Royal Society open science. 2016 Nov 23;3(11):160405.





Important resources

- OpenFOAM Guides
 - https://www.openfoam.com/documentation/overview
 - User Guide: Gain understanding of how OpenFOAM cases are assembled and evaluated in the OpenFOAM user guide:
 - Tutorial Guide: A collection of tutorials to help users get started with OpenFOAM covering a range of topics, including incompressible, compressible and multiphase flows, and stress analysis
 - Extended Code Guide: see how OpenFOAM operates under-the-hood. As an open source code, users can directly see how the code is written and learn how the functionality is implemented.
- Finite volume and time discretisation
 - https://spiral.imperial.ac.uk/bitstream/10044/1/8335/1/Hrvoje_Jasak-1996-PhD-Thesis.pdf
- Numerics of OpenFOAM
 - https://www.researchgate.net/publication/307546712
- VOF
 - http://dx.doi.org/10.17196/OS_CFD#YEAR_2017



Scientific Computing





Thank you







