Scientific Computing

Part 4: Complex Dynamic Systems
Introduction to Computational Fluid Dynamics

29th November 2022

Contents

SCC Part 4

What is Computational Fluid Dynamics

What is CFD?

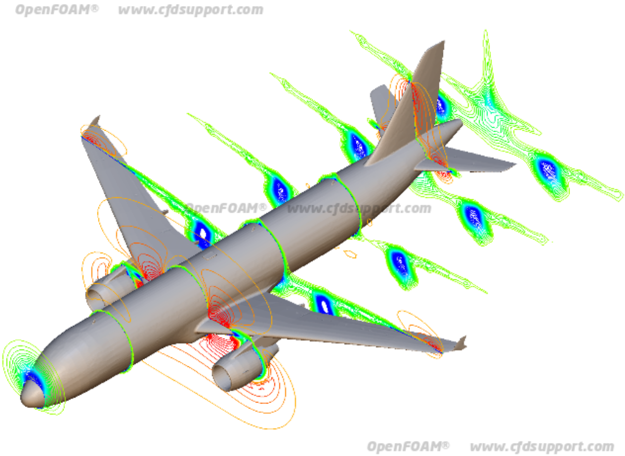
- Computational fluid dynamics (CFD for short) is the analysis of systems involving fluid flow, heat transfer and associated phenomena such as chemical reactions by means of computer-based simulation.
- The technique is very powerful and spans a wide range of industrial and non-industrial application areas.

What is CFD?

Some examples are:

- aerodynamics of aircraft and vehicles: lift and drag
- hydrodynamics of ships
- power plant: combustion in internal combustion engines and gas turbines
- turbomachinery: flows inside rotating passages, diffusers etc.
- electrical and electronic engineering: cooling of equipment including microcircuits
- chemical process engineering: mixing and separation, polymer moulding
- external and internal environment of buildings: wind loading and heating/ventilation
- marine engineering: loads on off-shore structures
- environmental engineering: distribution of pollutants and effluents
- hydrology and oceanography: flows in rivers, estuaries, oceans
- meteorology: weather prediction
- biomedical engineering: blood flows through arteries and veins

What is CFD?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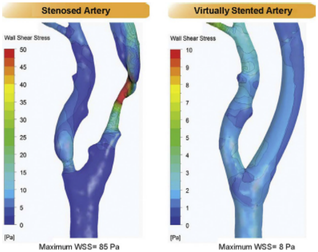
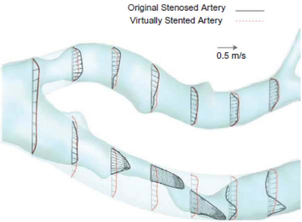
What is CFD?



Example of CFD prediction of wall shear stress (WSS) for originally stenosed and virtually stented arteries.



Example of predicted velocity profiles for originally stenosed and virtually stented arteries

Governing Equations of Fluid Flow and Heat Transfer

Governing Equations

- The aim of CFD simulations is to determine the velocity field $\boldsymbol{u} = \boldsymbol{u}(x, y, z, t)$, the pressure distribution $p = p(x, y, z, t)$, the density distribution $\rho = \rho(x, y, z, t)$ and temperature distribution $T = T(x, y, z, t)$ of a fluid flow at any given point (x, y, z) and at any given time t in three-dimensional space.
- Note that $\boldsymbol{u}$ is a vector field, while p, ρ, T are scalar fields. For historic reasons, the velocity vector $\boldsymbol{u}$ in CFD applications has the component u in $x-$direction, v in $y-$direction and w in $z-$direction, i.e.

$$\boldsymbol{u} = \begin{pmatrix} u \\ v \\ w \end{pmatrix}.$$

Governing Equations

- These properties can be calculated using a set of PDEs, which are introduced in this section.
- The full derivation of the corresponding PDEs is complex and cannot be covered in this script.
- We will merely introduce the concepts behind, state the PDEs and solve some applications. For a more detailed description see [6] and [7].

The Conservation Laws of Physics

The conservation laws of physics

The governing equations of fluid flow represent mathematical statements of the conservation laws of physics:

- **1. The mass of a fluid is conserved.**
  - This leads to the mass conservation or continuity equation (see Def. 2.1):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$

The conservation laws of physics

- **2. The rate of change of momentum equals the sum of the forces on a fluid particle** (Newton's second law).
  - Newton's second law states that the rate of change of momentum of a fluid particle equals the sum of the forces on the particle:

$$\dot{\boldsymbol{p}} = m\dot{\boldsymbol{v}} = \sum_{i=1}^{n} \boldsymbol{F}_i$$

  - We distinguis two types of forces on fluid particles (after [6]):
    - surface forces: pressure forces / viscous forces (i.e. internal friction) /gravity force
    - body forces: centrifugal force / Coriolis force / electromagnetic force
  - Adding up these forces and equating the sum with the rate of change of momentum leads to the Navier-Stokes equations , named after the two nineteenth-century scientists who derived them independently.

The conservation laws of physics

- **3. The rate of change of energy is equal to the sum of the rate of heat addition to and the rate of work done on a fluid particle** (first law of thermodynamics).

The conservation laws of physics

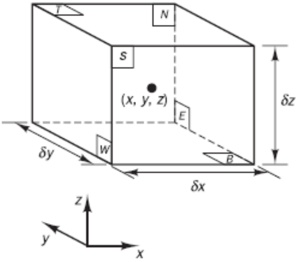
- To derive the governing PDEs for each conservation law, Consider a small element of fluid with sides δx, δy and δz as shown on the next slide.
- The volume V of this fluid element is

$$V = \delta x \delta y \delta z,$$

the mass m is (according to "mass = density x volume")

$$m = \rho V = \rho \delta x \delta y \delta z.$$

The conservation laws of physics



The conservation laws of physics

- The six faces of the fluid element are labelled N, S, E, W, T and B, which stands for North, South, East, West, Top and Bottom.
- The positive directions along the coordinate axes are also given.
- The centre of the element is located at position (x, y, z).
- The element under consideration is so small that fluid properties at the faces can be expressed accurately enough by means of the first two terms of a Taylor series expansion.
- So, for example, the pressure at the W and E faces, which are both at a distance of $\frac{1}{2}\delta x$ from the element centre, can be expressed as

$$p - \frac{\partial p}{\partial x} \cdot \frac{1}{2}\delta x \text{ and } p + \frac{\partial p}{\partial x} \cdot \frac{1}{2}\delta x$$

The conservation laws of physics

- A systematic account of changes in the mass, momentum and energy of the fluid element due to fluid flow across its boundaries and, where appropriate, due to the action of sources inside the element, leads to the fluid flow equations.

An Example: The Conservation of Mass

The conservation of mass

The first step in the derivation of the mass conservation equation is to write down a mass balance for the fluid element:

Rate of increase of mass in fluid element
=
Net rate of flow of mass into fluid element

Rate of increase of mass

The rate of increase of mass in the fluid element on the right hand side of this balance is

$$\frac{\partial m}{\partial t} = \frac{\partial}{\partial t}(\rho \cdot V) = \frac{\partial \rho}{\partial t} \cdot V = \frac{\partial \rho}{\partial t} \cdot \delta x \delta y \delta z \tag{1}$$

since the volume V of the fluid element is constant.

Net rate of flow of mass

- The mass flow rate across a face of the fluid element is defined by the product of density ρ, area A and the velocity component normal to the face.
- Hence the mass flow rate $\partial m_u / \partial t$ in $x-$direction with velocity u across the Area $A = \delta y \delta z$ at the center (x, y, z) would be

$$\frac{\partial m_u}{\partial t} = \rho \cdot u \cdot A = \rho \cdot u \cdot \delta y \delta z.$$

Net rate of flow of mass

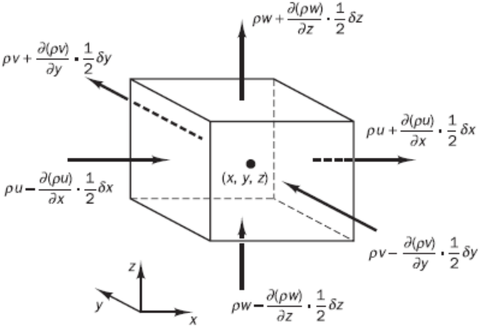
- Accordingly, the flow rate across the W and E faces of the fluid element is (see Fig. on the next slide)

$$\left(\rho u - \frac{\partial(\rho u)}{\partial x} \cdot \frac{1}{2}\delta x\right)\delta y \delta z \text{ and } \left(\rho u + \frac{\partial(\rho u)}{\partial x} \cdot \frac{1}{2}\delta x\right)\delta y \delta z$$

and the net rate of flow across both faces is

$$\begin{aligned} &\text{flow rate across E face - flow rate across W face} \\ &= \left(\rho u - \frac{\partial(\rho u)}{\partial x} \cdot \frac{1}{2}\delta x\right)\delta y \delta z - \left(\rho u + \frac{\partial(\rho u)}{\partial x} \cdot \frac{1}{2}\delta x\right)\delta y \delta z. \\ &= -\frac{\partial(\rho u)}{\partial x} \cdot \delta x \delta y \delta z \end{aligned}$$

Net rate of flow of mass



Net rate of flow of mass

- Repeating this step for each pair of faces and addidng each term, the net rate of flow of mass into the fluid element yields the net flow rate of mass into the fluid element:

$$-\frac{\partial(\rho u)}{\partial x}\cdot\delta x\delta y\delta z-\frac{\partial(\rho v)}{\partial y}\cdot\delta x\delta y\delta z-\frac{\partial(\rho w)}{\partial z}\cdot\delta x\delta y\delta z \quad (2)$$

Conservation of mass

- Equating Eqn. 1 and 2 yields

$$
\begin{aligned}
\frac{\partial \rho}{\partial t}\cdot \delta x \delta y \delta z &= -\frac{\partial(\rho u)}{\partial x}\cdot \delta x \delta y \delta z - \frac{\partial(\rho v)}{\partial y}\cdot \delta x \delta y \delta z - \frac{\partial(\rho w)}{\partial z}\cdot \delta x \delta y \delta z \\
\frac{\partial \rho}{\partial t} &= -\frac{\partial(\rho u)}{\partial x} - \frac{\partial(\rho v)}{\partial y} - \frac{\partial(\rho w)}{\partial z} \\
\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} &= 0 \qquad (3)
\end{aligned}
$$

Conservation of mass

- Using the Nabla-operator $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)^T$ we can write

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = \nabla \cdot (\rho \boldsymbol{u})$$

  as the dot product of the Nabla-operator and the vector $\rho \boldsymbol{u}$. This is also referred to as the "divergence" of the vector $\rho \boldsymbol{u}$.

- Equation 3 can thus be writen in vector notation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0.$$

Conservation of mass

Definition 2.1: Mass Conservation for a compressible fluid

- The equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$

or in longhand notation

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = 0$$

is the unsteady, three-dimensional **mass conservation** or **continuity equation** at a point in a **compressible fluid**.

Conservation of mass

Remarks:

1. The first term on the left hand side is the rate of change in time of the density (mass per unit volume). The second term describes the net flow of mass out of the element across its boundaries and is called the **convective** term.
2. For compressible fluids (i.e. a gas), the density

$$\rho = \rho(x, y, z, t)$$

is not constant.

Conservation of mass

- For incompressible fluids (i.e. a liquid), the density is constant and we have

$$\begin{aligned}\rho &= \text{const.}\\ \frac{\partial \rho}{\partial t} &= 0\\ \nabla\cdot(\rho \boldsymbol{u}) &= \rho\nabla\cdot(\boldsymbol{u})\end{aligned}$$

The mass conservation equation the simply becomes

$$\begin{aligned}\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho \boldsymbol{u}) &= 0\\ \Rightarrow 0+\rho\nabla\cdot\boldsymbol{u} &= 0\\ \Rightarrow \nabla\cdot\boldsymbol{u} &= 0\end{aligned}$$

Conservation of mass

Definition 2.2: Mass Conservation for an incompressible fluid

- For incompressible fluids (i.e. a liquid), the density ρ is constant, and the mass conservation equation becomes

$$\nabla \cdot \boldsymbol{u} = 0$$

or in longhand notation

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

The General Structure of the Governing Equations

General Structure of Governing Equations

- Despite their complexity, the PDEs used to describe the relevant conservation laws of physics for mass, momentum and energy all have the same structure.
- For generality, we shall pick a dummy physical quantity and call it ϕ (phi). It can be the temperature, the velocity, the concentration, the density, the electric field etc.

General Structure of Governing Equations

- There are three mechanisms that the terms in a PDE usually describe for this dummy quantity ϕ: accumulation, convection and diffusion. Let us have a quick look at each of these processes:

1. **Accumulation**
   - The accumulation or transient process accounts for the temporal rate of change of the a given quantity within an infinitesimal volume. This will have the form

$$\frac{\partial(\rho\phi)}{\partial t}$$

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- The accumulation or transient process accounts for the temporal rate of change of the a given quantity within an infinitesimal volume.
- This will have the form

$$\frac{\partial(\rho\phi)}{\partial t}$$

2. Convection

- The convection process accounts for the transport of the quantity due to any existing velocity field.
- This term is almost always described by a first derivative multiplied by a velocity.
- Convection occurs at the macro level and it is the source of nonlinearity in the NS equations.
- This will have the form

$$\nabla \cdot (\rho \boldsymbol{u} \phi)$$

3. Diffusion

- Finally, the diffusion process describes the tranport of the quantity due to the presence of any gradients of that quantity (e.g. the concentration of a chemical substance such as salt in water).
- This happens at the molecular level. By itself, diffusion is a linear process provided the diffusion coefficient is a constant.
- This will have the form

$$\nabla \cdot (\Gamma \nabla \phi)$$

where Γ is called the diffusion coefficient. This is equivalent to the thermal conductivity in heat transfer, which is a diffusion process.

Remarks:

- Notice that several simplifications may be made to the forms given above when certain properties hold. For example, when compressibility effects are negligible, one may extract the density outside the differential operators.
- In certain cases, there are terms that cannot be cast into the transient, convective, and diffusive terms. These are then lumped into what is a called a **source term**. For example, the gravitational effects, the pressure gradient, and any other body forces are part of the source term in the Navier-Stokes equations.
- The universality of the three mechanisms discussed above makes it possible for us to construct a general differential equation that describes the conservation principle of a physical quantity ϕ (remember that ϕ can be temperature, velocity, density, etc.).

General Structure of Governing Equations

- The generic scalar transport equation then has the form

$$\underbrace{\frac{\partial \rho\phi}{\partial t}}_{\text{Accumulation}} + \underbrace{\nabla\cdot(\rho\boldsymbol{u}\phi)}_{\text{Convection}} = \underbrace{\nabla\cdot(\Gamma\nabla\phi)}_{\text{Diffusion}} + \underbrace{S_\phi}_{\text{Source}} \qquad (4)$$

which can be specialized to any process in the realm of heat, mass, and momentum transfer.In words:

Rate of increase of ϕ of fluid element	+ Net rate of flow of ϕ out of fluid element	= Rate of increase of ϕ due to diffusion	+ Rate of increase of ϕ due to sources

The Full Set of Governing Equations for CFD

Full Set of Governing Equations

- Let us now derive the full set of governing equations (i.e. PDEs) for CFD using the generic scalar transport equation 4 for mass conservation, momentum conservatoin and energy conservation.

Full Set of Governing Equations

Mass conservation

- To obtain the mass conservatoin or continuity equation (for compressible flows) set $\phi = 1$. Since diffusion is not present and in the absence of sources set those to zero to obtain

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$

which is the same result as seen before.

Full Set of Governing Equations

Momentum conservation

- When we apply the generic scalar transport equation to each component u, v, w of the velocity vector $\boldsymbol{u} = (u, v, w)$, we get the Navier-Stokes equations for a so-called Newtoninan fluid[1]
- Thus, we replace ϕ by one velocity component at a time

[1] In a Newtonian fluid the viscous stresses are proportional to the rates of deformation.

Full Set of Governing Equations

Momentum conservation

- Thus, we replace ϕ by one velocity component at a time

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} u) = \nabla \cdot (\mu \nabla u) - \frac{\partial p}{\partial x} + S_{Mx} \quad (5)$$

$$\frac{\partial \rho v}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} v) = \nabla \cdot (\mu \nabla v) - \frac{\partial p}{\partial y} + S_{My} \quad (6)$$

$$\frac{\partial \rho w}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} w) = \nabla \cdot (\mu \nabla w) - \frac{\partial p}{\partial z} + S_{My} \quad (7)$$

Full Set of Governing Equations

Momentum conservation

- Here μ is the (dynamic) viscosity. The source terms S_{Mx}, S_{My}, S_{Mz} describe the effects of body forces such as the centrifugal force, Coriolis force and electromagnetic force and also viscuous forces of second order.
- Viscosity is a measure of a fluid's resistance to flow. It describes the internal friction of a moving fluid. For instance, honey has a much higher viscosity than water.

Full Set of Governing Equations

Energy conservation

- To obtain the energy equation for a fluid, simply set $\phi = i$ in Eq. 4:

$$\frac{\partial \rho i}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} i) = \nabla \cdot (k \nabla T) - p \nabla \cdot \boldsymbol{u} + S_{Dis} \qquad (8)$$

where i is the spedfic internal energy, k is the thermal conductivity. The effects due to the viscous stresses in the energy equation are described by the dissipation function S_{Dis}.

Full Set of Governing Equations

Equations of state

- The motion of a fluid in three dimensions is described by a system of five partial differential equations: mass conservation x-, y- and z-momentum equations and the energy equation.
- Among the unknowns are four thermodynamic variables: ρ, p, i and T. Relationships between the thermodynamic variables can be obtained through the assumption of thermodynamic equilibrium. The equations of state then relate these four thermodynamic variables:

$$\begin{aligned} p &= p(\rho, T) \\ i &= i(\rho, T) \end{aligned}$$

- For an ideal gas, the following, well-known equations of state are useful:

$$\begin{aligned} p &= \rho R T \\ i &= C_V T \end{aligned}$$

where R is the gas constant for an ideal gas and C_V is the heat

Full Set of Governing Equations

Remarks:

- In the flow of compressible fluids the equations of state provide the linkage between the energy equation on the one hand and mass conservation and momentum equations on the other.
- Liquids and gases flowing at low speeds behave as incompressible fluids. Without density variations there is no linkage between the energy equation and the mass conservation and momentum equations. The flow field can often be solved by considering mass conservation and momentum equations only. The energy equation only needs to be solved alongside the others if the problem involves heat transfer.

Full Set of Governing Equations

SCC Part 4

Overview:

Conservation of mass	$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$
Conservation of momentum	$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} u) = \nabla \cdot (\mu \nabla u) - \frac{\partial p}{\partial x} + S_{Mx}$ $\frac{\partial \rho v}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} v) = \nabla \cdot (\mu \nabla v) - \frac{\partial p}{\partial y} + S_{My}$ $\frac{\partial \rho v}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} v) = \nabla \cdot (\mu \nabla v) - \frac{\partial p}{\partial y} + S_{My}$

Full Set of Governing Equations

Overview:

Conservation of energy	$\frac{\partial \rho i}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} i) = \nabla \cdot (k \nabla T) - p \nabla \cdot \boldsymbol{u} + S_{Dis}$
Equations of state	$p = p(\rho, T) \text{and} i = i(\rho, T)$

Numerical Solutions of CFD Applications Using OpenFOAM

OpenFOAM

- The objective of all discretization techniques (Finite Difference, Finite Element, Finite Volume, Boundary Element...) is to devise a mathematical formulation to transform each of these terms into an algebraic equation.
- Once applied to all control volumes in a given mesh, we obtain a full linear system of equations that needs to be solved.
- There is a variety of commercial and open source applications that can be used to solve CFD applications.
- We are going to use the OpenFOAM library.

OpenFOAM

- The open source software OpenFOAM (see http://openfoam.org/) is a C++ library that allows for the numerical solution of the full set of PDEs of viscuous fluids as described in the previous chapter.
- The name OpenFOAM stands for Open Source Field Operation and Manipulation.
- It uses the method of finite volumes to solve the governing equations of CFD.
- The user guide for the current version 4.1 can be downloaded at http://foam.sourceforge.net/docs/Guides-a4/OpenFOAMUserGuide-A4.pdf or acessed online at http://cfd.direct/openfoam/user-guide/.

OpenFOAM

- OpenFOAM is used primarily to create executables, known as applications.
- The applications fall into two categories:
  - solvers, that are each designed to solve a specic problem in CFD;
  - and utilities, that are designed to perform tasks that involve data manipulation.

OpenFOAM

- The Open- FOAM distribution contains numerous solvers and utilities covering a wide range of problems.
- One of the strengths of OpenFOAM is that new solvers and utilities can be created by its users with some pre-requisite knowledge of the underlying method, physics and programming techniques involved.
- OpenFOAM is supplied with pre- and post-processing environments.
- The interface to the pre- and post- processing are themselves OpenFOAM utilities, thereby ensuring consistent data handling across all environments.

OpenFOAM

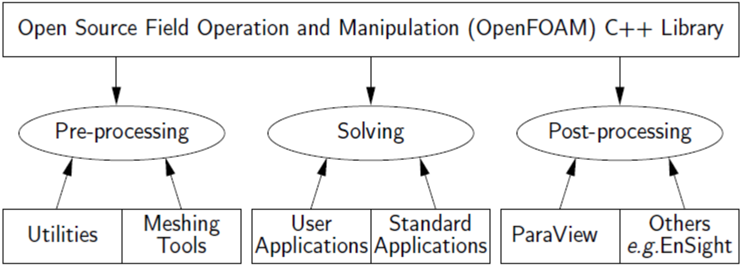
- OpenFOAM does not have a generic solver applicable to all cases.
- Instead, users must choose a specific solver for a class of problems to solve.
- The solvers with the OpenFOAM distribution are in the $FOAM_SOLVERS directory, reached quickly by typing app at the command line.
- An overview of the currently available solvers is available on the internet: http://www.openfoam.com/documentation/user-guide/standard-solvers.php.

OpenFOAM

- The utilities with the OpenFOAM distribution are in the $FOAM_UTILITIES directory, reached quickly by typing util at the command line.
- An overview is available at http://www.openfoam.com/documentation/user-guide/standard-utilities.php.

OpenFOAM

- The overall structure of OpenFOAM is shown in this figure:



OpenFOAM

- The objective of all discretization techniques (Finite Difference, Finite Element, Finite Volume, Boundary Element...) is to devise a mathematical formulation to transform each of these terms into an algebraic equation.
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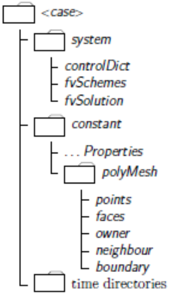
File Structure of OpenFOAM Cases

File Structure of OpenFOAM Cases

- The basic directory structure for a OpenFOAM case, that contains the minimum set of files required to run an application, is shown in the following Figure and described as follows (from [9]):



File Structure of OpenFOAM Cases

- **A *constant* directory** that contains a full description of the case mesh in a subdirectory *polyMesh* and files specifying physical properties for the application concerned, e.g. *transportProperties*.

File Structure of OpenFOAM Cases

- **A *system* directory** for setting parameters associated with the solution procedure itself. It contains at least the following 3 files:
  - *controlDict* where run control parameters are set including start/end time, time step and parameters for data output;
  - *fvSchemes* where discretisation schemes used in the solution may be selected at run-time; and,
  - *fvSolution* where the equation solvers, tolerances and other algorithm controls are set for the run.

File Structure of OpenFOAM Cases

- **The 'time' directories** containing individual files of data for particular fields, e.g. velocity and pressure. The data can be: either, initial values and boundary conditions that the user must specify to define the problem; or, results written to file by OpenFOAM. Note that the OpenFOAM fields must always be initialised, even when the solution does not strictly require it, as in steady-state problems. The name of each time directory is based on the simulated time at which the data is written. It is sufficient to say now that since we usually start our simulations at time t = 0, the initial conditions are usually stored in a directory named 0. For example, in the following tutorials, the velocity field U and pressure field p are initialised from files 0/U and 0/p respectively.

Tutorial 1: Plane-Parallel Plates With Laminar Flow

Tutorial 1

- Let us now start with a simple case, taken from [8]: OpenFOAM GUIDE FOR BEGINNERS, Jordi Casacuberta Puig, 2014.
- You can download the PDF-File Tutorial1_Chapter2_Plates_corrected.pdf and the case directory Tutorial1_ppWall from Moodle to your virtual machine.
- Alternatively, if you experiency network connection problems, the files are provided on a USB-stick.
- Please follow the description for Chapters 2.1 to 2.5 in the PDF step-by-step.

Sources

- [6] An Introduction to Computational Fluid Dynamics, H. K. Versteeg and W. Malalasekera, Springer, 2007
- [7] Computational Fluid Dynamics: A Practical Approach, J. Tu et al., Elsevier, 2013
- [8] OpenFOAM GUIDE FOR BEGINNERS, Jordi Casacuberta Puig, 2014
- [9] OpenFOAM User Guide, version 4.0, 24th June 2016, http://openfoam.org