Introduction to Computational Fluid Dynamics (CFD)

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What is computational fluid dynamics (CFD)?

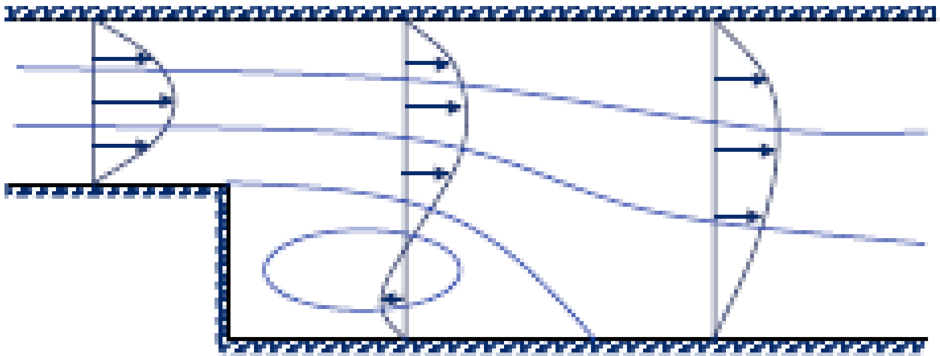
Course goals

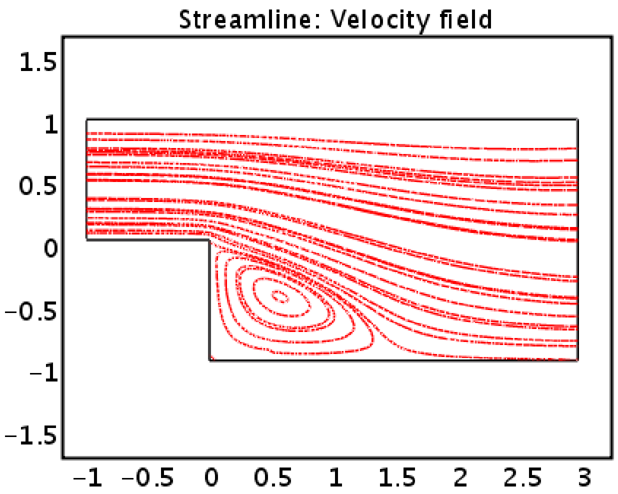
Course content

Homework and projects

What is computational fluid dynamics?

CFD –gives a prediction of fluid flows (and other transport phenomena) in different domains with different conditions

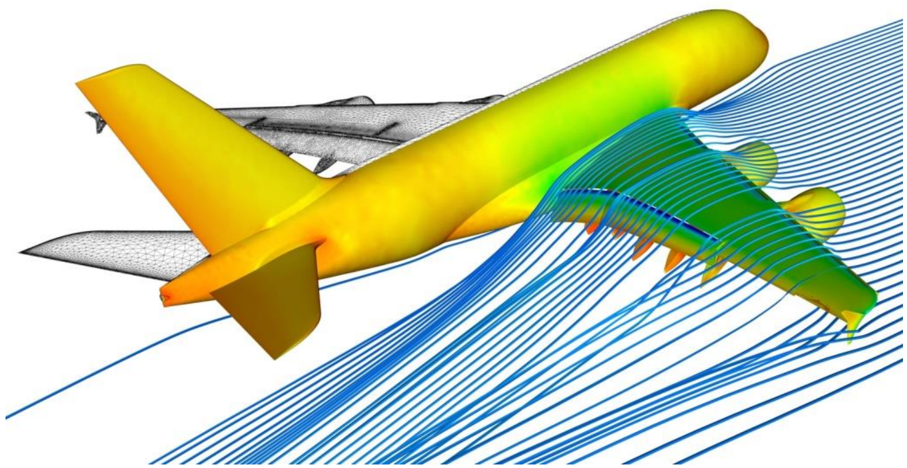


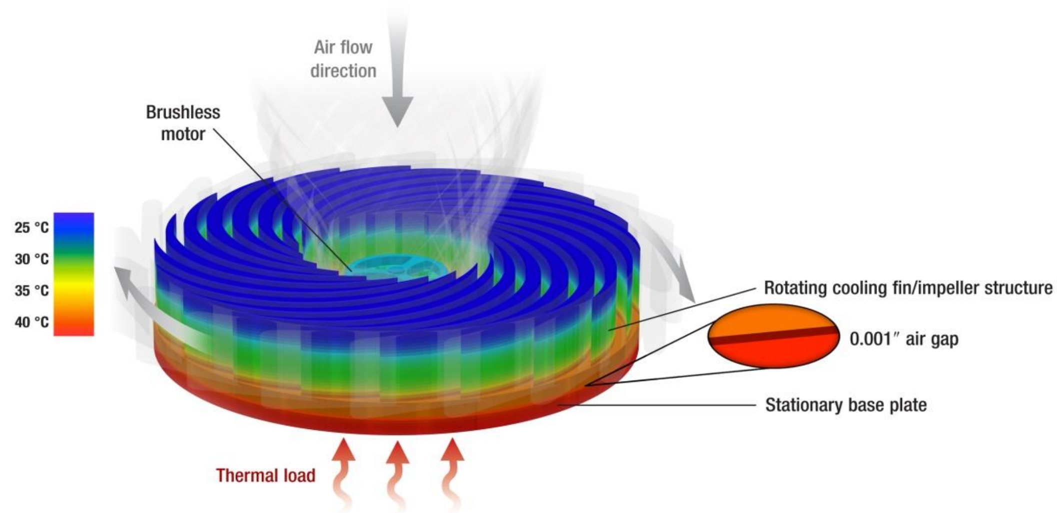


Flow over a backstep

Applications of CFD

- fluid flow
- heat transfer
- mass transfer
- reactive flow
- etc





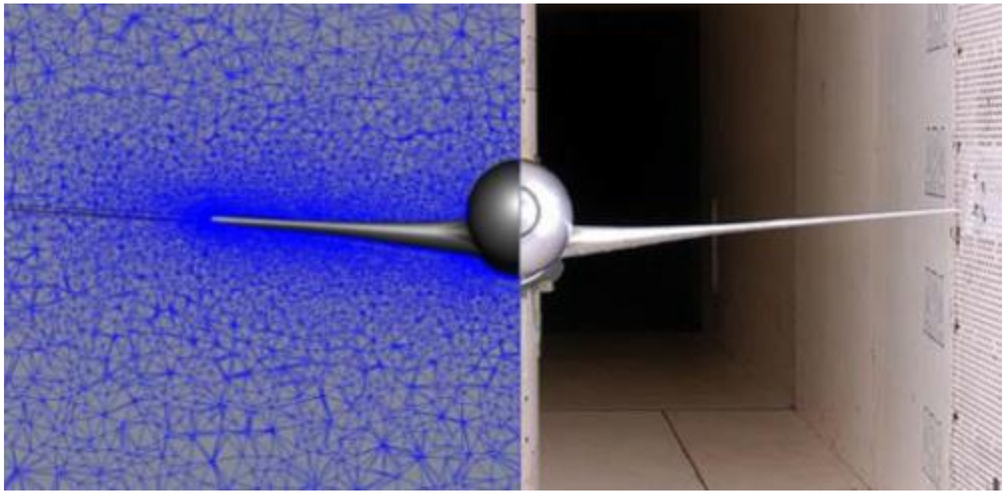
Advantages and limitations of CFD

Simulations

(quantitative prediction of flow phenomena using CFD software for all desired quantities)

- with high resolution in space and time
- for the actual flow domain
- for virtually any problem and realistic operating conditions

Error sources:
- modeling, discretization
- iteration
- implementation



Error sources:
- measurement errors,
- flow disturbances by the probes

Experiments

(give a quantitative description of flow phenomena using measurements)

- for one quantity at a time at a limited number of points and time instants
- for a laboratory-scale model
- for a limited range of problems and operating conditions

CFD **does** not replace the measurements completely but the amount of experimentation and the overall cost can be significantly reduced.

Simulations		Experiments	
	• cheap(er) • fast(er) • parallel • multiple-purpose •portable, easy to modify		• expensive • slow • sequential • single-purpose • dedicated equipment

The results of a CFD simulation are never 100% reliable because

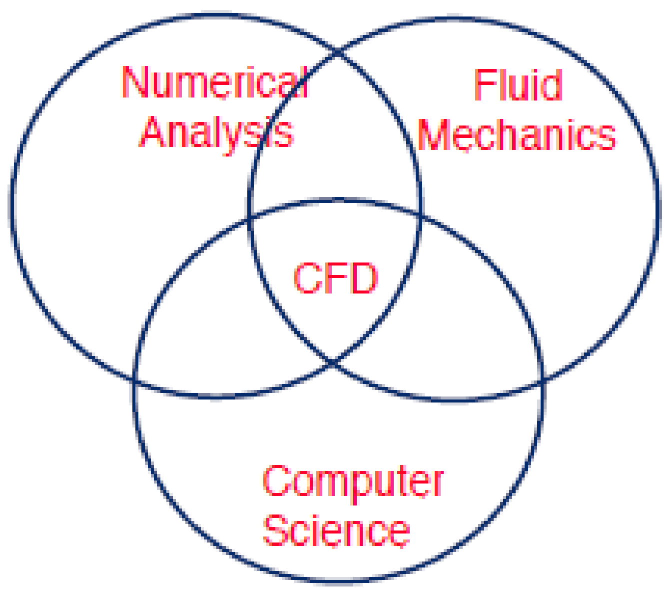
- the input data may be imprecise
- the mathematical model may be inadequate
- the accuracy of the results is limited by the available computing power

Introduction to Computational Fluid Dynamics

In order to predict the flow one need:

- mathematical modeling (partial differential equations of fluid mechanics)
- numerical methods (numerical analysis- discretization and solution techniques)
- computer science (software tools, solvers, pre- and postprocessing utilities)

CFD is an interdisciplinary topic



Steps:

Problem statement
(information about the flow)

Mathematical model
(IBVP = PDE + IC + BC)

Mesh generation
(nodes/cells, time instants)

Space/time discretization
(algebraic system Ax = b)

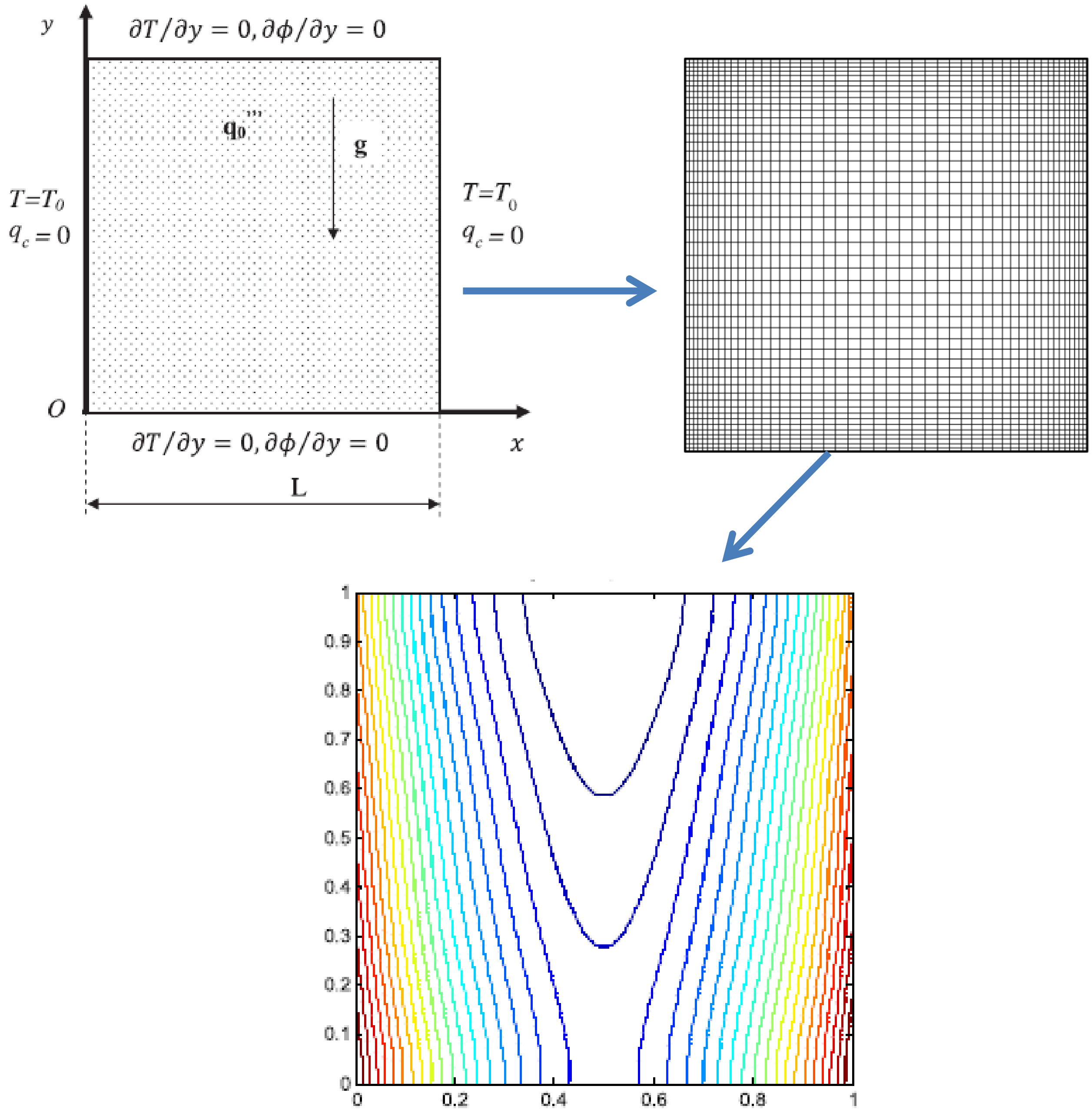
Iterative solver
(discrete function values)

CFD software
(implementation, debugging)

Simulation run
(parameters, stopping criteria)

Postprocessing
(visualization, data analysis)

Verification
(model validation / adjustment)



Problem statement

- What is known about the flow problem to be dealt with?
- What physical phenomena need to be taken into account?
- What is the geometry of the domain and operating conditions?
- What is the type of flow (laminar/turbulent, steady/unsteady)?
- What is the objective of the CFD analysis to be performed?
    - computation of integral quantities (lift, drag, yield)
    - snapshots of field data for velocities, concentrations etc.
    - shape optimization aimed at an improved performance
- What is the easiest/cheapest/fastest way to achieve the goal?

Mathematical model

- Choose a suitable flow model (viewpoint) and reference frame.
- Identify the forces which cause and influence the fluid motion.
- Define the computational domain in which to solve the problem.
- Formulate conservation laws for the mass, momentum, and energy.
- Simplify the governing equations to reduce the computational effort:
  - use available information about the prevailing flow regime
  - check for symmetries and predominant flow directions (1D/2D)
  - neglect the terms which have little or no influence on the results
  - model the effect of small-scale fluctuations that cannot be captured
  - incorporate a priori knowledge (measurement data, CFD results)
- Add constitutive relations and specify initial/boundary conditions.

Discretization process

The PDE system is transformed into a set of algebraic equations

- Mesh generation (decomposition into cells/elements)
  - structured or unstructured, triangular or quadrilateral?
  - CAD tools + grid generators (Delaunay, advancing front)
  - mesh size, adaptive refinement in ‘interesting’ flow regions
- Space discretization (approximation of spatial derivatives)
  - finite differences/volumes/elements
  - high- vs. low-order approximations
- Time discretization (approximation of temporal derivatives)
  - explicit vs. implicit schemes, stability constraints
  - local time-stepping, adaptive time step control

Iterative solution strategy

The coupled nonlinear algebraic equations must be solved iteratively

- Outer iterations: the coefficients of the discrete problem are updated using the solution values from the previous iteration so as to
  - get rid of the nonlinearities by a Newton-like method
  - solve the governing equations in a segregated fashion
- Inner iterations: the resulting system is typically solved by an iterative method (conjugate gradients, multigrid) because direct solvers (Gaussian elimination) are prohibitively expensive
- Convergence criteria: it is necessary to check the residuals, relative solution changes and other indicators to make sure that the iterations converge.

As a rule, the algebraic systems to be solved are very large (millions of unknowns) but sparse, i.e., most of the matrix coefficients are equal to zero.

CFD / Simulations

The computing times for a flow simulation depend on

- the choice of numerical algorithms and data structures
- linear algebra tools, stopping criteria for iterative solvers
- discretization parameters (mesh quality, mesh size, time step)
- cost per time step and convergence rates for outer iterations
- programming language (most CFD codes are written in Fortran)
- many other things (hardware, vectorization, parallelization etc.)

The quality of simulation results depends on

- the mathematical model and underlying assumptions
- approximation type, stability of the numerical scheme
- mesh, time step, error indicators, stopping criteria . . .

Postprocessing and analysis

Postprocessing of the simulation results is performed in order to extract the desired information from the computed flow field

- calculation of derived quantities (streamfunction, vorticity)
- calculation of integral parameters (lift, drag, total mass)
- visualization (representation of numbers as images)
  - 1D data: function values connected by straight lines
  - 2D data: streamlines, contour levels, color diagrams
  - 3D data: cutlines, cutplanes, isosurfaces, isovolumes
  - arrow plots, particle tracing, animations . . .
- Systematic data analysis by means of statistical tools
- Debugging, verification, and validation of the CFD model

Validation/Verification of CFD codes

- Verify the code to make sure that the numerical solutions are correct.
- Compare the results with available experimental data (making a provision for measurement errors) to check if the reality is represented accurately enough.
- Perform sensitivity analysis and a parametric study to assess the inherent uncertainty due to the insufficient understanding of physical processes.
- Try using different models, geometry, and initial/boundary conditions.
- Report the findings, document model limitations and parameter settings.

Commercial CFD (selection)

Major current players include

- Ansys (Fluent and other codes)

  http://www.ansys.com/

- Simens: (starCD and other codes)

  http://mdx.plm.automation.siemens.com

Others

- CHAM

  http://www.cham.co.uk/
- COMSOLE

  https://www.comsol.com/cfd-module

Free

- OpenFOAM

  http://www.openfoam.com

Course goals

Learn how to solve some transfer phenomena equations (e.g. Navier-Stokes, Darcy, Darcy-Brinkman, energy, etc.) for different classical problems (lid driven cavity, differentially heated cavity, etc.)

Hear about various concepts to allow continuing studies of the literature.

Background needed:

- Numerical Analysis
- Fluid Mechanics
- Basic computer skills (MATLAB)

Course content

Introduction

Fluid Mechanics and Heat Transfer. Basic equations.

Numerical methods for ODE

Numerical methods for BVP

Finite difference method for PDE

Case study. Lid driven fluid flow

Case study. Differentially heated cavity

Introduction to finite volume method

Introduction to finite elements method.

Literature

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- Petrila, T; Trif, D. (2005) Basics of Fluid Mechanics and Introduction to Computational Fluid Dynamics, Springer.
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- H K Versteeg and W Malalasekera (2007), An Introduction to Computational Fluid Dynamics, Pearson Education Limited

Homework and projects (proposal)

Two projects

- an intermediary project
- a final project

Two groups of students (4 students in one group) working on

- mathematical model
- numerical model
- simulation
- validation
- results' discussions

One student will be the group coordinator. In a group one student will be responsible for one phase.

Fluid Mechanics and Heat Transfer. Basic equations.

Fluid can be defined as a substance which can deform continuously when being subjected to shear stress at any magnitude. In other words, it can flow continuously as a result of shearing action. This includes any liquid or gas

Fluid characteristics

Macroscopic properties

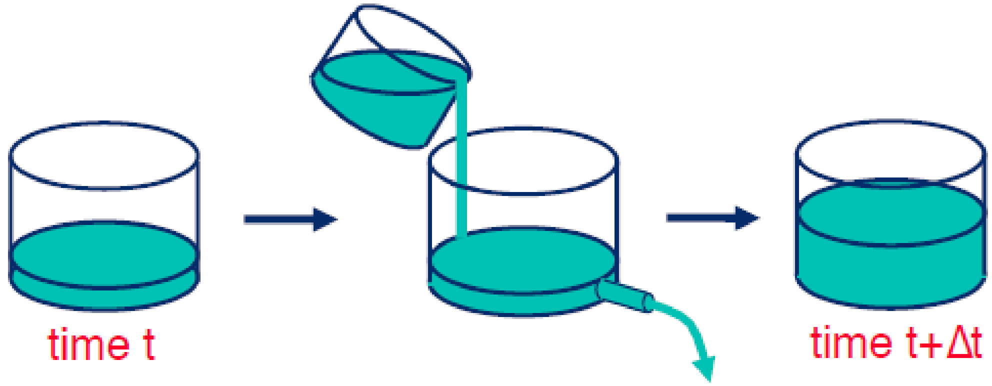
ρ	density
μ	viscosity
p	pressure
T	temperature
$\mathbf{v}$	velocity

Classification of fluid flows

viscous	inviscid
compressible	incompressible
steady	unsteady
laminar	turbulent
single-phase	multiphase

Continuity (Mass Conservation)

In general, mass can be added or removed:



The conservation law must be stated as:

Final Mass = Original Mass + Mass Added - Mass Removed

Rate of increase of mass = Net influx of mass

$$\frac{\partial \rho}{\partial t} + div(\rho\,\vec{v}) = 0$$

$$div(\vec{v}) = 0$$

incompressible

Momentum Equation (for fluid)

The equation of motion of the viscous (Newtonian) compressible fluid is given by

$$\rho\left(\frac{\partial \vec{v}}{\partial t}+(\vec{v}\cdot\nabla)\vec{v}\right)=\rho\vec{F}-grad\,p+div(\mu\,a_{jk})\vec{i}_j-\frac{2}{3}grad(\mu\,div\vec{v})$$

where

$$D_{ik}=a_{ik}=\frac{1}{2}\left(\frac{\partial v_i}{\partial x_k}+\frac{\partial v_k}{\partial x_i}\right)$$

is the strain rate tensor (rate of deformation tensor)

Particular cases

1. Inviscid incompressible fluid ($\mu=0,\ \rho=\rho_0=$ constant)

$$\rho_0\left(\frac{\partial \vec{v}}{\partial t}+(\vec{v}\cdot\nabla)\vec{v}\right)=\rho_0\vec{F}-grad\,p$$

2. Incompressible viscous fluid ($\mu = \text{constant}, \;\; \rho = \text{constant}$)

$$\rho\left(\frac{\partial \vec{v}}{\partial t} + \left(\vec{v}\cdot\nabla\right)\vec{v}\right) = \rho\vec{F} - grad\; p + \mu\Delta\vec{v}$$

(incompressible Navier-Stokes equations)

in Cartesian coordinates:

$$\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z}\right) = -\frac{\partial p}{\partial x} + \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) + \rho g_x$$

$$\rho\left(\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z}\right) = -\frac{\partial p}{\partial y} + \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2}\right) + \rho g_y$$

$$\rho\left(\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z}\right) = -\frac{\partial p}{\partial z} + \mu\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right) + \rho g_z\,.$$

3. Inviscid compressible fluid ($\mu = 0,\ \rho =$ variabil)

$$\rho\left(\frac{\partial \vec{v}}{\partial t} + (\vec{v}\cdot\nabla)\vec{v}\right) = \rho\vec{F} - grad\ p$$

(Euler equations)

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + X\,,$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + Y\,,$$

$$\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial z} + Z\,,$$

Energy equation

$$\rho \frac{dE}{dt} = -p\rho \frac{d}{dt}\left(\frac{1}{\rho}\right) + \phi + div\left(k \, grad \, T\right)$$

where E is the internal energy of a fluid particle (viscous compressible fluid)

- gas heating due to the compression

$$-p\rho \frac{d}{dt}\left(\frac{1}{\rho}\right) \underset{continuity\ equation}{=} -p \, div\vec{v}$$

- mechanical work of the viscous forces transformation in heat

$$\Phi = \tfrac{1}{2}\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)^2$$

By taking into account that the enthalpy of a unit of mass is $i = E + \frac{p}{\rho}$ we obtain

$$\rho \frac{di}{dt} = \frac{dp}{dt} + \phi + div(k\, grad\, T)$$

But for a perfect gas we have

$$di = c_p dT$$

and energy equation becomes

$$\rho \frac{d}{dt}(c_p T) = \frac{dp}{dt} + \phi + div(k\, grad\, T)$$

where

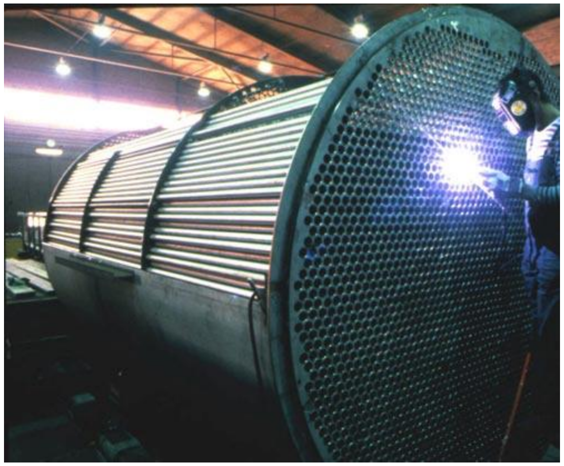
$$\frac{df}{dt} = \frac{Df}{Dt} = \frac{\partial f}{\partial t} + (\vec{v} \cdot \nabla) f \qquad \frac{Df}{Dt} \equiv \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x_1} v_1 + \frac{\partial f}{\partial x_2} v_2 + \frac{\partial f}{\partial x_3} v_3$$

is the substantial derivative.

Momentum Equation (for fluid saturated porous media)

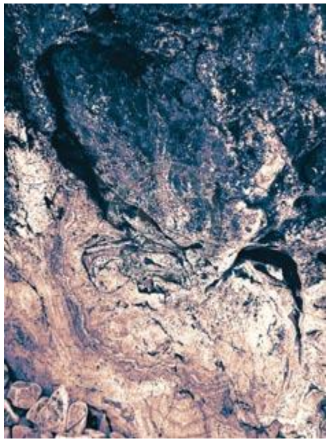
By a porous medium we mean a material consisting of a solid matrix with an interconnected void.

Porous media are present almost always in the surrounding medium, very few materials excepting fluids being non-porous.



heat exchanger

processor cooler



porous rock

Darcy's (law) equation (momentum equation)

$$\langle \vec{v} \rangle = -\frac{K}{\mu}\, grad\, p + \rho\, \vec{g}$$

where

- $\langle v \rangle$ is the average velocity (filtration velocity, superficial velocity, seepage velocity or Darcian velocity)
- $K = k\mu / \rho g$ is the permeability of the porous medium

Darcy' law expresses a linear dependence between the pressure gradient and the filtration velocity. It was reported that this linear law is not valid for large values of the pressure gradient.

Darcy's law extensions

Forchheimer's extension

$$\nabla p = -\frac{\mu}{K}\langle\vec{v}\rangle - \frac{c_F}{\sqrt{K}}\rho\left|\langle\vec{v}\rangle\right|\langle\vec{v}\rangle$$

where c_F is a dimensionless parameter depending on the porous medium

Brinkman's extension

$$\nabla p = -\frac{\mu}{K}\langle\vec{v}\rangle + \tilde{\mu}\,\Delta\langle\vec{v}\rangle$$

where $\tilde{\mu}$ is an effective viscosity

Brinkman-Forchheimer's extension

$$\nabla p = -\frac{\mu}{K}\langle\vec{v}\rangle - \frac{c_F}{\sqrt{K}}\rho\left|\langle\vec{v}\rangle\right|\langle\vec{v}\rangle + \tilde{\mu}\,\Delta\langle\vec{v}\rangle$$

Energy equation for porous media

$$\left(\rho c_p\right)_m \frac{\partial \langle T \rangle}{\partial t} + \left(\rho c_p\right)_{fluid} \langle \vec{v} \rangle \nabla \langle T \rangle = \nabla \left(k_e \nabla \langle T \rangle \right)$$

where

$$\left(\rho c_p\right)_m = \phi \left(\rho c_p\right)_{fluid} + (1-\phi)\left(\rho c_p\right)_{solid}$$

$$k_e = \phi k_{fluid} + (1-\phi) k_{solid}$$

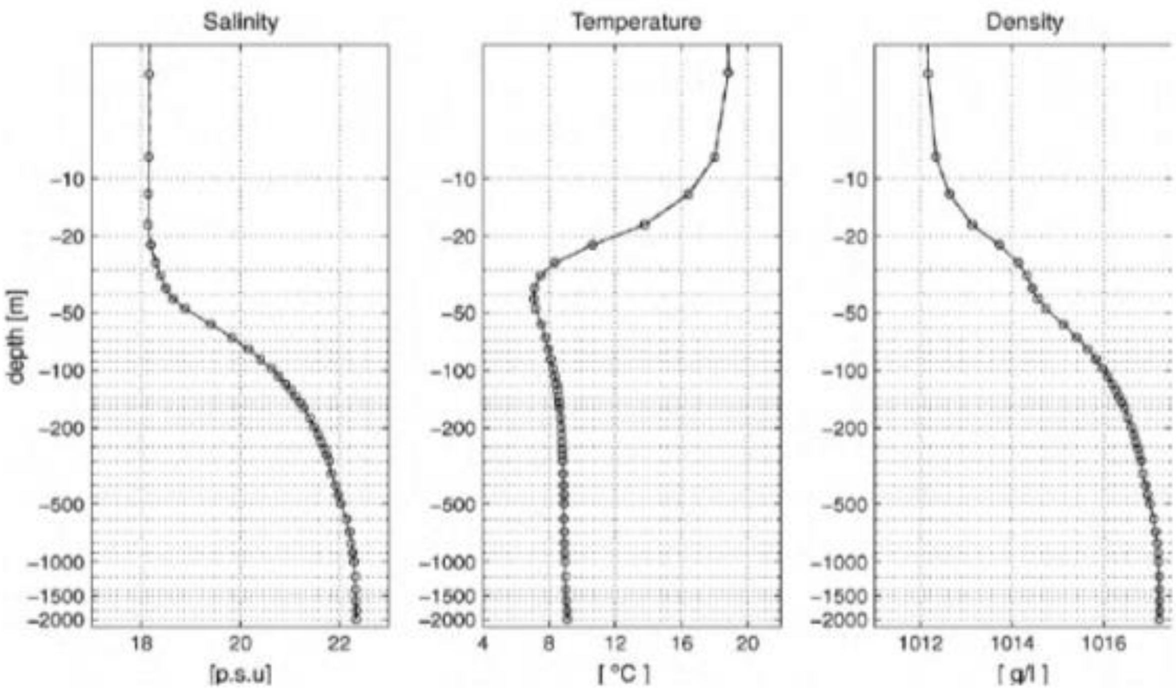
Bouyancy driven flow[1]

- There exists a large class of fluid flows in which the motion is caused by buoyancy in the fluid.
- Buoyancy is the force experienced in a fluid due to a variation of density in the presence of a gravitational field. According to the definition of an incompressible fluid, variations in the density normally mean that the fluid is compressible, rather than incompressible.
- For many of the fluid flows of the type mentioned above, the density variation is important only in the body-force term of the momentum equations. In all other places in which the density appears in the governing equations, the variation of density leads to an insignificant effect.
- Buoyancy results in a force acting on the fluid, and the fluid would accelerate continuously if it were not for the existence of the viscous forces.
- The situation depicted above occurs in natural convection.

[1] I.G. Currie, Fundamental Mechanics of Fluids, 3rd ed., Marcel Dekker, New York, 2003

Generally, density is a function of temperature and concentration

$$\rho = \rho(T, c)$$



Black Sea salinity, temperature and density

(Ecological Modelling, 221, 2010, p. 2287-2301)

Boussinesq's approximation

$$\left(\rho-\rho_{ref}\right)=\rho\beta_T\left(T_{ref}-T\right)+\rho\beta_S\left(C_{ref}-C\right)$$

$$\beta_T=-\frac{1}{\rho}\left(\frac{\partial\rho}{\partial T}\right)_p, \qquad \beta_S=-\frac{1}{\rho}\left(\frac{\partial\rho}{\partial C}\right)_{p,T}$$

Momentum

$$\rho\frac{\partial\mathbf{u}}{\partial t}+\rho(\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{u}=-\boldsymbol{\nabla}p+\mu\nabla^2\mathbf{u}+\rho g\beta(T-T_0)\mathbf{e}_z$$