

Introduction to CFD

Basic course

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Content

- Introduction
- Literature
- Modeling
- Discretization
- Iteration

Introduction

- Exercise – which CFD limitations do you know?

Reality	Simulation

Introduction

- Exercise – which CFD limitations do you know?

Reality	Simulation
All laws of physics taken into account	Only selected laws of physics taken into account
Exact physical property variations	Modeled physical property variations
Electrical, chemical, ... influences	Selected or no other influences
Infinite time resolution	Discrete time resolution
Infinite spatial resolution	Discrete space resolution
Infinite domain	Limited domain
Real boundary conditions	Estimated boundary conditions
...	...

Introduction

- Exercise – which CFD advantages do you know?

Reality – experimental testing	Simulation

Introduction

- Exercise – which CFD advantages do you know?

Reality – experimental testing	Simulation
Measuring errors	Exact “probing”
Approximate boundary conditions	Possibly “perfect” boundary conditions
Size limitations	No size limitations
Cost of the test setup	Virtual test setup
Number of measuring points	Probing at location of choice
Difficult visualization	Good visualization
...	...

Introduction

- What is a fluid(um)?
 - Substance whose molecular structure offers no resistance to external shear forces
 - A fluid does not have a fixed shape
 - A fluid can be both a liquid or a gas



Introduction

- Fluidum properties & effects - examples
 - Viscosity: measure for the forces generated during shearing of the liquid
 - Non-newtonian liquids: shear force does not vary linearly with the speed gradient perpendicular to the shear surface.
- <https://www.youtube.com/watch?v=D-wxnID2q4A>

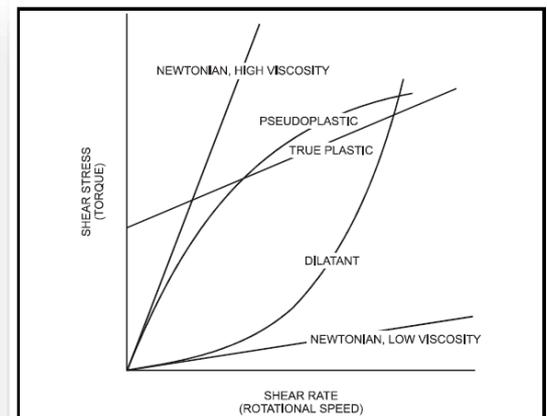
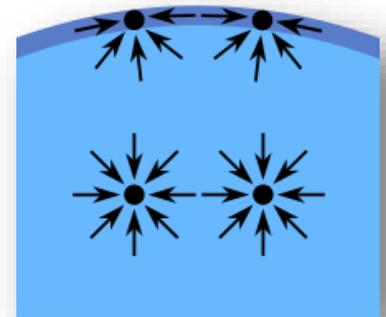


Figure 3-12. Behavior of Newtonian and Non-Newtonian Fluids

Introduction

- Fluidum properties & effects - examples
 - Surface tension:
 - Molecules at the surface lack neighbours, causing them to be pulled inward
 - This creates some internal pressure and forces liquid surfaces to contract to the minimal area
 - <https://www.youtube.com/watch?v=ynk4vJa-VaQ>



Introduction

- Fluidum properties & effects - examples
 - Multiphase flows:
 - A substance can be in a solid, liquid or gaseous state
 - Different substances in different states can interact
 - <https://www.youtube.com/watch?v=Op0U3PE2L5A>
 - <https://www.youtube.com/watch?v=bb9lhV6HgMQ>



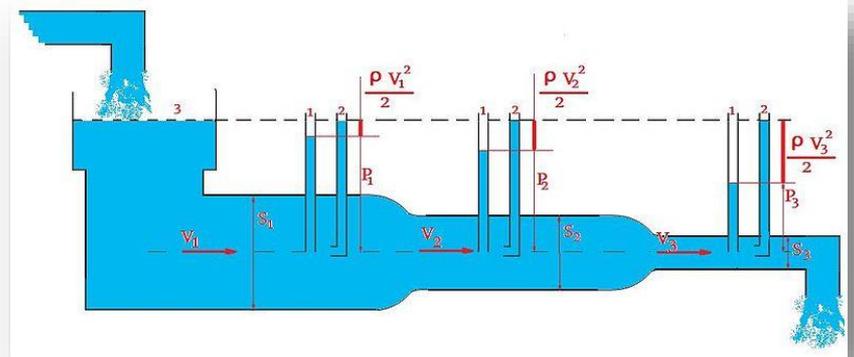
Introduction

- Fluidum properties & effects - examples
 - Vortex shedding:
 - Also called a Von Karman vortex
 - Typical example: flow around a cilinder
 - Vortices created at the back of the body detach periodically from either side
 - <https://www.youtube.com/watch?v=yMzrk-FlhKw>



Introduction

- Fluidum properties & effects - examples
 - Bernoulli effect:
 - $\frac{1}{2}\rho v^2 + \rho gh + P = \text{constant}$
 - Pressure decreases as velocity goes up
 - <https://www.youtube.com/watch?v=epesl-fWvrY>



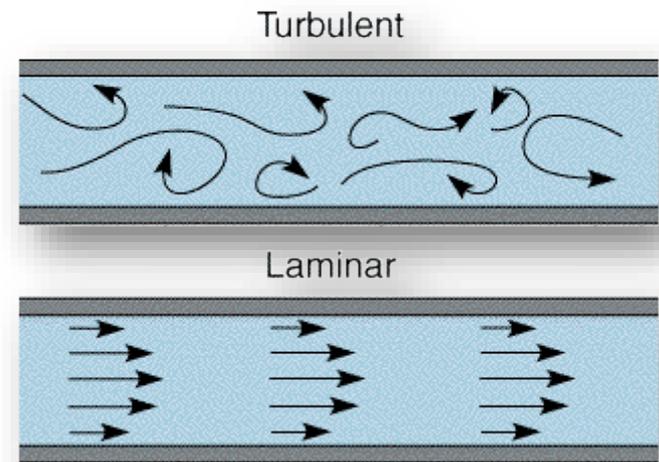
Introduction

- Fluidum properties & effects - examples
 - Combustion:
 - Extra equations to model the combustion
 - High amounts of turbulence possible
 - <https://www.youtube.com/watch?v=b6wfODEp0VE>



Introduction

- Fluidum properties & effects - examples
 - Laminar versus turbulent flow:
 - Laminar flow:
 - Viscous forces are dominant
 - No cross-currents perpendicular to the flow direction, no swirls
 - Orderly flow: steady streamlines
 - Turbulent flow:
 - Inertia forces are dominant
 - Less orderly flow
 - Eddies: small packets of fluid particles creating lateral mixing



Introduction

- Fluidum properties & effects - examples
 - Laminar versus turbulent flow:
 - Reynolds number:

$$Re = \frac{v \cdot L \cdot \rho}{\mu} = \frac{v \cdot L}{\nu}$$

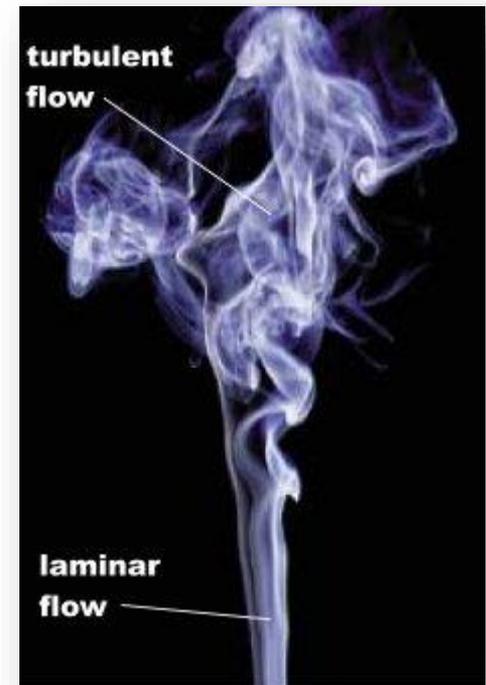
with

v = characteristic speed

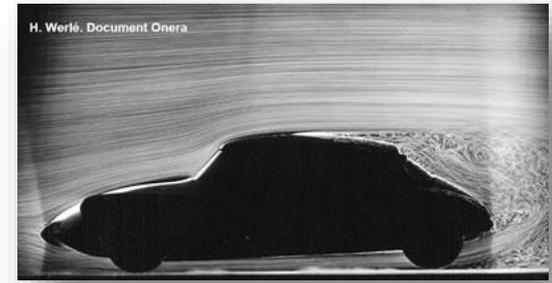
L = characteristic length

μ = dynamic viscosity

ν = kinematic viscosity



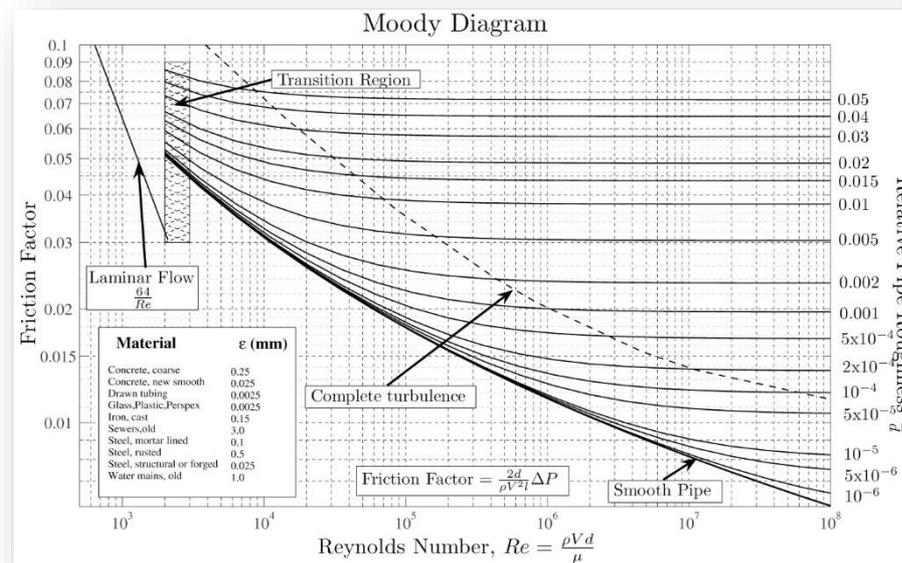
Introduction



- Fluidum properties & effects - examples
 - Laminar versus turbulent flow:
 - Reynolds number:
 - Measure for the inertia forces over the viscous forces
 - At low Re , flow is laminar, at high Re , flow is turbulent
 - In between, there is a transition zone
 - **Caution:** the Reynolds number is an application-specific parameter with subjective definition:
 - » no unique definition of the characteristic length and speed
 - » Transition points can occur at different Reynolds numbers

Introduction

- Fluidum properties & effects - examples
 - Laminar versus turbulent flow:
 - Reynolds number:
 - Moody diagram – example for pipe flow:

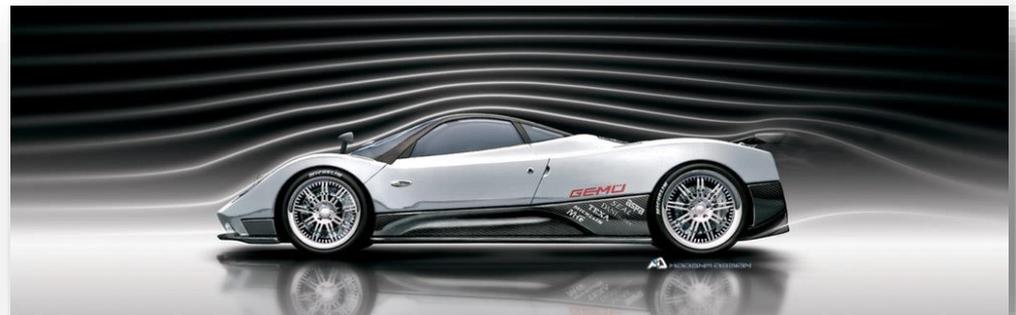


Introduction

- Fluidum properties & effects - examples
 - Laminar versus turbulent flow:
 - Reynolds number:
 - Scaled testing (e.g. Lab test, wind tunnel tests): scaled and full flow are identical if Re is equal:

$$Re^* = Re, \quad \frac{p^*}{\rho^* v^{*2}} = \frac{p}{\rho v^2}$$

- Then, the scaled model results can be extrapolated towards the real flow



Introduction

- Fluidum properties & effects - examples
 - Laminar versus turbulent flow:
 - Extreme amounts of calculation time required for exact simulation of turbulence (DNS – direct numerical simulation)
 - This is due to the very small spatial and time scale of the eddies, requiring very small grids and time steps
 - Turbulence models are used to reduce calculation time: (part of) the swirls are taken into account through models based on experimental values

Literature

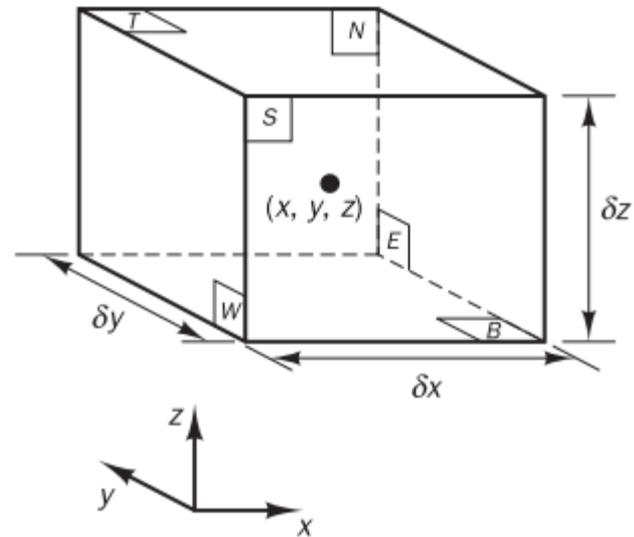
- *Computational methods for fluid dynamics* – Ferziger & Peric (basis for this CFD intro)
- *An introduction to computational fluid dynamics* – Versteeg & Malalasekera

Modeling

- Reality:
 - Things happen and there seems to be a consistency: a relationship between parameters
 - All physical, chemical, ... aspects always count
- CFD:
 - Describe reality by formulating a mathematical relationship between variables
 - Only the selected models count, rest is ignored

Modeling

- Consider a control volume (finite volume approach) to which we can apply models:
 - Volume Ω
 - Surface S
 - Dimensions δx , δy , δz
 - CV = control volume
 - CM = control mass



Modeling

- The variation of conservative properties
 - Intensive property ϕ : a physical property of the fluid expressed per unit mass (independent of the amount of mass considered)
 - Extensive property Φ : the summation over a certain volume:

$$\Phi = \int_{\Omega_{CM}} \rho \phi \, d\Omega$$

With Ω_{CM} = volume occupied by the control mass

Modeling

- The variation of conservative properties
 - General conservation law for conservative physical properties

$$\frac{d}{dt} \int_{\Omega_{CM}} \rho \phi \, d\Omega = \frac{d}{dt} \int_{\Omega_{CV}} \rho \phi \, d\Omega + \int_{S_{CV}} \rho \phi (v - v_b) \cdot n \, dS$$

Rate of change of the amount of the property Φ in the control mass

Rate of change of the property Φ within the control volume

Net flux of the property Φ through the CV boundary due to fluid motion relative to CV boundary

Modeling

- Navier stokes equations:
 - General conservation law with $\Phi = 1$ and $\Phi = v$
 - Equations that explain the movement of liquids
 - Description of the force balance for each point within the liquid

Modeling

- Navier stokes equations:
 - Mass conservation (continuity): $\Phi = 1$
 - Integral form:

$$\frac{\partial}{\partial t} \int_{\Omega} \rho \, d\Omega + \int_S \rho v \cdot n \, dS = 0$$

- Differential coordinate-free form:

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

Modeling

- Navier stokes equations:
 - Mass conservation (continuity): $\Phi = 1$
 - Differential form - cartesian coordinate system:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i}$$
$$= \frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_x)}{\partial x} + \frac{\partial(\rho u_y)}{\partial y} + \frac{\partial(\rho u_z)}{\partial z} = 0$$

Modeling

- Navier stokes equations:
 - Momentum conservation: $\Phi = v$
 - Integral form:

$$\frac{\partial}{\partial t} \int_{\Omega} \rho v \, d\Omega + \int_S \rho v v \cdot n \, dS = \sum f$$

with f the forces acting on the fluid in the CV:

- Surface forces: pressure, normal and shear stress, surface tension etc, ... \rightarrow stress tensor T (for newtonian fluids)
- Body forces: gravity, centrifugal and Coriolis forces, electromagnetic forces, ... \rightarrow body forces “ b ” (per unit mass)

Modeling

- Navier stokes equations:
 - Momentum conservation: $\Phi = v$
 - Integral form

Adding these forces to the equations results in the final integral form:

$$\frac{\partial}{\partial t} \int_{\Omega} \rho v \, d\Omega + \int_S \rho v v \cdot n \, dS = \int_S T \cdot n \, dS + \int_{\Omega} \rho b \, d\Omega$$

Velocity rate of change	Convective flux	Diffusive flux	Body forces
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Modeling

- Navier stokes equations:
 - Momentum conservation: $\Phi = v$
 - Differential coordinate-free form:

$$\frac{\partial(\rho v)}{\partial t} + \text{div}(\rho v v) = \text{div } T + \rho b$$

with stress tensor T – (surface forces):

$$T = - \left(p + \frac{2}{3} \mu \text{div } v \right) I + 2\mu D$$

with rate of strain (deformation) tensor D :

$$D = \frac{1}{2} [\text{grad } v + (\text{grad } v)^T]$$

Modeling

- Navier stokes equations:
 - Momentum conservation: $\Phi = v$
 - Differential form – cartesian coordinate system:

$$\frac{\partial(\rho u_i)}{\partial t} + \text{div}(\rho u_i v) = \text{div } t_i + \rho b_i$$

with

$$t_i = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) i_j - \left(p + \frac{2}{3} \mu \frac{\partial u_j}{\partial x_j} \right) i_i$$

Modeling

- Navier stokes equations:
 - Simplified models:
 - Incompressible flow $\rightarrow \frac{\partial \rho}{\partial t} = 0$
 - Inviscid (Euler) flow \rightarrow high Re-number flows
 - Potential flow
 - Creeping (Stokes) flow \rightarrow low Re-number flows
 - Boussinesq approximation \rightarrow small density variations
 - Boundary layer approximation

Modeling

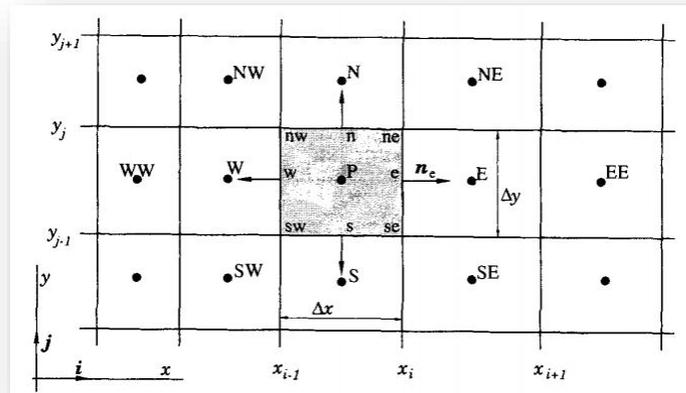
- Modeling error (Ferziger & Peric):
 - *“The difference between the real flow and the exact solution of the mathematical model”*
 - Modeling approximation and/or neglection (chemical, multi-phase, combustion, magnetism, ...)
 - Turbulence models
 - Approximation of boundary conditions
 - Dependency of properties on temperature, ...
 - Finite computational domain
 - Geometry simplifications

Discretization

- Reality: matter is continuous, almost infinite “resolution” down to the the molecular level
- CFD:
 - Analytical solution of the model equations is not possible (except for very simple cases)
 - Chop up reality into pieces (control volumes) that are small enough to describe the phenomena we want to simulate
 - Approximate the model by algebraic equations and apply them to the control volumes

Discretization

- 2D case – example volume in gray:
 - Computational node P at the center: for this location, the value of ϕ is calculated and stored
 - 4 cell faces: S_e (East surface), S_s , S_w , S_n
 - 8 locations on the cell faces: e, se, s, sw, w, wn, n, ne



Discretization

- 2D case – steps to discretize an equation:
 - Starting point: only the values at computational nodes (CV centers) are known.
 - Express surface integrals in function of values at face locations
 - Express volume integrals in function of values of face locations
 - Express values at face locations in function of values at computational nodes
 - End point: value at a CV center is calculated using only the values at neighbouring CV centers (this group is called a computational molecule).

Discretization

- Surface integral approximation:
 - Net flux through the CV boundary: summation of the fluxes through each of the CV surfaces

$$\int_S f dS = \sum_k \int_{S_k} f dS$$

Discretization

- Surface integral approximation:
 - Midpoint rule:

$$F_e = \int_{S_e} f dS = \bar{f}_e S_e \approx f_e S_e$$

- Trapezoid rule:

$$F_e = \int_{S_e} f dS \approx \frac{S_e}{2} (f_{ne} + f_{se})$$

- Simpson's rule:

$$F_e = \int_{S_e} f dS \approx \frac{S_e}{6} (f_{ne} + 4f_e + f_{se})$$

Discretization

- Volume integral approximation:
 - Simplest method – multiple value at P with CV volume:

$$Q_P = \int_{\Omega} q d\Omega = \bar{q} \Delta\Omega \approx q_P \Delta\Omega$$

- Example of higher order approximation

$$Q_P = \frac{\Delta x \Delta y}{36} (16q_p + 4q_s + 4q_n + 4q_w + 4q_e + 4q_{se} + 4q_{sw} + 4q_{ne} + 4q_{nw})$$

→ Value of q needs to be known at more locations

Discretization

- Values at cell face locations:
 - Values at locations other than the CV centers need to be calculated using interpolation between CV center values.
 - UDS – upwind differencing scheme:
 - Use the upstream value
 - Easy to calculate, but:
 - Numerically diffusive
 - Only first order accurate

$$\phi_e = \begin{cases} \phi_P & \text{if } (v \cdot n)_e > 0 \\ \phi_E & \text{if } (v \cdot n)_e < 0 \end{cases}$$

Discretization

- Values at cell face locations:
 - CDS – central differencing scheme:
 - Linear interpolation between 2 neighbouring nodes
 - Second order accurate (up to second order variations of the value are calculated correctly)

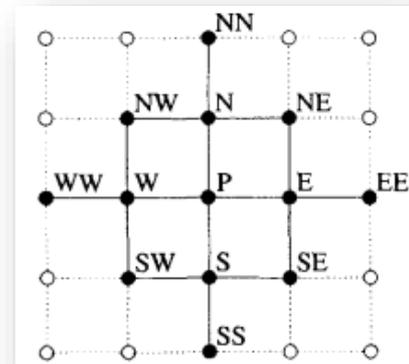
$$\phi_e = \phi_E \lambda_e + \phi_P (1 - \lambda_e)$$

with the linear interpolation factor defined as:

$$\lambda_e = \frac{x_e - x_P}{x_E - x_P}$$

Discretization

- Calculating the cell value:
 - Summation of all the flux approximations and source terms results in a set of algebraic equations
 - Result: computational molecule in which the values at node center P are calculated using the values at the neighbouring node centers



Discretization

- Calculating the cell value:
 - This results in a system of linear algebraic equations (if the original equation was linear):

$$A_P \Phi_P + \sum_I A_I \Phi_I = Q_P$$

with P the node being examined and “I” the involved neighbouring nodes.

- Grouping all these equations for the cells in the domain results in a matrix notation:

$$A\Phi = Q$$

Discretization

- Discretization error (Ferziger & Peric):
 - “The difference between the exact solution of the governing equations and the exact solution of the discrete approximation”*
 - Refine the grid locally where variable changes are large
 - Approximations become more accurate with a finer grid
 - Higher order approximations can be more accurate, but require more programming effort & computing power
 - Higher order approximations are only accurate on a grid that is fine enough and can cause oscillations

Iteration

- Reality:
 - The solution is always exact
- CFD:
 - Exact solution of algebraic equations is not possible or too expensive.
 - Therefore, use iteration techniques that converge towards the solution until you are “close enough”.

Iteration

- Properties of CFD equations
 - Discretized convection-diffusion equations are **algebraic equations**.
 - Depending on the original partial differential equation, these are **linear or non-linear**.
 - Matrices of these equations are always **sparse**: this property can be used to speed up the calculation.
 - The equations are often **coupled**: the dominant variable of one equations occurs in other equations

Iteration

- Linear equations – solution methods:
 - Direct methods:
 - Basic: Gauss elimination
 - General technique for full matrices

Forward elimination

$$\begin{array}{c}
 \boxed{\begin{bmatrix} 1 & 3 & -2 & | & 5 \\ 3 & 5 & 6 & | & 7 \\ 2 & 4 & 3 & | & 8 \end{bmatrix} \sim \begin{bmatrix} 1 & 3 & -2 & | & 5 \\ 0 & -4 & 12 & | & -8 \\ 2 & 4 & 3 & | & 8 \end{bmatrix} \sim \begin{bmatrix} 1 & 3 & -2 & | & 5 \\ 0 & -4 & 12 & | & -8 \\ 0 & -2 & 7 & | & -2 \end{bmatrix} \sim \begin{bmatrix} 1 & 3 & -2 & | & 5 \\ 0 & 1 & -3 & | & 2 \\ 0 & -2 & 7 & | & -2 \end{bmatrix}} \\
 \sim \begin{bmatrix} 1 & 3 & -2 & | & 5 \\ 0 & 1 & -3 & | & 2 \\ 0 & 0 & 1 & | & 2 \end{bmatrix} \sim \begin{bmatrix} 1 & 3 & -2 & | & 5 \\ 0 & 1 & 0 & | & 8 \\ 0 & 0 & 1 & | & 2 \end{bmatrix} \sim \begin{bmatrix} 1 & 3 & 0 & | & 9 \\ 0 & 1 & 0 & | & 8 \\ 0 & 0 & 1 & | & 2 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 0 & | & -15 \\ 0 & 1 & 0 & | & 8 \\ 0 & 0 & 1 & | & 2 \end{bmatrix}
 \end{array}$$

Back substitution

- <https://www.youtube.com/watch?v=2j5lc2V7wq4>

Iteration

- Linear equations – solution methods:
 - Direct methods:
 - More advanced: LU decomposition
 - Matrix A is factored into the product of 2 separate matrices:
 $A = LU$
 - U is an upper diagonal matrix: produced by the forward elimination phase of the Gauss elimination
 - L is a lower diagonal matrix: produced by the back substitution used in the Gauss elimination phase

Iteration

- Linear equations – solution method:
 - Direct methods:
 - More advanced: LU decomposition
 - Solution is performed in 2 steps:
 1. $LY = Q$
 2. $U\phi = Y$
 - Main disadvantage: triangular factors for sparse matrices are not sparse
 - Main advantage: factorization can be performed without knowing $Q \rightarrow$ investing in this factorization can pay off later when applying it in an iterative method

Iteration

- Linear equations – solution methods:
 - Iterative methods:
 - Why:
 - Discretization error is much larger than the accuracy of the computer → solution up to an accuracy (just) higher than the discretization is enough
 - Usually much cheaper (less computational effort) than direct methods
 - How:
 - Guess an initial solution
 - Use the equation to improve it over and over

Iteration

- Non-linear equations – solution method:
 - Solution strategy:
 - Guess an initial solution
 - Linearize the equations around that solution
 - Improve the solution through iteration

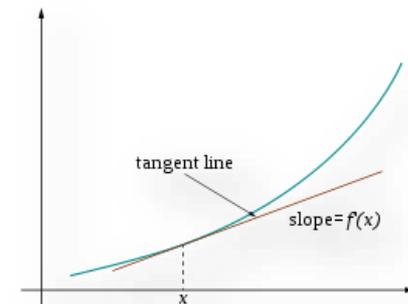
Iteration

- Non-linear equations – solution method:
 - How to linearize the equations – Newton-like method:
 - Approximate the non-linear curve by it's tangent using the first two terms of the Taylor series:

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0) \rightarrow x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

Or more generally:

$$x_k = x_{k-1} - \frac{f(x_{k-1})}{f'(x_{k-1})}$$



Iteration

- Coupled equations – solution method:
 - Simultaneous solution:
 - Put all the equations into one large matrix
 - Result: a block-band matrix
 - Best solution when equations are both linear and tightly coupled
 - Example: pressure-velocity coupling
 - Simple method
 - PISO method