CFD - An Overview

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Computational

- Complex problems
- No analytical solution
- Numerical approximation
- Using computers

Fluid

- Continually deforms when force is applied

Images: game-icons.net, Lorc and Delapouite

Dynamics

- Considering the forces in fluids
- Studying the resulting fluid motion
- May be stationary or instationary

Classes of Fluids

- Liquids
  – Forms free surface

- Gases
  – Freely diffuse

- *Plasma*
  – *Ionized, highly electrical conductive*

Images: game-icons.net, Lorc and Delapouite

Some Defining Properties of Fluids

- Viscosity
  - Relation of shear stress to speed of deformation

- Compressibility
  - Relation of volume change under pressure

- Heat conductivity

- Density

Images: game-icons.net, Cathelineau, Skoll, Lorc and Delapouite

Modelling

- Reality
- Physical Model
- Mathematical Model
- Numerical Approximation
- Simulation code
- Usage of the simulation code
- Analysis of results

Physical Model for Fluids

- Level of detail
  - Quantum – Molecular – Continuum
- Consideration of effects
  - Electrodynamics? Gravity? Relativity? Chemical reactions?

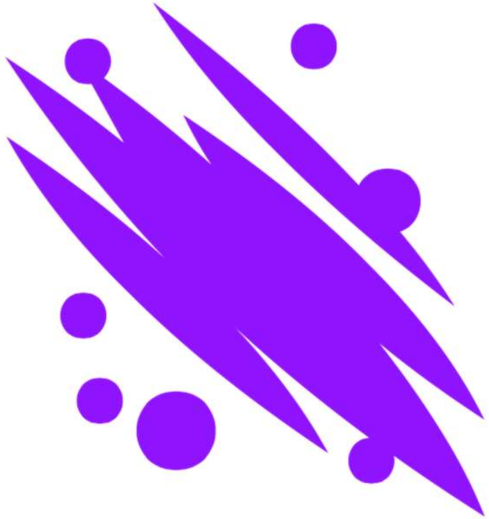
Continuum Assumption

- On the considered scale:
  - Fluid covers complete space
  - Infinitisimal small decomposition possible

- Knudsen number:

$$\mathbf{Kn} = \frac{\text{mean free path}}{\text{reference length scale}}$$

Continuum Classification



- High **Kn** (>0.5):
  - (For example rarefied gases)
  - Physical model: Kinetic gas theory
- *Knudsen flow (0.01 < Kn < 0.5)*

- Low **Kn** (<0.01):
  - (For example air around plane)
  - Physical model: Continuum mechanics

Image: game-icons.net, Lorc

Physical Continuum Model

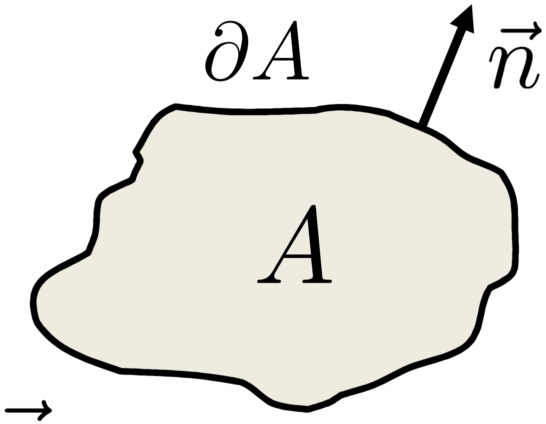
- Newtonian mechanics
- Conservation laws:
  - Conservation of mass
  - Conservation of momentum
  - Conservation of energy

Mathematical Model

- Conservation laws yield compressible Navier-Stokes equations
- System of partial differential equations
- Describes evolution of state due to spatial fluid variations

Conservation Laws

- Quantity can neither vanish nor appear
- Observing a given volume:
  - Quantity only changed by transport through the surface



- Mathematical:

$$\frac{\partial}{\partial t}\int_A u(\vec{x},t)\mathrm{d}A = -\oint_{\partial A}\vec{f}(u)\vec{n}\mathrm{d}s$$

Integral Conservation

$$\frac{\partial}{\partial t}\int_A u(\vec{x},t)\mathrm{d}A = -\oint_{\partial A}\vec{f}(u)\cdot\vec{n}\mathrm{d}s$$

t time

$\vec{x}$ location

u conserved quantity

$\vec{f}$ flux

A volume

∂A surface

$\vec{n}$ surface normal

Convective Transport

- Quantity transported by velocity $\vec{v}$

- Convective flux:

$$\vec{f} = u \cdot \vec{v}$$

Conservation in Continuum

- Conservation law holds for infinitisimal volumes
- Conservation in each point
  - ➢ <u>Differential formulation</u>

- Continuously differentiable:
  - **Divergence Theorem** *(replace surface by volume integral)*
  - **Leibniz Rule** *(exchange integration and differentiation)*

Replacing Surface by Volume Integral

- Divergence Theorem: $\oint_{\partial A} \vec{f} \cdot \vec{n} \mathrm{d}s = \int_A \nabla \cdot \vec{f} \mathrm{d}A$

- Incoporate in the conservation law

$$\frac{\partial}{\partial t} \int_A u(\vec{x}, t) \mathrm{d}A = - \oint_{\partial A} \vec{f}(u) \cdot \vec{n} \mathrm{d}s$$

- Yields: $\frac{\partial}{\partial t} \int_A u(\vec{x}, t) \mathrm{d}A = - \int_A \nabla \cdot \vec{f}(u) \mathrm{d}A$

Differential Conservation Law

- Using Leibniz's rule and pulling everything into one integral:

$$\int_A \left(\frac{\partial u(\vec{x},t)}{\partial t} + \nabla \cdot \vec{f}(u) \right) \mathrm{d}A = 0$$

- Conservation holds for any volume
  - ➢Conservation in each point

$$\frac{\partial u(\vec{x},t)}{\partial t} + \nabla \cdot \vec{f}(u) = 0$$

Conservation of Mass

- *Conserved*: Mass density ρ
- *Changed by*:
  - Convection $\vec{f} = \rho\vec{v}$
- *Integral form:* $\frac{\partial}{\partial t}\int_A \rho(\vec{x},t)\mathrm{d}A = -\oint_{\partial A} \rho\vec{v}\cdot\vec{n}\mathrm{d}s$
- *Differential form:* $\frac{\partial\rho(\vec{x},t)}{\partial t} + \nabla\cdot(\rho\vec{v}) = 0$

Conservation of Momentum

- *Conserved*: Momentum density $\vec{m} = \rho\vec{v}$
- *Changed by*:
  - Convection $\overline{\overline{f^c}} = \vec{m} \circ \vec{v}$ *(Dyadic product)*
  - Surface forces
    - pressure $\overline{\overline{f^p}} = p\overline{\overline{I}}$ *(Identity tensor)*
    - friction $\overline{\overline{f^v}} = -\overline{\overline{\tau}}$ *(Stress deviator tensor)*
  - *Possible volume forces* (gravity, electromagnetism) $\vec{F}^e$

Conservation of Momentum

- *Integral form:*

$$\frac{\partial}{\partial t}\int_A \vec{m}(\vec{x},t)\mathrm{d}A = -\oint_{\partial A}\Big(\overbrace{\vec{m}\circ\vec{v}}^{\text{convect.}} + \overbrace{p\overline{\overline{I}}}^{\text{pres.}} - \overbrace{\overline{\overline{\tau}}}^{\text{fri.}}\Big)\vec{n}\mathrm{d}s + \int_A \vec{F}^e\mathrm{d}A$$

- *Differential form:*

$$\frac{\partial\vec{m}(\vec{x},t)}{\partial t} + \nabla\cdot\big(\overbrace{\vec{m}\circ\vec{v}}^{\text{convect.}} + \overbrace{p\overline{\overline{I}}}^{\text{pres.}}\big) = \overbrace{\nabla\cdot\overline{\overline{\tau}}}^{\text{fric.}} + \vec{F}^e$$

Stress Deviator Tensor

- Deformation tensor: $(\mathrm{def}\ \vec{v})_{ij} = \frac{\partial v_j}{\partial x_i} + \frac{\partial v_i}{\partial x_j}$

- Stress tensor in Navier-Stokes equations:

$$\overline{\overline{\tau}} = \lambda \left(\nabla \cdot \vec{v}\right) \overline{\overline{I}} + \mu \cdot \mathrm{def}\ \vec{v}$$

λ volume viscosity

μ dynamic shear viscosity

Newtonian Fluids

- Newtonian fluid:
  - Viscosity **independent** of shear rate
  - Still may depend on thermodynamic quantities (often temperature)
- Non-Newtonian fluids:
  - Viscosity varies with shear rate
  - Rheology

Conservation of Energy

- *Conserved*: Energy density $e = \rho\varepsilon + \frac{\rho}{2}\vec{v}\cdot\vec{v} + \rho g h$
- *Changed by*:
  - Convection $\vec{f}^c = e \cdot \vec{v}$
  - Work of surface forces $\vec{f}^s = p \cdot \vec{v} - \overline{\overline{\tau}}\vec{v}$
  - Heat conduction $\vec{f}^h = -\kappa \nabla T$
- Possible work by volume forces; Heat sources (e.g. chemical reactions, radiation) $\vec{F}^e \cdot \vec{v} + Q$

Conservation of Energy

- *Integral form:*

conv. pres. fric. heat

$$\frac{\partial}{\partial t}\int_A e(\vec{x},t)\mathrm{d}A = -\oint_{\partial A}(e\cdot\vec{v} + p\cdot\vec{v} - \overline{\overline{\tau}}\vec{v} - \kappa\nabla T)\vec{n}\mathrm{d}s + \int_A(\vec{F}^e\cdot\vec{v} + Q)\mathrm{d}A$$

- *Differential form:*

$$\frac{\partial e(\vec{x},t)}{\partial t} + \nabla(e + p)\vec{v} = \nabla\cdot\left(\overline{\overline{\tau}}\vec{v}\right) + \nabla\cdot\left(\kappa\nabla T\right) + \vec{F}^e\cdot\vec{v} + Q$$

Equation of State

- Relation of thermodynamic quantities density, pressure and temperature

- Simplest thermodynamic model is the **ideal gas** assumption:

$$\frac{p}{\rho} = R \cdot T$$

R gas constant

Calorically Perfect Gas

- Specific heat capacity c_v assumed to be constant
- Direct proportional relation between inner energy and temperature: $\varepsilon = c_v \cdot T$

- Together with the ideal gas model:

$$\varepsilon = \frac{p}{\rho(\gamma - 1)}$$

with γ as ratio of specific heats

Real Gas

- Usually ideal gas sufficient
- More complex models required for
  - close to phase changes
  - close to critical points
  - high pressures
  - low temperatures
- Compressibility factor as measure

Real Gas Models

- Virial model: Series of perturbative terms
- Van der Waals: Most prominent 2 term model
- Redlich-Kwong: 2 term model often more accurate than van der Waals
- Many more of varying complexity

Compressible Navier-Stokes Equations

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

$$\frac{\partial \vec{m}(\vec{x}, t)}{\partial t} + \nabla \cdot (\vec{m} \circ \vec{v} + p\bar{\bar{I}}) = \nabla \cdot \bar{\bar{\tau}}$$

$$\frac{\partial e(\vec{x}, t)}{\partial t} + \nabla \cdot (e + p)\vec{v} = \nabla \cdot \bar{\bar{\tau}}\vec{v} + \nabla \cdot (\kappa \nabla T)$$

+ Equation of state
  - Perfect gas: $p = (\gamma - 1) \cdot \left(e - \frac{\rho}{2}|\vec{v}|^2\right)$

Image: game-icons.net, Lorc

Nondimensionalization

- Introduce suitable reference values
- Define all quantities in relation to reference values
- Useful for classification of flows
- Helps to limit value range

Reference Values

- Choose a characteristic length, pressure, density and velocity $L,\ p_{ref},\ \rho_{ref},\ v_{ref}$
- Accordingly you get a characteristic time scale, speed of sound and temperature

$$t_{ref} = \frac{L}{v_{ref}},\ c_{ref} = \sqrt{\gamma \frac{p_{ref}}{\rho_{ref}}},\ T_{ref} = \frac{p_{ref}}{R\rho_{ref}}$$

- Normalize all quantities with the references

Similarity Parameters

- Ratios of flow effects, experiments with the same parameters show same behavior

- **Mach number** $$Ma = \frac{v}{c}$$ $\frac{\text{Flow velocity}}{\text{Speed of sound}}$

- **Reynolds number** $$Re = \frac{\rho v L}{\mu}$$ $\frac{\text{Fictitious force}}{\text{Friction}}$

- **Prandtl number** $$Pr = \frac{\mu c_p}{\kappa}$$ $\frac{\text{Momentum diff.}}{\text{Thermal diff.}}$

Nondimensional Navier-Stokes Equations

- Similarity parameters of reference, perfect gas:

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

$$\frac{\partial \vec{m}(\vec{x},t)}{\partial t} + \nabla \cdot (\vec{m} \circ \vec{v} + \frac{p}{\gamma Ma^2} \overline{\overline{I}}) = \frac{\nabla \cdot \overline{\overline{\tau}}}{Re}$$

$$\frac{\partial e(\vec{x},t)}{\partial t} + \nabla \cdot (e + \frac{p}{\gamma Ma^2}) \vec{v} = \frac{1}{Re} \left(\nabla \cdot \overline{\overline{\tau}} \vec{v} + \frac{\Delta T}{(\gamma - 1) Ma^2 \cdot Pr} \right)$$

$$p = (\gamma - 1) \cdot \left(e - \frac{\rho}{2} |\vec{v}|^2 \right) \gamma Ma^2$$

Image: game-icons.net, Lorc

Other Similarity Parameters

- Depending on the problem
- Some examples:
  - Péclet number **Pe** (transport)
  - Froude number **Fr** (gravitation)
  - Richardson number **Ri** (weather)
  - Rayleigh number **Ra** (free convection)
  - Strouhal number **St** (vortex shedding)

Simplifications

- Two important simplifications often deployed:
  - Inviscous flows: Euler equations
    - Neglecting diffusive processes
  - Incompressible flows
    - Density independent of pressure
    - Infinite speed of sound

Simplification Overview

Compressible Navier-Stokes equations include friction and thermal conduction

hyperbolic - parabolic

$Re \to \infty$

Euler equations
Gas dynamics
hyperbolic

$Ma \to 0$

Incompressible Navier-Stokes equations
parabolic - elliptic

Flow Regimes

- Different classes of PDEs

➢ Different numerical methods

Image: game-icons.net, Lorc

Simplification to Euler Equations

Compressible Navier-Stokes equations include friction and thermal conduction

hyperbolic - parabolic

$Re \to \infty$

Euler equations
Gas dynamics
hyperbolic

$Ma \to 0$

Incompressible Navier-Stokes equations
parabolic - elliptic

Neglect Friction and Heat Transport

- Compressible Navier-Stokes -> Euler equations

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

$$\frac{\partial \vec{m}(\vec{x},t)}{\partial t} + \nabla \cdot (\vec{m} \circ \vec{v} + p\overline{\overline{I}}) = \nabla \cdot \overline{\overline{\tau}}$$

$$\frac{\partial e(\vec{x},t)}{\partial t} + \nabla \cdot (e + p)\vec{v} = \nabla \cdot \overline{\overline{\tau}}\vec{v} + \nabla \cdot (\kappa \nabla T)$$

Gas Dynamics: The Euler Equations

- Hyperbolic system (wave transport)

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

$$\frac{\partial \vec{m}(\vec{x},t)}{\partial t} + \nabla \cdot (\vec{m} \circ \vec{v} + p\overline{\overline{I}}) = 0$$

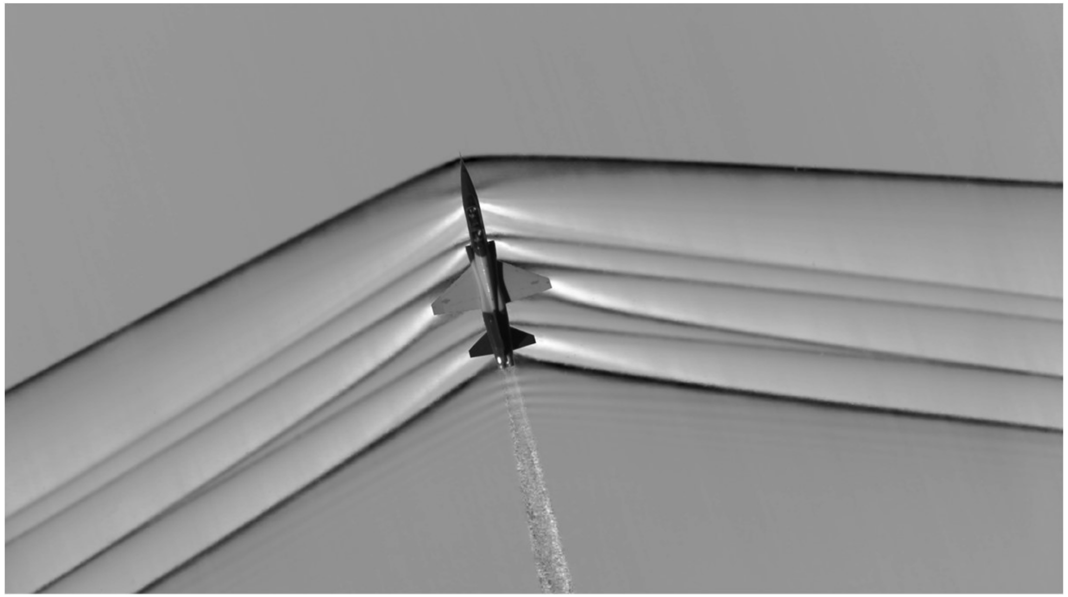
$$\frac{\partial e(\vec{x},t)}{\partial t} + \nabla (e + p)\vec{v} = 0$$

\+ Equation of state (usually ideal gas)

Image: game-icons.net, Lorc

Gas Dynamics

- Nonlinear transport problem
- State travels along characteristics
- Formation of discontinuities (shocks)



Schlieren image of supersonic aircraft with shock waves.

Image: NASA Photo

Vectorial Notation (1D, Perfect Gas)

- Gather state in one vector: $\vec{u}(x,t) = \begin{bmatrix} \rho(x,t) \\ m(x,t) \\ e(x,t) \end{bmatrix}$

- Also the flux:

$$\vec{f}(\vec{u}) = \begin{bmatrix} m \\ \frac{(3-\gamma)m^2}{2\rho} + (\gamma - 1)e \\ \frac{m}{\rho}\left(\gamma e + \frac{(1-\gamma)m^2}{2\rho}\right) \end{bmatrix}$$

- *(Equation of state for perfect gas in flux)*

Compact Notation of the System with Vectors

$$\frac{\partial \vec{u}(x,t)}{\partial t} + \frac{\partial \vec{f}(\vec{u})}{\partial x} = 0$$

- First order, nonlinear PDE system
- Conservative variables $\vec{u}$
- Compact notation shows structure of the PDEs

More Spatial Dimensions

- Space coordinate becomes a vector $\vec{x}$
- Momentum becomes a vector $\vec{m}$
  - (more components in the state vector)
- Get a flux for each spatial dimension

Compact Notation, Multiple Spatial Dimensions

- For *d* dimensions we have:

$$\frac{\partial \vec{u}(\vec{x},t)}{\partial t} + \sum_{i=1}^{d} \frac{\partial \vec{f_i}(\vec{u})}{\partial x_i} = 0$$

- For example in 2D, 2 fluxes with 4 components:

$$\vec{f_1}(\vec{u}) = \begin{bmatrix} m_1 \\ \frac{(3-\gamma)m_1^2}{2\rho} + (\gamma - 1)(e - \frac{m_2^2}{2\rho}) \\ \frac{m_1 \cdot m_2}{\rho} \\ \frac{m_1}{\rho}\left(\gamma e + \frac{(1-\gamma)(m_1^2+m_2^2)}{2\rho}\right) \end{bmatrix} \vec{f_2}(\vec{u}) = \begin{bmatrix} m_2 \\ \frac{m_2 \cdot m_1}{\rho} \\ \frac{(3-\gamma)m_2^2}{2\rho} + (\gamma - 1)(e - \frac{m_1^2}{2\rho}) \\ \frac{m_2}{\rho}\left(\gamma e + \frac{(1-\gamma)(m_1^2+m_2^2)}{2\rho}\right) \end{bmatrix}$$

Simplification To Incompressible

Compressible Navier-Stokes equations include friction and thermal conduction

hyperbolic - parabolic

$Re \to \infty$

Euler equations
Gas dynamics
hyperbolic

$Ma \to 0$

Incompressible Navier-Stokes equations
parabolic - elliptic

Neglect Density and Temperature Changes

- Compressible Navier-Stokes -> Incompressible

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

$$\frac{\partial \vec{m}(\vec{x},t)}{\partial t} + \nabla \cdot (\vec{m} \circ \vec{v} + p\overline{\overline{I}}) = \nabla \cdot \overline{\overline{\tau}}$$

$$\frac{\partial e(\vec{x},t)}{\partial t} + \nabla \cdot (e + p)\vec{v} = \nabla \cdot \overline{\overline{\tau}}\vec{v} + \nabla \cdot (\kappa \nabla T)$$

Divergence Free Flow

- Constant density:
  - One variable less
  - mass conservation reduces to divergence free constrained for the velocity field:

$$\nabla \vec{v} = 0$$

- Note: no time dependency in this equation

One Equation Less

- With $\nabla \vec{v} = 0$
- And constant temperature ($\nabla T = 0$)

➢ The energy balance does not provide any additional information

Incompressible Navier-Stokes Equations

- Parabolic – Elliptic system of PDEs:

$$\nabla \cdot \vec{v} = 0$$

$$\frac{\partial \vec{v}(\vec{x},t)}{\partial t} + \nabla \cdot \left(\vec{v} \circ \vec{v} + \frac{p}{\rho}\overline{\overline{I}}\right) = \nabla \cdot \frac{\overline{\overline{\tau}}}{\rho}$$

- Variables:

  Velocity $\vec{v}$

  Pressure p

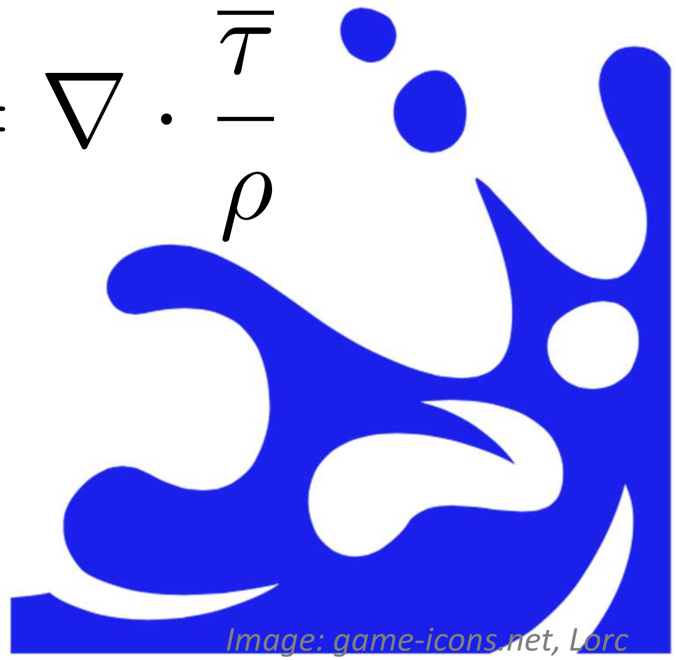


Image: game-icons.net, Lorc

Potential Flow

- Incompressible and inviscid
- Can use a scalar potential to describe the velocity field

Numerical Methods

- **Finite Differences**
- **Finite Volumes**
- **Finite Elements**
  - continuous
  - discontinuous
- Finite Points
- Smoothed Particle Hydrodynamics

- Lattice Boltzmann
- Pseudo-Spectral
- Boundary Elements
- Panel Method (potential flows)
- Vortex Lattice (potential flows)

Finite Differences

- Approximates differentials by difference quotients on a grid with point values
- Will be briefly discussed on Tuesday
- Solver using this scheme:
  – Overture (http://www.overtureframework.org/)

Finite Volume

- Utilizes an integral formulation with integral means in control volumina and the fluxes between those
- Will be discussed on Tuesday
- Solvers using this scheme:
  - OpenFOAM (dedicated course)
  - Code Saturne (https://www.code-saturne.org/cms/)
  - Gerris (http://gfs.sourceforge.net/wiki/index.php/Main_Page)

Finite Elements

- Utilizes functions in elements to represent the solution
- Will be discussed on Wednesday (continuous) and Thursday (discontinuous)
- Solvers using this scheme:
  - Elmer (https://www.csc.fi/web/elmer)
  - Nektar++ (https://www.nektar.info/)
  - Ateles (http://www.apes-suite.org/pages/ateles)

Finite Points

- Meshfree method based on scattered point values with a solution construction from a local point neighborhood
- Least-Square fitting of unknowns
- Interesting for moving/deforming boundary problems

Smoothed-Particle Hydrodynamics

- Meshless, lagrangian method: particles build the fluid and a kernel function describes the “range“ of the properties of the particle
- Especially interesting for free-surface flows
- Solvers implementing this scheme:
  - AQUAgpusph (http://canal.etsin.upm.es/aquagpusph/)
  - Pysph (https://pysph.readthedocs.io/en/latest/)
  - FLUIDS (http://fluids3.com/)

Lattice-Boltzmann

- Works on the Boltzmann equation with a discrete space
- Cellular automata on a mesoscopic level reproduce Navier-Stokes equations in a macroscopic view
- Solvers with this scheme:
  - Palabos (http://www.palabos.org/)
  - Musubi (http://www.apes-suite.org/pages/musubi)
  - OpenLB (http://www.openlb.net/)

(Pseudo)-Spectral

- Approximation of the solution by a function series
- Highly efficient for smooth problems
- Limitations by function choice an geometrical layout
- Example: http://dedalus-project.org/
- Spectral Element Method solver:
  - Nek5000 (https://nek5000.mcs.anl.gov/)

Boundary Elements

- Uses boundary values to define solution to integral equation
- Requires Green's function to be computable for the given problem
- Solvers for this scheme:
  - FastBEM (http://www.yijunliu.com/Software/)
  - Nemoh (https://lheea.ec-nantes.fr/logiciels-et-brevets/nemoh-presentation-192863.kjsp)

Panel Method

- Represents a potential flow by superposition of various singularities
- Singularities organized in panels to represent walls in the flow
- Solvers implementing this scheme:
  - XFOIL (http://web.mit.edu/drela/Public/web/xfoil/)
  - Panair (http://www.pdas.com/panair.html)
  - Q-Blade (http://www.q-blade.org/)

Vortex Lattice

- For potential flows
- Prandtl's lifting lines theory
- Model lifting surfaces by discrete vortex lines
- Surfaces discretized into panels with horseshoe vortices
- Implementation:
  - OpenVOGEL (https://sites.google.com/site/gahvogel/main)

Focus of This Course

- We will look at the „classical“ methods (FDM, FVM and FEM)
- We will use the batch system to run larger computations on a parallel HPC system
- We use Ateles as a solver and look at the workflow from mesh generation to visualization