Scientific Computing I

Module 9: Case Study – Computational Fluid Dynamics

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Fluid mechanics as a Discipline

Prominent discipline of application for numerical simulations:

- *experimental* fluid mechanics: wind tunnel studies, laser Doppler anemometry, hot wire techniques, ...
- *theoretical* fluid mechanics: investigations concerning the derivation of turbulence models, e.g.
- *computational* fluid mechanics (CFD): numerical simulations

Many fields of application:

- aerodynamics: aircraft design, car design,. . .
- thermodynamics: heating, cooling,. . .
- process engineering: combustion
- material science: crystal growth
- astrophysics: accretion disks
- geophysics: mantle convection, climate/weather prediction, tsunami simulation, . . .

Part I: Modelling

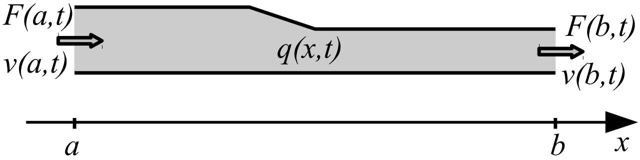
Fluids and Flows

- *ideal* or *real* fluids
  $\rightarrow$ "ideal": no resistance to tangential forces
- *compressible* or *incompressible* fluids
  $\rightarrow$ volume change of gases (vs. liquids?) under pressure
- *viscous* or *inviscid* fluids
  $\rightarrow$ think of the different characteristics of honey and water
- *Newtonian* and *non-Newtonian* fluids
  $\rightarrow$ the latter may show some elastic behaviour (e.g. in liquids with particles like blood)
- *laminar* or *turbulent* flows
  $\rightarrow$ turbulence: unsteady, 3D, high vorticity, vortices of different scales, high transport of energy between scales

Mathematical Models for CFD

- typically: all require different models
- our focus here: incompressible, viscous, Newtonian, laminar
  - $\rightarrow$ **incompressible Navier-Stokes Equations**
  - $\rightarrow$ **Shallow Water Equations**
- starting point: continuum mechanics
  - $\rightarrow$ macroscopic properties (pressure, density, velocity field) in contrast to stochastic or micro-/mesoscopic approaches (lattice Boltzman method, e.g.)
- relies on basic conservation laws (remember the heat equation): conservation of *mass* and *momentum* (and energy)
- additionally: slight focus on *Finite Volume Methods*

Advection Equation



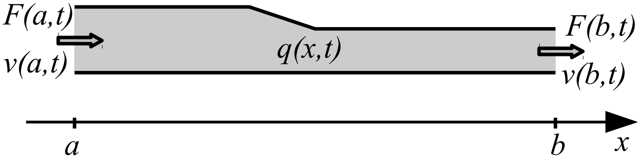
Conservation of some quantity q in a fluid domain $\Omega = [a, b]$ with given velocity $v(x, t)$:

- total amount/mass of q in $\Omega = [a, b]$ is given by $\int_a^b q(x, t)\,\mathrm{dx}$
- change of mass can only happen due to in-/outflow at a and b:

$$\frac{\partial}{\partial t} \int_a^b q(x, t)\,\mathrm{dx} = F(a, t) - F(b, t) = -F(x, t)\Big|_a^b = -\int_a^b \frac{\partial}{\partial x} F(x, t)\,\mathrm{dx}$$

- note: $F(a, t)$ and $-F(b, t)$ denote an inflow into the domain Ω

Advection Equation (2)



Consider

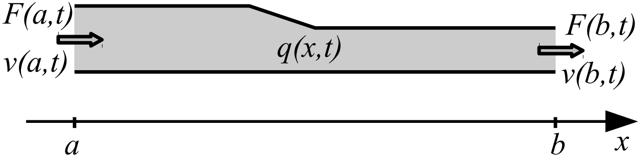
- flux function $F(x,t)$ depends on velocity $v(x,t)$, density $q(x,t)$ and the pipe's cross-sectional area $A(x)$:

$$F(x,t) = A(x)v(x,t)q(x,t)$$

- for simplicity, we set $A(x) = 1$, and obtain:

$$\frac{\partial}{\partial t}\int_a^b q(x,t)\,\mathrm{dx} = -\int_a^b \frac{\partial}{\partial x}F(x,t)\,\mathrm{dx} = -\int_a^b \frac{\partial}{\partial x}\big(v(x,t)q(x,t)\big)\,\mathrm{dx}$$

Advection Equation (3)



Advection Equation:

- for smooth functions, we may write:

$$\int_a^b \frac{\partial}{\partial t} q(x,t)\,\mathrm{dx} = \frac{\partial}{\partial t}\int_a^b q(x,t)\,\mathrm{dx} = -\int_a^b \frac{\partial}{\partial x}\big(v(x,t)q(x,t)\big)\,\mathrm{dx}$$

- as this equation has to hold for any $\Omega = [a,b]$, we demand:

$$\frac{\partial}{\partial t} q(x,t) = -\frac{\partial}{\partial x}\big(v(x,t)q(x,t)\big) \quad \text{or short:} \quad q_t + (vq)_x = 0$$

Advection and Diffusion

Diffusion

- even in a fluid at rest, an inhomogeneous density $q(x,t)$ will slowly change towards a uniform density q_0 due to molecular processes $\rightarrow$ **diffusion**
- *Fick's law of diffusion*: resulting flux is prop. to gradient of q

$$-F_{\text{diff}} = \beta q_x$$

- to model both advection and diffusion, we have $-F = -vq + \beta q_x$, and thus

$$q_t + (vq)_x = \beta q_{xx}$$

"advection-diffusion equation"

- special case $q_t = 0$:

$$-\beta q_{xx} + (vq)_x = 0$$

1D Euler Equations

- with our quantity q being the mass density ρ, we obtain an equation for the **conservation of mass**:

$$\rho_t + (v\rho)_x = 0 \tag{1}$$

- another conservation property is that of momentum ρv; here, the flux term includes the pressure p:

$$F_{\text{mom}} = \rho v^2 + p$$

- thus, we obtain as equation for the **conservation of momentum**:

$$(\rho v)_t + (\rho v^2 + p)_x = 0 \tag{2}$$

- we obtain a system of two PDEs, the **1D Euler Equations** (1)–(2)
- to close the system, we need a relation between ρ and p (using the ideal gas law, e.g.)
- we might add an equation for temperature (derived from the conservation of internal energy)

Conservation Laws in Higher Dimensions

- in 2D, a conservation law for quantity q takes the form:

$$q_t + F(q)_x + G(q)_y = 0$$

- or similar in 3D:

$$q_t + F(q)_x + G(q)_y + H(q)_z = 0$$

- for advection, the flux functions are

$$F(q) = uq \qquad G(q) = vq \qquad H(q) = wq$$

  where u, v, w are the velocity components in the three space dimensions x, y, z
- hence, for 2D we obtain a conservation law such as

$$q_t + (uq)_x + (vq)_y = 0$$

2D Euler Equations

- in 2D, with velocity components $u(x, y, t)$ and $v(x, y, t)$ the equation for **conservation of mass** reads:

$$\rho_t + (\rho u)_x + (\rho v)_y = 0$$

- similar, the two equation for **conservation of momentum** are:

$$(\rho u)_t + (\rho u^2 + p)_x + (\rho uv)_y = 0$$
$$(\rho v)_t + (\rho uv)_x + (\rho v^2 + p)_y = 0$$

- again, we assume constant temperature, and we need a relation between ρ and p to close the system
- the Euler equations model an inviscid (ideal) fluid
- we also neglect additional source terms, such as for gravity forces, etc.

Navier-Stokes Equations

- mass conservation/continuity equation is the same as for the Euler equations:

$$\rho_t + (\rho u)_x + (\rho v)_y + (\rho w)_z = 0$$

or, written in vector notation:

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho \vec{u}) = 0, \qquad \nabla \cdot \vec{u} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}$$

- momentum conservation/momentum equations

$$\frac{\partial}{\partial t}(\rho \vec{u}) + \nabla \cdot (\vec{u} \otimes \rho \vec{u}) - \nabla \sigma - f = 0$$

- with σ being the *stress tensor*, which includes the pressure p and viscous forces: $\sigma = -pI + \ldots$
- f models external (volume) forces (gravity, e.g.)

Navier-Stokes Equations

Conservation and Convection Form

- the equations for mass and momentum, on the previous slide, are given in the so-called **conservation form**
- with the equations

  $$\nabla\cdot(\rho\vec{u}) = \vec{u}\cdot\nabla\rho+\rho\nabla\cdot\vec{u} \quad \text{and} \quad \nabla\cdot(\rho\vec{u}\otimes\vec{u}) = \vec{u}\big(\nabla\cdot(\rho\vec{u})\big)+(\rho\vec{u}\cdot\nabla)\vec{u},$$

  we obtain:

  $$\frac{\partial}{\partial t}\rho + \vec{u}\cdot\nabla\rho + \rho\nabla\cdot\vec{u} = 0$$

  $$\frac{\partial}{\partial t}(\rho\vec{u}) + \vec{u}\big(\nabla\cdot(\rho\vec{u})\big) + (\rho\vec{u}\cdot\nabla)\vec{u} - \nabla\sigma - f = 0$$

- with $\frac{\partial}{\partial t}(\rho\vec{u}) = \rho\frac{\partial}{\partial t}\vec{u} + \vec{u}\frac{\partial}{\partial t}\rho$

  and applying $\vec{u}\frac{\partial}{\partial t}\rho + \vec{u}\big(\nabla\cdot(\rho\vec{u})\big) = \vec{u}\big(\frac{\partial}{\partial t}\rho + \nabla\cdot(\rho\vec{u})\big) = 0$,

  we obtain for the momentum equation in **convection form**

  $$\rho\left(\frac{\partial}{\partial t}\vec{u} + (\vec{u}\cdot\nabla)\vec{u}\right) - \nabla\sigma - f = 0$$

Navier-Stokes Equations

Incompressible Equations

- in the convection form

$$\frac{\partial}{\partial t}\rho + \vec{u} \cdot \nabla \rho + \rho \nabla \cdot \vec{u} = 0$$

$$\rho \left(\frac{\partial}{\partial t}\vec{u} + (\vec{u} \cdot \nabla)\vec{u} \right) - \nabla \sigma - f = 0$$

we assume that the density ρ is constant: $\frac{\partial}{\partial t}\rho = 0$, $\nabla \rho = 0$

- we obtain obtain the **incompressible Navier-Stokes equations**:

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

$$\rho \left(\frac{\partial}{\partial t}\vec{u} + (\vec{u} \cdot \nabla)\vec{u} \right) - \nabla \sigma - f = 0$$

- “incompressible”: the density does not change due to pressure or temperature, e.g.

Viscous Forces

Open question: stress tensor σ

- σ includes pressure p and viscosity tensor τ: $\sigma = -pI + \tau$
- *Newtonian* fluids: viscous stresses proportional to the strain rate (first derivatives)
- isotropic, **incompressible** fluids, Stokes assumption (no volume viscosity), then $\nabla\sigma = -\nabla p + \mu\Delta\vec{u}$
- μ the dynamic viscosity

Viscous Forces

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- isotropic, **incompressible** fluids, Stokes assumption (no volume viscosity), then $\nabla\sigma = -\nabla p + \mu\Delta\vec{u}$
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Incompressible Navier-Stokes equations:

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

$$\rho\left(\frac{\partial}{\partial t}\vec{u} + (\vec{u}\cdot\nabla)\vec{u}\right) = -\nabla p + \mu\Delta\vec{u} + f$$

Dynamic Similarity of Flows

Dimensionless Form of the Navier-Stokes Equations

- we scale our unknowns to typical length scale L and velocity u_∞:

$$x \to \frac{x}{L} \qquad t \to \frac{u_\infty t}{L} \qquad u \to \frac{u}{u_\infty} \qquad p \to \frac{p - p_\infty}{\rho u_\infty^2}$$

- and obtain the dimensionless form of the Navier-Stokes equations:

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

$$\frac{\partial}{\partial t}\vec{u} + (\vec{u} \cdot \nabla)\vec{u} = -\nabla p + \frac{1}{\text{Re}}\Delta \vec{u} + f$$

introducing the **Reynolds number** $\text{Re} := \dfrac{\rho u_\infty L}{\mu}$

- important corollary: flows with the same Reynolds number will show the same behaviour

Boundary Conditions (here only velocity)

- **no-slip:** the fluid can not penetrate the wall and sticks to it
$$\vec{u} = 0.$$
- **free-slip:** the fluid can not penetrate the wall but does not stick to it
$$u_{\vec{n}} = 0, \frac{\partial \vec{u}_{\|}}{\partial \vec{n}} = 0.$$
- **inflow:** both tangential and normal velocity components are prescribed
$$\vec{u} = \vec{u}_{\text{inflow}}.$$
- **outflow:** should be “do nothing”; simple option: all velocity components do not change in normal direction
$$\frac{\partial \vec{u}}{\partial \vec{n}} = 0.$$
- **periodic:** same velocity and pressure at inlet and outlet
$$\vec{u}_{\text{in}} = \vec{u}_{\text{out}}.$$