Mathematical modelling in science and engineering

Lecture 7 CFD and thermodynamics

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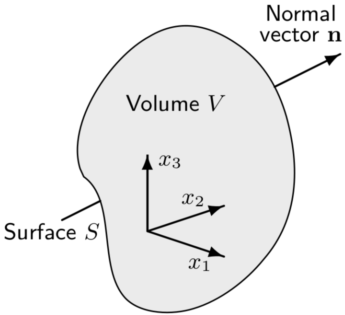
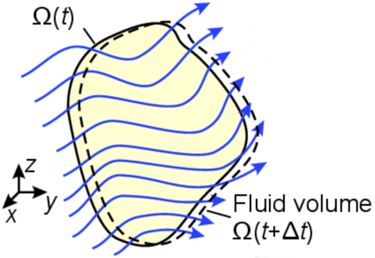
Derivation of fundamental equations in mechanics and thermodynamics

The setting for the derivation of fundamental equations in mechanics and thermodynamics in 2D and 3D





The conservation of mass principle – mass balance

Mass is neither created nor destroyed

- the rate of change of mass inside any domain must be equal to the mass flux through the boundary of the domain:

$$\frac{d}{dt}\int_{\Omega} \rho dV = - \int_{\partial\Omega} \rho v_i n_i dS$$

where:

- $\rho(\mathbf{x}, t)$ – density at time t and point $\mathbf{x} \in \Omega$,
- $\mathbf{v}(\mathbf{x}, t)$ – velocity,
- $\mathbf{n}$ – the unit outward normal to $\partial\Omega$

After applying the divergence theorem and taking into account that the equation holds for any domain Ω we arrive at the differential equation

The continuity equation (mass balance)

$$\frac{\partial \rho}{\partial t} + (\rho v_i)_{,i} = 0$$

The conservation of momentum principle

Newton's second law of mechanics

- the rate of change of momentum of a group of particles is equal to the sum of all forces exerted on this group

$$\frac{d}{dt}\int_{\Omega_t} \rho v_j dV = \int_{\partial\Omega_t} \sigma_{ji} n_i dS + \int_{\Omega_t} b_j dV$$

where

- Ω_t – portion of space occupied by the group of particles
  - Ω_t may vary in time
- $\boldsymbol{\sigma}$ – stress tensor, b_j – body forces

The transport theorem

$$\frac{d}{dt}\int_{\Omega_t} f dV = \int_{\Omega_t} \left(\frac{\partial f}{\partial t} + (f v_i)_{,i} \right) dV$$

valid for any smooth function $f(\mathbf{x}, t)$

The transport theorem and the momentum balance

Material assumptions (constitutive equations):

- stress tensor σ_{ji} symmetric due to the conservation of angular momentum
- stresses split according to the formula (δ_{ji} – Kronecker's delta):

$$\sigma_{ji} = -p\delta_{ji} + \tau_{ji}$$

  - p – thermodynamic pressure as isotropic normal stresses $p = -\frac{1}{3}\sigma_{ii}$
  - τ_{ji} – viscous stresses
    - isotropic Newtonian fluid, viscous stresses proportional to the rate of change of deformation tensor (gradient of velocity tensor), $\tau_{ji} = \mu(v_{i,j} + v_{j,i}) + \lambda\delta_{ji}v_{k,k}$
    - no volume viscosity (Stokes hypothesis, $\tau_{ii} = 0$), $\tau_{ji} \approx \mu(v_{i,j} + v_{j,i} - \frac{2}{3}\delta_{ji}v_{k,k})$

Assuming the above constitutive equations and applying the transport theorem together with the divergence theorem to the momentum balance leads to:

Momentum equation

$$\frac{\partial(\rho v_j)}{\partial t} + (\rho v_j v_i)_{,i} + p_{,i} - \tau_{ji,i} = b_j$$

Thermodynamic considerations

Basic principles

- the principle of energy conservation, energy balance:
  - specific total energy (energy per unit volume): $e = e_I + e_K + e_p$
  - specific internal energy, e_I, expressed in specific forms for different materials and processes
  - specific kinetic energy, $e_K = \frac{1}{2} v_i v_i$
  - specific potential energy, e_P, possible for external force fields (further neglected)
- the first law of thermodynamics (general statement): $\Delta U = Q - W$
  - the change in internal energy ΔU of a system
  - the amount of heat supplied to the system Q
  - the work done by the system W
- the first law of thermodynamics (in practical calculations):
  - the expression for specific internal energy: $de_I = Tds - pdV$
    - T – temperature, s – entropy, p – pressure, $V = \frac{1}{\rho}$ – volume

Thermodynamic considerations

Constitutive equations

- ideal gas law: $\frac{pV}{T} = const$
  - for practical calculations: $e_I = \frac{p}{(\gamma-1)\rho} = c_V T$
  - heat capacity ratio $\gamma = \frac{c_p}{c_V}$
  - specific heat capacities:
    - at constant volume, $c_V = \left(\frac{\partial Q}{\partial T}\right)_{V=const}$
    - at constant pressure, $c_p = \left(\frac{\partial Q}{\partial T}\right)_{p=const}$
  - the speed of sound c, $c^2 = \frac{\gamma p}{\rho}$
- heat flux q_i
  - Fourier's law: $q_i = -\kappa T_{,i}$
  - κ - the coefficient of thermal conductivity
- $\mu = \frac{1.45\, T^{\frac{3}{2}}}{T+110} \cdot 10^{-6}$ – Sutherland's law for viscosity as function of temperature

The conservation of energy principle

The energy balance

- the rate of change of the total energy for a group of particles is equal to the rate at which work is done by the external forces plus an explicit inflow of energy through the boundary

$$\frac{d}{dt}\int_{\Omega_t}(\rho e)dV = -\int_{\partial\Omega_t} v_j(p\delta_{ji} - \tau_{ji})n_i dS - \int_{\partial\Omega_t} q_i n_i dS$$

Additional terms possible for e.g.

- heat sources
- body forces

The standard procedure comprised of applying the transport and the divergence theorems leads to :

Energy balance equation

$$\frac{\partial(\rho e)}{\partial t} + ((\rho e + p)v_i - \tau_{ji}v_j + q_i)_{,i} = 0$$

Compressible fluid flow equations in conservative form

The equations for the three conservation principles in vector form

$$\begin{pmatrix} \rho \\ \rho v_j \\ \rho e \end{pmatrix}_{,t} + \begin{pmatrix} \rho v_i \\ \rho v_i v_j + p\delta_{ij} - \tau_{ij} \\ (\rho e + p)v_i - \tau_{ij}v_j + q_i \end{pmatrix}_{,i} = 0$$

Defining:

- $\boldsymbol{U} = (\rho, \rho v_j, \rho e)^T$ - vector of conservation variables
- $\boldsymbol{f}_i^E = (\rho v_i, \rho v_i v_j + p\delta_{ij}, (\rho e + p)v_i)^T$ – vector of Eulerian (inviscid) fluxes
- $\boldsymbol{f}_i^\mu = (0, \tau_{ij}, \tau_{ij}v_j - q_i)^T$ - vector of viscous and heat fluxes

leads to:

The Navier-Stokes equations of compressible fluid flow

$$\boldsymbol{U}(\boldsymbol{x}, t)_{,t} + \boldsymbol{f}_i^E(\boldsymbol{U})_{,i} = \boldsymbol{f}_i^\mu(\boldsymbol{U}, \nabla \boldsymbol{U})_{,i}$$

Compressible fluid flow equations

Nondimensional form of the compressible Navier-Stokes equations and the similarity of flows

- definitions of non-dimensional quantities (based on constant reference quantities with $_\infty$ subscript)

$$\rho' = \frac{\rho}{\rho_\infty}, \qquad p' = \frac{p}{p_\infty}, \qquad v_i' = \frac{v_i}{v_\infty}$$

- reference length L characterizing the problem (e.g. the length of airplane, the width of channel, etc.)
- the change of variables:

$$x_i' = \frac{x_i}{L} \quad \text{implying} \quad (\cdot)_{,i} = \frac{\partial(\cdot)}{\partial x_i} = \frac{\partial(\cdot)}{\partial x_i'}\frac{1}{L} = \frac{1}{L}(\cdot)_{,i'}$$

and

$$t' = \frac{v_\infty}{L}t \quad \text{– a new time scale implying} \quad (\cdot)_{,t} = \frac{v_\infty}{L}(\cdot)_{,t'}$$

Compressible fluid flow equations

Nondimensional form of the compressible Navier-Stokes equations and the similarity of flows

- After a few transformations the Navier-Stokes equations expressed in terms of the new nondimensional variables look as follows:

$$\rho'_{,t'} + (\rho' v'_i)_{,i'} = 0$$

$$(\rho' v'_j)_{,t'} + (\rho' v'_i v'_j + \frac{p_\infty}{\rho_\infty v_\infty^2} p' \delta_{ij})_{,i'} = \frac{1}{L \rho_\infty v_\infty} \left(\mu (v'_{i,j'} + v'_{j,i'}) + \lambda \delta_{ij} v'_{k,k'} \right)_{,i'}$$

$$\frac{p_\infty}{\rho_\infty v_\infty^2} \frac{1}{\gamma - 1} p'_{,t'} + (\rho' e'_K)_{,t'} + \left((\frac{p_\infty}{\rho_\infty v_\infty^2} \frac{\gamma}{\gamma - 1} p' + \rho' e'_K) v'_i \right)_{,i'} =$$
$$\frac{1}{L \rho_\infty v_\infty} \left(\mu v'_k (v'_{i,k'} + v'_{k,i'}) + \lambda v'_i v'_{k,k'} + \frac{1}{\gamma - 1} \frac{\kappa}{c_V} \frac{p_\infty}{\rho_\infty v_\infty^2} (\frac{p'}{\rho'})_{,i'} \right)_{,i'}$$

Compressible fluid flow equations

Nondimensional form of the compressible Navier-Stokes equations and the similarity of flows

- there are only four coefficients in the nondimensional compressible Navier-Stokes equations, all defined in terms of reference quantities
- the coefficients can be expressed using special numbers used in fluid dynamics:
  - Mach number
  $$M_\infty^2 = \frac{v_\infty^2}{c_\infty^2} = \frac{\rho_\infty v_\infty^2}{\gamma p_\infty}$$
  - Reynolds number
  $$Re_\infty = \frac{L \rho_\infty v_\infty}{\mu}$$
  - Prandtl number
  $$Pr = \frac{\gamma c_V \mu}{\kappa}$$
- the special numbers are usually defined using the values on the inflow part of the boundary (so called "free stream" values)

Compressible fluid flow equations

Nondimensional form of the compressible Navier-Stokes equations and the similarity of flows

- after substituting the relations for coefficients, the final form of the nondimensional Navier-Stokes equations is obtained:

$$\rho_{,t} + (\rho v_i)_{,i} = 0$$

$$(\rho v_j)_{,t} + \left(\rho v_i v_j + \frac{1}{\gamma M_\infty^2} p \delta_{ij}\right)_{,i} = \frac{1}{Re_\infty}\left(v_{i,j} + v_{j,i} - \frac{2}{3}\delta_{ij} v_{k,k}\right)_{,i}$$

$$\frac{1}{\gamma M_\infty^2}(\rho e_I)_{,t} + (\rho e_K)_{,t} + \left(\left(\frac{1}{\gamma M_\infty^2}\rho e_I + \rho e_K + \frac{1}{\gamma M_\infty^2} p\right) v_i\right)_{,i} =$$

$$\frac{1}{Re_\infty}\left(v_k (v_{i,k} + v_{k,i}) - \frac{2}{3} v_i v_{k,k} + \frac{1}{Pr M_\infty^2}\left(\frac{p}{\rho}\right)_{,i}\right)_{,i}$$

Compressible fluid flow equations

Nondimensional form of the compressible Navier-Stokes equations and the similarity of flows

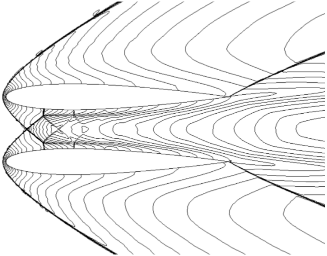
- the same change of variables applied to an initial and boundary conditions leads to an initial condition and boundary conditions for the nondimensional variables.
- a solution to the non-dimensional equations, satisfying also the nondimensional initial and boundary conditions, is similar (i.e. can be obtained by the simple scalings defined previously) to any flow which:
  - has the same shape of its domain as the nondimensional flow
  - has the same parameters γ, M_∞, Re_∞ and Pr
  - its initial and boundary conditions can be obtained by the scaling from the initial and boundary conditions of the nondimensional flow
  - has the same time scale as the nondimensional flow (if not, additional scaling in time has to be performed)
- two flows similar to the same nondimensional flow are similar to each other.

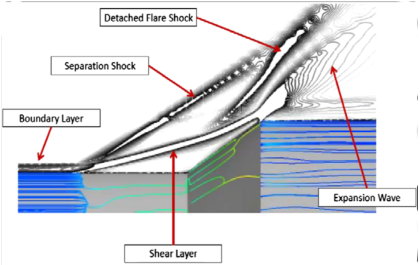
Different models for fluid flow

- Compressible Navier-Stokes equations are the most general model of fluid flow
- For many flows, especially for liquids but also for gases at relatively low speeds, the equations become difficult to solve due to the terms with the coefficient $\frac{1}{M_\infty^2} = \frac{c_\infty^2}{v_\infty^2}$, that becomes very large
  - it is possible for such cases to develop a set of approximate equations, so called incompressible Navier-Stokes equations
- Compressible Navier-Stokes equations describe the fluids as continuum objects (without going to atomic level), but still the range of length scales is very large
  - for applications in aerodynamics the length of an object (e.g. aircraft) can be of order 10^1 meters, while the sizes of flow features (e.g. the width of shock waves) may be as small as several hundreds nanometers (order 10^{-7}m)
  - with today's computing power it is impossible in most of practical applications to discretize the compressible Navier-Stokes equations on meshes that would guarantee the full resolution of all flow features
  - the size of grid cells or elements would have to be smaller than flow features sizes

Different models for fluid flow

- The full set of compressible (or incompressible) Navier-Stokes equations on meshes that guarantee the resolution of all flow features can be solved only in special situations
- In order to determine large scale flow features (such as the position of shock waves) the viscous effects can be neglected leading to the Euler equations of inviscid fluid flow (with Mach number as the only parameter)

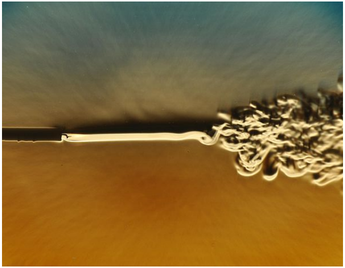


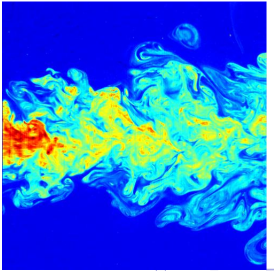


- Euler equations neglect e.g. the effect of boundary layers and their impact on flow features

Different models for fluid flow

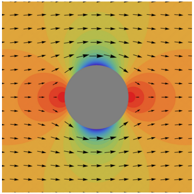
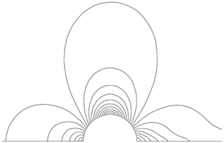
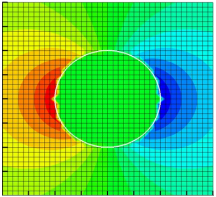
- In order to take into account the effects of small, unresolved flow scales (e.g. turbulent, chaotic motion of fluid particles) the unknowns in the Navier-Stokes equations (compressible or incompressible) can be represented as the sum of (resolved) averaged values and (unresolved) fluctuations, that lead to the standard Navier-Stokes equations for the averaged quantities coupled with special equations for fluctuations
  - the turbulent effects are important for high Reynolds number flows
  - the equations for fluctuations of unknowns are usually discretized using sets of additional assumptions that lead to different turbulence models





Different models for fluid flow

- The Mach number measures the importance of compressibility for the character of the flow
  - for low Mach number inviscid flows (compressible and incompressible) the character of the flow can be approximately determined by the solution of the equation formulated for the velocity potential (potential flow, below left)
- The Reynolds number measures the ratio of inertial forces to viscous forces
  - for low Reynolds number flows the effects of inertia forces can be neglected, leading to the Stokes flow (creeping flow, below right)

- etc., etc., etc. - there are many models in CFD (Computational Fluid Dynamics) developed for specific types of flows and specific fluids

Finite volume method

Finite volume method (FVM) is a method for finding approximate solutions to partial differential equations, especially PDEs formulated as conservation laws

- The idea of the finite volume method for compressible Euler equations:

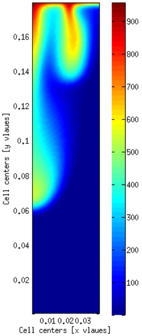
$$\boldsymbol{U}(\boldsymbol{x},t)_{,t} + \boldsymbol{f}_i^E(\boldsymbol{U})_{,i} = 0$$

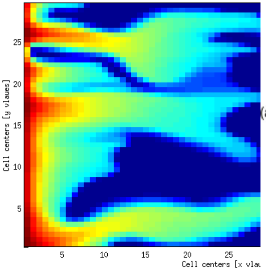
  - discretization of the computational domain into cells (control volumes) – the cells can be either simple (as finite elements) or can be constructed as Voronoi diagrams based on standard meshes
  - integration of the PDEs over the computational domain, splitting the global integral into the sum of integrals over each cell, the application of the Green-Gauss-Ostrogradski theorem for fluxes – the exchange of volume integrals to surface integrals

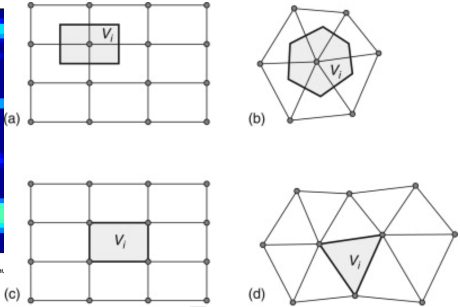
$$\int_{V_c} \boldsymbol{U}(\boldsymbol{x},t)_{,t} dV = -\int_{\partial V_c} \boldsymbol{f}_i^E(\boldsymbol{U}) n_i dS$$

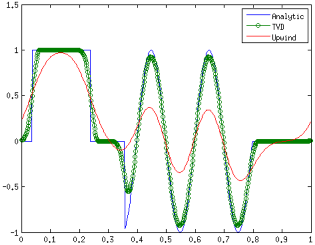
  - the application of special techniques for calculating approximations to integrals of fluxes based on discrete values and for updating these values based on calculated fluxes

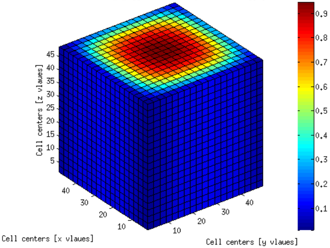
Finite volume method











Finite volume method

- Based on suitable extensions of the basic scheme, the FVM can be applied to inviscid and viscous, compressible and incompressible flows, as well as different than fluid dynamics application areas
- The main advantage of the finite volume method is its conservative character, related to the direct application of conservative principles for each cell
- Moreover, due to special methods for constructing flux approximations, the FVM, for many problems, can eliminate oscillations of solutions in the regions of rapid gradient changes (such as e.g. shocks)
- The FVM does not introduce higher order cells – the values are associated either with cells or mesh vertices
- *h*-adaptivity and remeshing (usually called Adaptive Mesh Refinement (AMR) techiques) are often applied to locally increase accuracy of solutions
- The FVM method for time dependent problems can use explicit or implicit time integration schemes
- In practical applications FVM is today the most popular discretization technique in computational fluid dynamics (CFD)

Incompressible fluid flow – the Navier-Stokes equations

Derivation of the Navier-Stokes equations for incompressible fluid flow:

- due to incompressibility density is assumed to be constant
  - $\rho = \rho_0 = const$, the volume for a group of particles remains the same
  - the terms in the fluid flow equations with the gradient of density vanish
  - the analysis of the thermodynamic relations indicates that the speed of sound is infinite for incompressible media
  - therefore the changes in the pressure field propagate immediately throughout the whole computational domain
  - although the model of incompressible flow is purely theoretical (there are no fully incompressible materials) the approximations to the real flows based on the model can be relatively easily computed and have great practical importance

Mass balance (the continuity equation) for incompressible fluid flow

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

Incompressible fluid flow – the Navier-Stokes equations

Derivation of the Navier-Stokes equations for incompressible fluid flow:

- since the density is constant, the pressure becomes the function of velocity field only, not the thermodynamic quantity
- the continuity and momentum equations decouple from the energy equation (the pressure and velocity fields do not depend on the temperature field)

Momentum balance for incompressible fluid flow

$$\rho_0\left(\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v} \cdot \boldsymbol{\nabla})\boldsymbol{v}\right) - \mu \boldsymbol{\nabla}^2 \boldsymbol{v} + \boldsymbol{\nabla} p \quad = \quad \boldsymbol{f}$$

Historically, the Navier-Stokes equations denoted the equations for fluid velocities, derived form the momentum balance. The name is also used for the whole system that must solved to find the velocity field in fluid flow and, hence, denotes the coupled equations for mass, momentum and energy balance for compressible flows and coupled equations for mass and momentum balance for incompressible flows

Incompressible fluid flow – the Navier-Stokes equations

Derivation of the Navier-Stokes equations for incompressible fluid flow:

- the Navier-Stokes equations assume the viscous stress tensor for the Newtonian incompressible fluid in the form:
  - $\tau_{ij} = \mu(v_{i,j} + v_{j,i})$
- usually the system is closed with the typical boundary conditions

Boundary conditions for incompressible fluid flow

$$\begin{aligned} \boldsymbol{v} &= \hat{\boldsymbol{v}}_0 \quad \text{on } \Gamma_D \\ (\mu \boldsymbol{\nabla} \boldsymbol{v})\boldsymbol{n} - p\boldsymbol{n} &= \boldsymbol{g} \quad \text{on } \Gamma_N \end{aligned}$$

- in the so called Boussinesq approximation for the buoyancy driven flows, the density in the momentum balance may be treated as linear function of the temperature
  - e.g. $\rho = \rho_0 + \Delta\rho(T) = \rho_0 - \alpha\rho_0(T - T_0)$
  - this approximation is used for modifying the body force due to gravity: $\boldsymbol{f} = \rho_0 \mathbf{g}\left(1 - \alpha(T - T_0)\right)$

Energy equation for incompressible fluid flow

- the energy balance equation formulated for the total energy $e = e_I + e_K$

$$\left(\rho(e_I + \frac{1}{2}v_j v_j)\right)_{,t} + \left((\rho(e_I + \frac{1}{2}v_j v_j) + p)v_i - \tau_{ij}v_j + q_i\right)_{,i} = 0$$

  can be transformed to the equation for the internal energy alone (by using the momentum balance to eliminate the mechanical energy $e_K = \frac{1}{2}v_j v_j$ from the equation):

$$(\rho e_I)_{,t} + (\rho e_I v_i)_{,i} + p v_{i,i} - \tau_{ij} v_{i,j} + q_{i,i} = 0$$

- the assumption of incompressibility leads to further simplifications of the model:

$$\rho c_p \left(\frac{\partial T}{\partial t} + T_{,i} v_i\right) - (\kappa T_{,i})_{,i} = 0$$

  due to the fact that: $v_{i,i} = 0$, $c_p = c_V = const$, $e_I = c_V T$, $q_i = -\kappa T_{,i}$ and $\tau_{ij} v_{i,j}$ (heat produced by fluid viscosity) is small and can be neglected

Energy equation for incompressible fluid flow

Convective heat transfer equation

$$\rho c \left(\frac{\partial T}{\partial t} + \boldsymbol{v} \cdot \boldsymbol{\nabla} T \right) - \boldsymbol{\nabla} \cdot (\kappa \boldsymbol{\nabla} T) = s$$

- temperature distribution depends on the velocity field
- velocity and pressure fields do not depend on the temperature field
  - the exception is the Bussinesq approximation with gravity causing hotter fluid to move up and the cooler fluid to move down