Introduction to Computational Fluid Dynamics

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Graduate course

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1 Principles and equations of Fluid Mechanics

1.1 Continuous media

- The continuum hypothesis.
- What is a material point?
- The Lagrangian frame.
- The Eulerian frame.

1.2 Cartesian vectors and tensors

We assume $\{x_1, x_2, x_3\}$ to be Cartesian coordinates, with

$$\breve{e}^{(1)}, \quad \breve{e}^{(2)}, \quad \breve{e}^{(3)} \tag{1.1}$$

the Cartesian basis of vectors.

<u>Vector field:</u>

$$\mathbf{u}(\mathbf{x}, t) = \sum_i u_i(\mathbf{x}, t)\, \breve{e}^{(i)} \tag{1.2}$$

<u>Gradient:</u>

$$\nabla\varphi = \sum_i \frac{\partial\varphi}{\partial x_i}\breve{e}^{(i)} = \varphi_{,i}\, \breve{e}^{(i)} \tag{1.3}$$

$$\underline{\nabla\varphi} = (\varphi_{,1}, \varphi_{,2}, \varphi_{,3})^T \tag{1.4}$$

<u>Divergence:</u>

$$\nabla \cdot \mathbf{u} = \sum_i \frac{\partial u_i}{\partial x_i} = u_{i,i} \tag{1.5}$$

<u>Tensor product of two vectors:</u>

$$\mathbf{u} \otimes \mathbf{v} = \sum_{i,j} u_i v_j \breve{e}^{(i)} \otimes \breve{e}^{(j)} \tag{1.6}$$

$$(\mathbf{u} \otimes \mathbf{v}) \cdot \mathbf{w} = (\mathbf{u} \otimes \mathbf{v})\mathbf{w} = \mathbf{u}\,(\mathbf{v} \cdot \mathbf{w}) \tag{1.7}$$

Double contraction:

$$(\mathbf{u} \otimes \mathbf{v}) : (\mathbf{w} \otimes \mathbf{z}) = (\mathbf{u} \cdot \mathbf{w})(\mathbf{v} \cdot \mathbf{z}) = \sum_{i,j} u_i v_j w_i z_j \tag{1.8}$$

$$\mathbf{T} : \mathbf{S} = \sum_{i,j} T_{ij} S_{ij} \tag{1.9}$$

Gradient of a vector field:

$$\nabla \mathbf{u} = \sum_{i,j} u_{i,j} \check{e}^{(i)} \otimes \check{e}^{(j)} \tag{1.10}$$

$$\left(\underline{\underline{\nabla \mathbf{u}}}\right)_{ij} = u_{i,j} \tag{1.11}$$

Theorem 1.1 *Volume integral of a gradient.*

$$\int_V \varphi_{,i} \; dV = \int_{\partial V} \varphi \, n_i \; dS \tag{1.12}$$

Theorem 1.2 *Gauss-Green,* $\check{\mathbf{n}}$ *is the outward normal.*

$$\int_V \nabla \cdot \mathbf{z} \; dV = \int_{\partial V} \mathbf{z} \cdot \check{\mathbf{n}} \; dS \tag{1.13}$$

Outer product, cross product:

$$\mathbf{w} \times \mathbf{z} = \varepsilon_{ijk}\, w_j\, z_k\, \check{\mathbf{e}}^{(i)} \tag{1.14}$$

Curl of a vector:

$$\nabla \times \mathbf{z} = \varepsilon_{ijk}\, z_{k,j}\, \check{\mathbf{e}}^{(i)} \tag{1.15}$$

Exo. 1.1 *Show that the divergence of $\nabla \times \mathbf{z}$ is zero, for any differentiable vector field $\mathbf{z}$. Show that the curl of $\nabla\varphi$ is zero, for any differentiable scalar function φ.*

Exo. 1.2 *Let V be a connected volume in 3D, with boundary ∂V. Assume that the fluid inside V is at constant pressure, exerting a force*

$$\mathbf{F} = p\, \check{\mathbf{n}} \tag{1.16}$$

per unit area on ∂V. Prove that the total force exerted by the inner fluid on the boundary is zero.

Exo. 1.3 *Let V be a volume in 3D, with boundary ∂V. Assume the volume is filled with a fluid of constant density ρ. Prove that the total weight can be obtained from surface integrals:*

$$\int_V \rho\, g\; dV = \frac{\rho\, g}{3} \int_{\partial V} \mathbf{x} \cdot \check{\mathbf{n}}\; dS = \rho\, g \int_{\partial V} x_3\, n_3\; dS \tag{1.17}$$

Exo. 1.4 *Prove Archimedes' principle. A body immersed in a stagnant homogeneous liquid (which has pressure proportional to its depth, $p = \rho\, g\, h$) experiences a net upward force equal to the weight of the displaced liquid.*

1.3 Material derivative and transport theorem

The trajectory of particles in a continuum can be described by a function $\mathcal{F}(\mathbf{x}, s, t)$ which gives *the position at time t of the particle that ocupies position $\mathbf{x}$ at time s.*

- $\mathcal{F}(\mathbf{x}, t, t) = \mathbf{x}$ for all t.
- Fixing s and t, considered just as function of $\mathbf{x}$, the function $\boldsymbol{\phi}(\mathbf{x}) = \mathcal{F}(\mathbf{x}, s, t)$ is the *deformation* field of the medium between times s and t.
- The velocity field is related to $\mathcal{F}$

$$\frac{\partial \mathcal{F}}{\partial t}(\mathbf{x}, s, t) = \mathbf{u}(\mathcal{F}(\mathbf{x}, s, t), t) \tag{1.18}$$

  Here the pair $(\mathbf{x}, s)$ are a label for the *particle*. Another usual label is $\mathbf{X}$, defined as the position occupied by the particle in some "reference configuration", which needs not correspond to an instant of time. This is the so-called Lagrangian frame.

- Trajectories are sometimes written as

$$\mathbf{x}(t) = \boldsymbol{\phi}(\mathbf{X}, t) \tag{1.19}$$

Exo. 1.5 *A continuum is rigidly rotating with angular velocity ω around the axis $\mathbf{a} = \check{\mathbf{e}}^{(1)} + \check{\mathbf{e}}^{(2)}$. Compute its Eulerian velocity field $\mathbf{u}(\mathbf{x}, t)$ and its kinematic history function $\mathcal{F}(\mathbf{x}, s, t)$.*

The *material* or *total* derivative of a quantity ψ at time t for the particle that at that time is located at $\mathbf{x}$ is defined as the "derivative following the particle", or, more precisely,

$$\frac{D\psi}{Dt} = \lim_{\delta \to 0} \frac{\psi(\mathcal{F}(\mathbf{x}, t, t+\delta), t+\delta) - \psi(\mathbf{x}, t)}{\delta} \tag{1.20}$$

Exo. 1.6 *Prove that*

$$\frac{D\psi}{Dt} = \partial_t \psi + \mathbf{u} \cdot \nabla \psi \tag{1.21}$$

The *acceleration* of a fluid is the material derivative of the velocity

$$\mathbf{a} = \frac{D\mathbf{u}}{Dt} = \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\, \mathbf{u} = \partial_t \mathbf{u} + (\nabla \mathbf{u}) \cdot \mathbf{u} \tag{1.22}$$

Exo. 1.7 *Compute the acceleration field of the rigid rotation described in Exo. 1.5.*

Let Ω be a region in space, and let $f(\mathbf{x}, t)$ be a scalar field defined in Ω. To fix ideas, let f be a *temperature* field.

Let us select, at time t, a region V of Ω. This defines a *material volume*, consisting of the set of material particles that are inside V at time t.

If one follows the particles that are in V at t, they will occupy another region of space $\mathcal{V}(t')$ at time t'. Obviously $\mathcal{V}(t) = V$.

For any t', let $I(t')$ be the integral of f, at time t', over the volume occupied $\mathcal{V}(t')$ by the particles

$$I(t') = \int_{\mathcal{V}(t')} f(\mathbf{x}, t') \; dV \; . \tag{1.23}$$

Clearly $I(t')$ is the integral of the temperature over the material volume, a volume that changes position in time but has fixed material identity.

Reynolds transport theorem.

$$\frac{DI}{Dt}(t) = \int_V \left[\partial_t f + \nabla \cdot (\mathbf{u}\, f)\right] \; dV = \int_V \partial_t f \; dV + \int_{\partial V} f \, \mathbf{u} \cdot \check{\mathbf{n}} \; dS \tag{1.24}$$

Exo. 1.8 *Use the previous formula to prove that a flow in which the volume of each material part is preserved must be solenoidal (*$\nabla \cdot \mathbf{u} = 0$*), also called incompressible.*

1.4 Conservation of mass

Let M be the mass contained at time t in volume V,

$$M = \int_V \rho \, dV \ . \tag{1.25}$$

Since *the mass is conserved*,

$$\frac{DM}{Dt} = 0 \ , \tag{1.26}$$

which implies that **(integral form)**

$$\int_V \partial_t \rho \, dV = - \int_{\partial V} \rho \, \mathbf{u} \cdot \check{\mathbf{n}} \, dS \tag{1.27}$$

and also that **(differential form)**

$$\partial_t \rho + \nabla \cdot (\rho \, \mathbf{u}) = 0 \tag{1.28}$$

This last equation can be written as

$$\frac{D\rho}{Dt} + \rho \, \nabla \cdot \mathbf{u} = 0 \ , \tag{1.29}$$

which shows that an incompressible flow ($\nabla \cdot \mathbf{u} = 0$) in which the density of the material particles does not change with time automatically satisfies mass conservation.

The **mass flux** is given by

$$\mathbf{j} = \rho\,\mathbf{u}\ . \tag{1.30}$$

The conservation of mass can be written as a *conservation law*:

$$\partial_t \rho + \nabla \cdot \mathbf{j} = g \tag{1.31}$$

where g represents the sources (in the case of mass equal to zero).

$$\frac{d}{dt}\int_V \rho\ dV = -\int_{\partial V} \underbrace{\mathbf{j}\cdot\check{\mathbf{n}}}_{J}\ dS\ +\ \int_V g\ dV \qquad \text{variation = inflow - outflow + internal sources} \tag{1.32}$$

Exo. 1.9 *Let* ψ *be the* mass density, *or* mass fraction, *of some species A dispersed in the medium. The mass of this species in some volume V is*

$$M_A = \int_V \rho\,\psi\ dV\ . \tag{1.33}$$

Derive conservation laws in differential and integral form for ψ*. Also prove that*

$$\frac{D\psi}{Dt} = 0\ . \tag{1.34}$$

1.5 Conservation of momentum

The total momentum contained by a region V of a continuum is

$$\mathbf{P} = \int_V \rho\, \mathbf{u}\; dV \; . \tag{1.35}$$

The principle of conservation of momentum states that changes in the momentum are equal to the applied (volumetric and surface) forces, i.e.

$$\frac{D\mathbf{P}}{Dt} = \int_V \mathbf{f}\; dV \; + \; \int_S \mathbf{F}\; dS \; . \tag{1.36}$$

Using the transport theorem one arrives at the integral form

$$\boxed{\frac{d}{dt}\int_V \rho\, \mathbf{u}\; dV \; = \int_V \mathbf{f}\; dV \; + \; \int_{\partial V} \left[\mathbf{F} - \rho\left(\mathbf{u}\otimes\mathbf{u}\right)\check{\mathbf{n}}\right]\; dS \; .} \tag{1.37}$$

The Cauchy stress tensor

The *action-reaction principle* requires that, if at a point $\mathbf{x}$ of ∂V the region is subject to a surface force density $\mathbf{F}(\mathbf{x})$, the continuum inside reacts with an equal and opposite force.
It can be proved that there exists a symmetric tensor, the *Cauchy stress tensor*, such that for all $\mathbf{x}$ and t

$$\mathbf{F}(\mathbf{x},t) = \boldsymbol{\sigma}(\mathbf{x},t) \cdot \check{\mathbf{n}}(\mathbf{x},t) \ , \tag{1.38}$$

in the sense that *the surface forces that a medium exerts on another body through a surface with normal* $\mathbf{n}$ *(pointing outwards) is equal to* $-\boldsymbol{\sigma} \cdot \check{\mathbf{n}}$.

Inserting the stress tensor in (1.37) one arrives at

$$\frac{d}{dt} \int_V \rho\, \mathbf{u} \, dV \ = \int_V \mathbf{f} \ dV \ + \ \int_{\partial V} (\boldsymbol{\sigma} - \rho\, \mathbf{u} \otimes \mathbf{u}) \cdot \check{\mathbf{n}} \ dS \ . \tag{1.39}$$

The momentum flux through a surface is, thus,

$$\boldsymbol{\zeta} = -\boldsymbol{\sigma} + \rho\, \mathbf{u} \otimes \mathbf{u} \tag{1.40}$$

Exo. 1.10 *From (1.39) deduce the following differential forms of momentum conservation:*

Conservative form:

$$\partial_t(\rho \mathbf{u}) + \nabla \cdot \boldsymbol{\zeta} = \mathbf{f} \qquad or \tag{1.41}$$

$$\partial_t(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f} \tag{1.42}$$

Non-conservative form:

$$\rho\, \partial_t \mathbf{u} + \rho\, (\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f} \tag{1.43}$$

Also, write the equations above in Cartesian components.

1.6 Conservation of energy

Exo. 1.11 *Read 1.6 and 1.7 from Wesseling.*

The energy of a part of a continuum which occupies volume V is

$$E = \int_V \rho \left(\frac{1}{2} |\mathbf{u}|^2 + e \right) \, dV \tag{1.44}$$

where e is the *internal energy per unit mass*, which expresses the capability of a medium storing energy and is a function of its *local state.* The principle of conservation of energy reads

$$\frac{DE}{Dt} = \mathcal{Q} + \mathcal{W} \ , \tag{1.45}$$

where the right-hand side is the sum of the heat and work received from the surroundings. Defining $\mathbf{q}$ as the heat flux and Q as the heat source per unit volume one gets

$$\frac{DE}{Dt} = \int_V (\mathbf{f} \cdot \mathbf{u} + Q) \, dV + \int_{\partial V} (\mathbf{u} \cdot \boldsymbol{\sigma} - \mathbf{q}) \cdot \check{\mathbf{n}} \, dS \tag{1.46}$$

Exo. 1.12 *From the equation above, prove the following differential form*

$$\rho \frac{De}{Dt} = -\nabla \cdot \mathbf{q} + \boldsymbol{\sigma} : \nabla \mathbf{u} + Q \tag{1.47}$$

1.7 Constitutive laws

If one counts the equations up to now we have

- Conservation of mass (1 equation).
- Conservation of momentum (3 equations).
- Conservation of energy (1 equation).

Total: **5 equations**.

Counting the unknowns: ρ (1), $\mathbf{u}$ (3), $\boldsymbol{\sigma}$ (6), e (1), $\mathbf{q}$ (3). Total: **14 unknowns**.

The 9 equations that are lacking come from the so-called *constitutive laws*, that describe the material behavior (notice that the equations up to now hold for *any* continuum).

Essentially we need laws for e, $\boldsymbol{\sigma}$ and $\mathbf{q}$. For the latter Fourier's law is almost universally adopted,

$$\mathbf{q} = -\boldsymbol{\kappa}\,\nabla T\ , \tag{1.48}$$

where T is the temperature and $\boldsymbol{\kappa}$ the thermal conductivity (in general a tensor).

1.8 Newtonian and quasi-newtonian behavior

- The stress of a fluid at a point $\mathbf{x}$ and instant t can in principle depend on the whole deformation history of the vicinity of $\mathbf{x}$.

- However, not all constitutive laws correspond to fluids. The definition of fluid requires that "if the vicinity of the point has not deformed at all, then the stress tensor must be spherical". Spherical, in this context, means that $\boldsymbol{\sigma}$ is a multiple of the identity.

- A most important class of fluid constitutive laws corresponds to the so-called *quasi-Newtonian fluids*:

$$\boldsymbol{\sigma} = (-p + \lambda \nabla \cdot \mathbf{u})\, \mathbf{1} + \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \tag{1.49}$$

  in which λ and μ can depend on the *instantaneous deformation rate tensor*

$$\boldsymbol{\varepsilon}(\mathbf{u}) = D\, \mathbf{u} = \frac{1}{2} \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \ . \tag{1.50}$$

- Since λ and μ are scalars, the model is *objective* only if they depend on $\boldsymbol{\varepsilon}(\mathbf{u})$ through is *invariants*:

$$I = \operatorname{trace} \boldsymbol{\varepsilon}(\mathbf{u}) = \mathbf{1} : \boldsymbol{\varepsilon}(\mathbf{u}) = \nabla \cdot \mathbf{u} \tag{1.51}$$

$$II = \frac{1}{2} \left[(\operatorname{trace} \boldsymbol{\varepsilon}(\mathbf{u}))^2 - \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) \right] \tag{1.52}$$

$$III = \det \boldsymbol{\varepsilon}(\mathbf{u}) \tag{1.53}$$

  Notice that, in particular, the *deformation rate*

$$\|\boldsymbol{\varepsilon}(\mathbf{u})\| = \sqrt{\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u})} \tag{1.54}$$

- If λ and μ are constants, eventually dependent on the temperature, the fluid is called *Newtonian.*

- Shear thinning (resp. shear thickening) describe fluids in which μ is a decreasing (resp. increasing) function of $\|\boldsymbol{\varepsilon}(\mathbf{u})\|$.

Exo. 1.13 *Knowing that the velocity field of a rigid body motion is given by*

$$\mathbf{u}(\mathbf{x},t) = \mathbf{z}(t) + \mathbf{r}(t) \times \mathbf{x} \ , \tag{1.55}$$

prove that $\boldsymbol{\varepsilon}(\mathbf{u})$ *is zero.*

- Incompressibility.
- Turbulence.

2 Brief overview of numerical methods for CFD

2.1 Differential, integral and variational formulations

Consider the general second-order differential equation

$$L\varphi = -(\mathrm{a}_{ij}\varphi_{,j})_{,i} + (\mathrm{b}_i\varphi)_{,i} + c\,\varphi = q \ . \tag{2.1}$$

This equation is said to be *uniformly elliptic* if there exists $C > 0$ such that

$$\mathbf{v}\cdot(\mathbf{a}(\mathbf{x})\cdot\mathbf{v}) = \mathrm{a}_{ij}(\mathbf{x})\,\mathrm{v}_i\mathrm{v}_j \geq C\,\|\mathbf{v}\|^2 \qquad\qquad \forall\,\mathbf{x}\ \ \forall\,\mathbf{v}\ . \tag{2.2}$$

This condition, together with suitable boundary conditions, guarantees the existence of a unique φ in the space $H^1(\Omega)$. This solution is continuous (a.e.) across any surface.

Equation (2.1) can be seen as a steady conservation law in differential formulation,

$$\nabla\cdot\mathbf{j} = g\ , \tag{2.3}$$

by taking

$$\mathbf{j} = \mathbf{J}(\varphi,\nabla\varphi) = -\,\mathbf{a}\,\nabla\varphi\, +\, \mathbf{b}\,\varphi \tag{2.4}$$

and

$$g = q - c\,\varphi\ . \tag{2.5}$$

There thus exists a unique $\varphi \in H^1(\Omega)$ that satisfies the boundary conditions and also (2.3) for all $\mathbf{x}$ in the domain Ω of the problem. This is the **differential formulation**, which is the start point of **finite difference** approximation methods.

The differential equation must be understood in a *weak sense*, i.e.,

$$-\int_{\Omega} \mathbf{j} \cdot \nabla\psi \; dV + \int_{\partial\Omega} \psi \, \mathbf{j} \cdot \check{\mathbf{n}} \; dS = \int_{\Omega} g \, \psi \; dV \tag{2.6}$$

for all $\psi \in H^1(\Omega)$. Notice that this formula has no derivative of $\mathbf{j}$ and thus makes sense in cases in which the strong form (2.3) does not.

Considering homogeneous Dirichlet boundary conditions, the **variational formulation** of the problem reads: "Find $\varphi \in H_0^1(\Omega)$ such that

$$-\int_{\Omega} \mathbf{J}(\varphi, \nabla\varphi) \cdot \nabla\psi \; dV = \int_{\Omega} g(\varphi) \, \psi \; dV \tag{2.7}$$

for all $\psi \in H_0^1(\Omega)$."

This formulation is adopted in **primal finite element methods**, in which φ_h belongs to some subspace V_h and satisfies (2.7) only for functions ψ belonging to V_h.

Let Γ be a surface that divides Ω into two parts, Ω_1 and Ω_2. Integrating by parts (2.7) in each Ω_i one obtains

$$\int_{\Omega_1} [\nabla\cdot\mathbf{J}(\varphi,\nabla\varphi)-g(\varphi)]\,\psi\,dV+\int_{\Omega_2} [\nabla\cdot\mathbf{J}(\varphi,\nabla\varphi)-g(\varphi)]\,\psi\,dV-\int_{\Gamma} [\![\mathbf{J}(\varphi,\nabla\varphi)\cdot\check{\mathbf{n}}]\!]\,\psi\,dS=0 \qquad \forall\,\psi\in H_0^1(\Omega)\,. \tag{2.8}$$

This implies that

- The solution of (2.7) satisfied the differential equation a.e. in Ω_1 and Ω_2.
- The normal flux $\mathbf{J}\cdot\check{\mathbf{n}}$ is continuous across Γ.

Exo. 2.1 *Give arguments to support (or prove) both previous statements.*

Let K be an open polyhedral subset of Ω, with facets $e \in \mathcal{E}$. Integrating (2.3) over K and using Gauss-Green formula one gets

$$\sum_{e \in \partial K} \int_e \mathbf{J}(\varphi, \nabla\varphi) \cdot \check{\mathbf{n}} \; dS = \int_K g(\varphi) \; dK \; . \tag{2.9}$$

Notice that $\mathbf{J} \cdot \check{\mathbf{n}}$ is well defined on e. The **integral formulation** of the problem corresponds to "find the unique $\varphi \in H^1(\Omega)$ such that (2.9) holds for all polyhedra K contained in Ω".

- The integral formulation is the basis of **finite volume methods**. The discretization methodology consists of selecting a finite number of polyhedra as the finite volume mesh $\mathcal{T}_h$, and obtaining a finite number of equations by only requiring that (2.9) holds for those polyhedra. This leads to

$$\sum_{e \in \partial K} \overline{F}_{K,e} = \int_K g \; dV \qquad\qquad \forall\, K \in \mathcal{T}_h \; . \tag{2.10}$$

- The next step is the selection of degrees of freedom for the discrete solution. The most usual choice is to have one unknown φ_K per finite volume K, i.e., N_V unknowns for N_V equations. In addition, a node $\mathbf{x}_K$ is defined for each K.

- Letting $\underline{\varphi} \in \mathbb{R}^{N_V}$ be the column array of unknowns, a **numerical flux function** $F_{K,e}(\underline{\varphi})$ is introduced satisfying a **consistency condition**

$$F_{K,e}(\underline{\varphi}^*) \simeq \overline{F}_{K,e}(\varphi, \nabla\varphi) \tag{2.11}$$

  where $\underline{\varphi}^* = (\varphi(\mathbf{x}_1, \varphi(\mathbf{x}_2, \ldots)^T$ is the array of nodal values of any **exact** solution φ of the problem.

- The discrete system of equations reads

$$\sum_{e \in \partial K} F_{K,e}(\underline{\varphi}) = \int_K g(\underline{\varphi}) \; dV \qquad\qquad \forall\, K \in \mathcal{T}_h \; . \tag{2.12}$$

- For the method to be strictly conservative, it must happen that if a given facet e separates cell K from cell L then

$$F_{K,e}(\underline{\varphi}) = -F_{L,e}(\underline{\varphi}) \ . \tag{2.13}$$

- An interesting alternative to our choice of degrees of freedom is to add an additional unknown per facet. Let $\mathcal{E}$ be the "skeleton" of the mesh, consisting of all facets e, and let $\hat{\varphi}_j$, with $j = 1, \ldots, N_E$ be the facet unknowns. One now has N_V equations and $N_V + N_E$ unknowns. The required additional equations are (2.13), closing the system.

- Other possibilities exist, such as overlapping finite volumes, but we will not discuss them here.

2.2 A one-dimensional example

Let us take

$$L\varphi = -(\mathrm{a}\,\phi_{,1})_{,1} = q \tag{2.14}$$

in the domain $(0,\ell)$, which has nodes $0 = x_0, x_1, \ldots, x_n = \ell$. Let $h_i = x_i - x_{i-1}$. Also, let $x_{i+\frac{1}{2}} = \frac{1}{2}(x_i + x_{i+1})$ and $h_{i+\frac{1}{2}} = \frac{1}{2}(h_i + h_{i+1})$.

Finite differences

$$(\mathrm{a}\,\varphi')'(x_j) \simeq \frac{\mathrm{a}(x_{j+\frac{1}{2}})\varphi'(x_{j+\frac{1}{2}}) - \mathrm{a}(x_{j-\frac{1}{2}})\varphi'(x_{j-\frac{1}{2}})}{h_{j+\frac{1}{2}}}$$

$$\simeq \frac{\frac{\mathrm{a}_j+\mathrm{a}_{j+1}}{2}\,\frac{\varphi(x_{j+1})-\varphi(x_j)}{h_{j+1}} - \frac{\mathrm{a}_{j-1}+\mathrm{a}_j}{2}\,\frac{\varphi(x_j)-\varphi(x_{j-1})}{h_j}}{h_{j+\frac{1}{2}}}\,. \tag{2.15}$$

For equispaced nodes this leads to the discrete scheme (3.9) of Wesseling.

Exo. 2.2 *Build a small code for this problem and solve the interface problem of page 84 of Wesseling. Compare to the results shown in the book.*

Finite volumes

Notice that $\mathrm{J}(\varphi, \varphi') = -\mathrm{a}\,\varphi'$. Letting the finite volumes be given by $V_j = (x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}})$ a reasonable numerical flux (for continuous a) is

$$F_{j+\frac{1}{2}} = -\frac{\mathrm{a}_j + \mathrm{a}_{j+1}}{2}\;\frac{\varphi_{j+1} - \varphi_j}{h_{j+1}}\;. \tag{2.16}$$

Exo. 2.3 *Build the corresponding finite volume method in terms of nodal quantities. Compare to the finite-difference scheme.*

Improved finite volumes

Let us introduce as additional degrees of freedom the values $\varphi_{j+\frac{1}{2}}$ and

$$F_{j,j+\frac{1}{2}} = -\,\mathrm{a}_j\,\frac{\varphi_{j+\frac{1}{2}} - \varphi_j}{h_{j+1}/2}\;. \tag{2.17}$$

Similarly, we have

$$F_{j+1,j+\frac{1}{2}} = \mathrm{a}_{j+1}\,\frac{\varphi_{j+1} - \varphi_{j+\frac{1}{2}}}{h_{j+1}/2}\;. \tag{2.18}$$

Conservation condition (2.13) then allows to eliminate the unknown $\varphi_{j+\frac{1}{2}}$,

$$F_{j+\frac{1}{2}} = F_{j,j+\frac{1}{2}} = -F_{j+1,j+\frac{1}{2}} \qquad \Rightarrow \qquad \varphi_{j+\frac{1}{2}} = \frac{\mathrm{a}_j\varphi_j + \mathrm{a}_{j+1}\varphi_{j+1}}{\mathrm{a}_j + \mathrm{a}_{j+1}}\;. \tag{2.19}$$

Exo. 2.4 *Build the finite volume scheme corresponding to the flux above. Compare to (3.17) de Wesseling. Modify the code of exercise 2.2 to implement it. Test it. Compute the convergence order in a smooth problem with analytical solution.*

Exo. 2.5 *Study and discuss cell-centered finite volumes for the 1D problem, in which the nodes are* $x_{j+\frac{1}{2}}$ *instead of* x_j *and the finite volumes are of the form* (x_j, x_{j+1}). *Modify the code to deal with cell-centered discretization and compare to previous results.*

Exo. 2.6 *Analyze the consistency (truncation error) of the fluxes and of the overall stencil of the vertex-centered scheme of Exo. 2.3. Consider* $\mathrm{a} \equiv 1$, $f = 1$ *and* h_i *equal to* h *if* i *is even and equal to* $h/2$ *when* i *is odd. Discuss the result together with a numerical experiment.*

Exo. 2.7 *Discuss and implement Dirichlet and Neumann boundary conditions for cell-centered and vertex-centered discretizations.*

3 Numerical approximation of fully developed flow

3.1 The physical setting

- Incompressible flow along a long cylinder of cross section $\Omega \subset \mathbb{R}^2$. The flow domain is $\mathcal{B} = \Omega \times (0, L)$.
- The flow is driven by a pressure gradient

$$\mathcal{G} = \frac{p(L) - p(0)}{L} \tag{3.1}$$

  notice that when $\mathcal{G} > 0$ we expect $w = u_3 < 0$ and viceversa.

- If L is sufficiently large, the entry and exit effects can be neglected and all cross sections are essentially identical, except for the pressure.
- Decomposing the stress tensor in pressure and non-pressure components, we assume

$$\boldsymbol{\sigma}(x_1, x_2, x_3, t) = -p(x_3, t)\,\mathbb{I} + \boldsymbol{\sigma}^*(x_1, x_2, t) \ . \tag{3.2}$$

- Let ω be an arbitrary region in Ω and let V be the corresponding cylinder, i.e.,

$$V = \omega \times (0, L) \ . \tag{3.3}$$

  We denote also $\omega_z = \omega \times \{z\}$ (the cross section at $x_3 = z$) and $\mathcal{S} = \partial\omega \times (0, L)$ (the lateral surface) so that

$$\partial V = \omega_0 \cup \mathcal{S} \cup \omega_L \ . \tag{3.4}$$

3.2 Conservation principles

- Mass: Because of incompressibility, and assuming ρ is a constant, this principle reads

$$0 = \int_{\partial V} \mathbf{u} \cdot \check{\mathbf{n}} \, dS = - \int_{\omega_0} w \, dS \; + \; \int_{\omega_L} w \, dS \; + \; \int_{\mathcal{S}} \mathbf{u} \cdot \check{\mathbf{n}} \, dS \; . \tag{3.5}$$

  This condition is automatically satisfied in *parallel flows* which we consider hereafter, i.e., flows in which the velocity is of the form

$$\mathbf{u}(x_1, x_2, x_3, t) = (0, 0, w(x_1, x_2, t)) \; . \tag{3.6}$$

- Momentum: In parallel flows,

$$L \, \frac{d}{dt} \int_{\omega} \rho \, w \, d\omega = -\mathcal{G} \, L \, |\omega| \; + L \int_{\partial\omega} \boldsymbol{\tau} \cdot \check{\boldsymbol{\nu}} \, d\partial\omega \tag{3.7}$$

  where

$$\underline{\boldsymbol{\tau}} = (\sigma_{13}, \sigma_{23})^T \qquad \text{and} \qquad \underline{\check{\boldsymbol{\nu}}} = (\mathrm{n}_1, \mathrm{n}_2)^T \; . \tag{3.8}$$

In incompressible isothermal flows the mass and momentum conservation principles form a closed system.

In this case one equation, which is (3.7), in one unknown w.

The **no-slip boundary condition** holds when a fluid is in contact with a solid surface, in this case it translates to

$$w(x_1, x_2, t) = 0 \qquad \forall \, (x_1, x_2) \, \in \, \partial\Omega \; . \tag{3.9}$$

3.3 Viscous parallel flow

If the fluid is Newtonian-like (Boussinesq),

$$\boldsymbol{\sigma}^* = \mu \begin{pmatrix} 0 & 0 & w_{,1} \\ 0 & 0 & w_{,2} \\ w_{,1} & w_{,2} & 0 \end{pmatrix} \qquad \Rightarrow \qquad \boldsymbol{\tau} = \mu \nabla w \ . \tag{3.10}$$

We can, applying Gauss-Green theorem, rewrite (3.7) as

$$\int_\omega \left[\rho\, \partial_t\, w + \mathcal{G} - \nabla \cdot (\mu \nabla w) \right] \, d\omega = 0 \tag{3.11}$$

and arrive at the differential form

$$\begin{cases} \rho\, \partial_t\, w + \mathcal{G}(t) - \nabla \cdot (\mu \nabla w) = 0 & \text{in } \Omega \ , \\ w = 0 & \text{on } \partial\Omega \ . \end{cases} \tag{3.12}$$

Writing it as a conservation law

$$\partial_t(\rho\, w) + \nabla \cdot \mathbf{j} = g \ , \qquad \mathbf{j} = -\mu \nabla w \ , \qquad g = -\mathcal{G} \ . \tag{3.13}$$

3.4 Discretization in Cartesian grids

3.4.1 Finite differences

Consider a rectangular pipe $\Omega = (0, L_1) \times (0, L_2)$ with a uniform vertex-centered Cartesian grid with nodes at positions

$$\mathbf{X}_{j_1 j_2} = ((j_1 - 1)h_1, (j_2 - 1)h_2), \qquad j_\alpha = 1, \ldots, n_\alpha + 1, \qquad \alpha \in \{1, 2\} \ , \tag{3.14}$$

where n_α is the number of subdivisions in the α direction and $n_\alpha h_\alpha = L_\alpha$.

Considering as unknowns the values at the nodes w_{j_1,j_2}, we have $w_{j_1,j_2} = 0$ if (j_1, j_2) is at the boundary. For an internal node, on the other hand, a FD space discretization of (3.12) with constant density and viscosity leads to

$$\rho \frac{d}{dt} w_{j_1,j_2} + \mathcal{G} - \mu \, \frac{w_{j_1+1,j_2} - 2\, w_{j_1,j_2} + w_{j_1-1,j_2}}{h_1^2} - \mu \, \frac{w_{j_1,j_2+1} - 2\, w_{j_1,j_2} + w_{j_1,j_2-1}}{h_2^2} = 0 \ . \tag{3.15}$$

Our first issue is the implementation of this method.

Node-to-unknown mapping:

There are $(n_1 + 1) \times (n_2 + 1)$ unknowns, they can be numbered by row or by column (or else) to get the mapping. Denoting $N_1 = n_1 + 1$, $N_2 = n_2 + 1$,

```
function ng = ij2n (i,j)
  global N1 N2
  if(N1 < N2)
    ng = i + (j-1)*N1;
  else
    ng = j + (i-1)*N2;
  endif
endfunction
```

Exo. 3.1 *Build a function* `n2ij(n)` *that is the inverse of the previous one.*

Viscous matrix:

```
pP=ij2n(i,j); pN=ij2n(i,j+1); pE=ij2n(i+1,j); pS=ij2n(i,j-1); pW=ij2n(i-1,j);
```

The following matrix row provides the viscous contribution $(L_\mu w)_P \simeq -\mu \nabla^2 w(P)$ to equation P (interior node):

```
aux1 = mu/dx^2; aux2 = mu/dy^2;
A(pP,pP) = 2*(aux1+aux2);
A(pP,pN)=-aux2; A(pP,pS)=-aux2;
A(pP,pE)=-aux1; A(pP,pW)=-aux1;
```

so that

$$-\mu \frac{w_{j_1+1,j_2} - 2\,w_{j_1,j_2} + w_{j_1-1,j_2}}{h_1^2} - \mu \frac{w_{j_1,j_2+1} - 2\,w_{j_1,j_2} + w_{j_1,j_2-1}}{h_2^2} = \left(\underline{\underline{A}}\ \underline{W}\right)_P \quad . \tag{3.16}$$

Considering just the interior nodes, we get the system

$$\rho \frac{d}{dt}\underline{W} \ + \ \underline{\underline{A}}\ \underline{W} \ = \ \underline{b}(t) \tag{3.17}$$

where $b_P(t) = -G(t)$. Discretizing now in time by the θ-method,

$$\left(\frac{\rho}{\Delta t}\underline{\underline{\mathbf{I}}} + \theta\,\underline{\underline{A}}\right) \underline{W}^{n+1} = \left(\frac{\rho}{\Delta t}\underline{\underline{\mathbf{I}}} - \ (1-\theta)\,\underline{\underline{A}}\right) \underline{W}^{n} + \ \underline{b}^{n+\theta} \tag{3.18}$$

or

$$\underline{\underline{M}}\,\underline{W}^{n+1} = \underline{\underline{R}}\,\underline{W}^{n} + \ \underline{b}^{n+\theta} \tag{3.19}$$

```
#-- Assembly: loop over nodes
for i=1:N1
   for j=1:N2
      if (i==1 || i==N1 || j==1 || j==N2)
         continue;
      else
# viscous matrix
         pP=ij2n(i,j); pN=ij2n(i,j+1); pE=ij2n(i+1,j); pS=ij2n(i,j-1); pW=ij2n(i-1,j);
         aux1 = mu/dx^2; aux2 = mu/dy^2;
         Af(pP,pP) = 2*(aux1+aux2);
         Af(pP,pN)=-aux2; Af(pP,pS)=-aux2; Af(pP,pE)=-aux1; Af(pP,pW)=-aux1;
# mass matrix
         Am(pP,pP)=rho/dt;  bm(pP)=dx*dy;
      endif
   endfor
endfor
#-- Timestepping Matrices: M, R
M = Am + theta*Af;
R = Am - (1-theta)*Af;
#-- Correct M for no-slip boundary conditions
for i=1:N1
   for j=1:N2
      if (i==1 || i==N1 || j==1 || j==N2)
         pP=ij2n(i,j); M(pP,pP)=1;
      endif
   endfor
endfor
```

3.5 Vertex-centered finite volumes

- The node-to-unknown mapping remains the same.
- From (3.7), the equation for the (interior) finite volume P is

$$F_{PN} + F_{PE} + F_{PS} + F_{PW} = \int_{\omega_P} (-\mathcal{G} - \rho\,\partial_t w)\; d\omega \simeq h_1\, h_2 \left(-\mathcal{G} - \rho\,\frac{dW_P}{dt}\right) \tag{3.20}$$

where we have treated $\partial_t w$ as a source and the left-hand side approximates $\int_{\partial\omega_P} \mathbf{j}\cdot\check{\boldsymbol{\nu}}\; ds$ (remember that $\mathbf{j} = -\mu\nabla w$).

- Now we have to define the discrete fluxes

$$\int_{e_N} \mathbf{j}\cdot\check{\boldsymbol{\nu}}\; dx_1 = \int_{e_N} \mathrm{j}_2\; dx_1 = \int_{e_N} (-\mu\, w_{,2})\; dx_1 \simeq \mu\,\frac{W_P - W_N}{h_2}\, h_1 \doteq F_{PN} \tag{3.21}$$

and analogously

$$F_{PE} \doteq \mu\,\frac{W_P - W_E}{h_1}\, h_2 \tag{3.22}$$

$$F_{PS} \doteq \mu\,\frac{W_P - W_S}{h_2}\, h_1 \tag{3.23}$$

$$F_{PW} \doteq \mu\,\frac{W_P - W_W}{h_1}\, h_2 \tag{3.24}$$

$$\tag{3.25}$$

- We divide everything by $h_1 h_2$ to arrive at the discrete equation

$$\rho\,\frac{dW_P}{dt} + \mu\,\frac{W_P - W_N}{h_2^2} + \mu\,\frac{W_P - W_S}{h_2^2} + \mu\,\frac{W_P - W_E}{h_1^2} + \mu\,\frac{W_P - W_W}{h_1^2} = -\mathcal{G}\;. \tag{3.26}$$

- The viscous matrix can now be decomposed into the contributions of each face:

```
# viscous matrix
         pP=ij2n(i,j); pN=ij2n(i,j+1); pE=ij2n(i+1,j); pS=ij2n(i,j-1); pW=ij2n(i-1,j);
         aux1 = mu/dx^2; aux2 = mu/dy^2;
# north face
         Af(pP,pP) = Af(pP,pP) + aux2;
         Af(pP,pN) = Af(pP,pN) - aux2;
# east face
         Af(pP,pP) = Af(pP,pP) + aux1;
         Af(pP,pE) = Af(pP,pE) - aux1;

etcetera
```

Exo. 3.2 *(Optional) Extend the previous method and code to the variable-spacing case. Assume that two arrays $\underline{x}$ and $\underline{y}$ are provided, such that node (i,j) is located at (x_i, x_j). Build the method starting from (3.7) for these vertex-centered finite volumes. Notice that in this case the first term, after cancelling L, will read*

$$\underline{\underline{E}}\,\frac{d\,\underline{W}}{dt}\,, \qquad \textit{with} \qquad E_{rs} = \rho\,|V_r|\,\delta_{rs}\ . \tag{3.27}$$

The viscous matrix is also different from the one shown earlier.

Exo. 3.3 *Implement the computation of the flow rate Q and the mean velocity $\overline{W}$, having as input the solution vector $\underline{W}$.*

$$Q \doteq \int_\Omega w\; d\Omega, \qquad \overline{W} = \frac{Q}{|\Omega|}\ . \tag{3.28}$$

- Variable viscosity: Let us assume that μ is taken as constant in each cell $(x_i, x_{i+1}) \times (y_j, y_{j+1})$. We thus have a matrix `mu(1:N1-1,1:N2-1)`, so that the node `(i,j)` has `mu(i,j)` in the NE quadrant, `mu(i,j-1)` in the SE quadrant, and so on. We then have

```
# viscous matrix
         pP=ij2n(i,j); pN=ij2n(i,j+1); pE=ij2n(i+1,j); pS=ij2n(i,j-1); pW=ij2n(i-1,j);
# north face
         muf = 0.5*(mu(i-1,j)+mu(i,j));
         Af(pP,pP) = Af(pP,pP) + muf/dy^2;
         Af(pP,pN) = Af(pP,pN) - muf/dy^2;
# east face
         muf = 0.5*(mu(i,j)+mu(i,j-1));
         Af(pP,pP) = Af(pP,pP) + muf/dx^2;
         Af(pP,pE) = Af(pP,pE) - muf/dx^2;

etcetera
```

- <u>Quasi-newtonian fluid</u>: Viscosity may depend on the shear rate, for incompressible flows given by

$$\dot{\gamma} \doteq \sqrt{D\,\mathbf{u} : D\,\mathbf{u}} \tag{3.29}$$

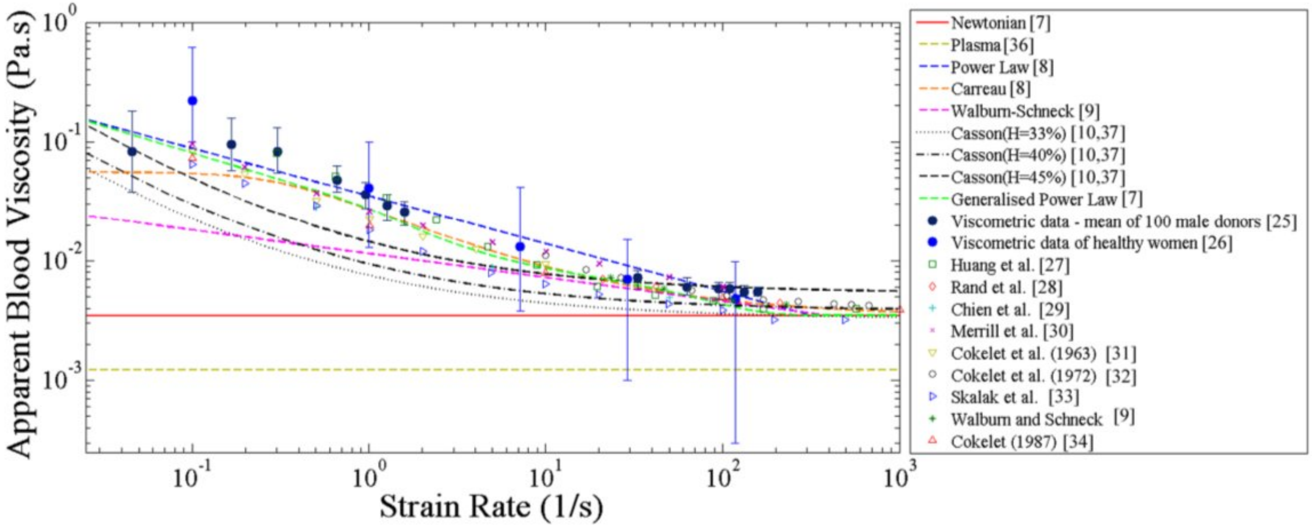

Fig 2. Experimental measurements of blood viscosity and non-Newtonian blood rheological models.

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Different models exist for blood

Table 1. Blood rheological model equations.

Blood Model	Effective Viscosity (Pa·s)
Newtonian [7]	$\mu = 0.00345\ Pa{\cdot}s$
Plasma [36]	$\mu = 0.00122\ Pa{\cdot}s$
Power Law (Modified) [8]	$\mu = \begin{cases} m(\dot{\gamma})^{n_p-1}, & \dot{\gamma} < 427 \\ 0.00345\, Pa\cdot s, & \dot{\gamma} \geq 427 \end{cases}$, $m = 0.035$, $n_p = 0.6$
Walburn-Schneck (Modified) [9]	$\mu = \begin{cases} C_1 e^{(C_2 H)} e^{\left(C_4\left(\frac{TPMA}{H^2}\right)\right)} (\dot{\gamma})^{-C_3 H}, & \dot{\gamma} < 414 \\ 0.00345\, Pa\cdot s, & \dot{\gamma} \geq 414 \end{cases}$, C1 = 0.00797, C2 = 0.0608, C3 = 0.00499, C4 = 14.585, H = 40, TPMA = 25.9
Casson [10,37]	$\mu = 0.1\left(\left[\sqrt{\eta} + \sqrt{\tau_y\left(\frac{1-e^{-m\lvert\dot{\gamma}\rvert}}{\lvert\dot{\gamma}\rvert}\right)}\right]^2\right)$, $\tau_y = (0.625H)3$, $\eta = \eta 0(1-H)^{-2.5}$, $\eta_0 = 0.012$, H = 40% (female normal), 33% (post-angioplasty) or 45% (male normal)
Carreau [8]	$\mu = \mu_{\infty C} + (\mu_0 - \mu_{\infty C})[1 + (\lambda\dot{\gamma})^2]^{\frac{n_C-1}{2}}$, $\lambda = 3.313$, $n_C = 0.3568$, $\mu_0 = 0.056$, and $\mu_{\infty C} = 0.00345$
Generalised Power Law [7]	$\mu = \lambda\lvert\dot{\gamma}\rvert^{n-1}, \lambda = \mu_{\infty G} + \Delta\mu exp\left[-\left(1 + \frac{\lvert\dot{\gamma}\rvert}{a}\right)exp\left(-\frac{b}{\lvert\dot{\gamma}\rvert}\right)\right]$, $n = n_\infty - \Delta n\, exp\left[-\left(1 + \frac{\lvert\dot{\gamma}\rvert}{c}\right)exp\left(-\frac{d}{\lvert\dot{\gamma}\rvert}\right)\right]$, $\mu_{\infty G} = 0.0035$, $n_\infty = 1.0$, $\Delta\mu = 0.025$, $\Delta n = 0.45$, a = 50, b = 3, c = 50, and d = 4

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Exo. 3.4 *(Optional) Develop and implement a code for simulating blood flow through a rectangular pipe of cross section $100\mu m \times 50\mu m$ using the Carreau model. Solve for several values of $\mathcal{G}$, chosen such as to have cases with low mean velocity ($< 1\mu m/s$), high mean velocity ($> 50\mu m/s$), and some intermediate values. Build a curve Q vs. $\mathcal{G}$ and compare with the same curve for the Newtonian case $\mu = \mu_{\infty C} = 3.45 \times 10^{-3}$ Pa-s. Compare the velocity profiles (newtonian vs. non-newtonian) at high and low velocity.*

- Viscous dissipation, heat conduction:

Exo. 3.5 *Explain how to compute, in fully developed flow, the viscous dissipation (in Watt/m^3)*

$$\Phi = \boldsymbol{\sigma} : D\,\mathbf{u} \tag{3.30}$$

Exo. 3.6 *(Optional) Develop a finite volume method to approximate the temperature distribution in fully developed flow, solving the energy equation*

$$\rho\, c_p\, \partial_t T - \kappa\, \nabla^2 T = \Phi \tag{3.31}$$

with $T = 0$ *imposed on the boundary.*