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

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

the Cartesian basis of vectors.

<u>Vector field:</u>

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

<u>Gradient:</u>

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

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

<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>

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

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

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*

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

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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.

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

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,

$$M = \int_V \rho \, dV \ .$$

$$(1.25)$$

Since *the mass is conserved*,

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

$$(1.26)$$

which implies that **(integral form)**

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

$$(1.27)$$

and also that **(differential form)**

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

$$(1.28)$$

This last equation can be written as

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

$$(1.29)$$

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).

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

$$\tag{1.32}$$

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

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

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:

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

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

Non-conservative form:

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

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

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

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*:

$$
\begin{aligned}
I &= \operatorname{trace} \boldsymbol{\varepsilon}(\mathbf{u}) = \mathbf{1} : \boldsymbol{\varepsilon}(\mathbf{u}) = \nabla \cdot \mathbf{u} & (1.51) \\
II &= \frac{1}{2} \left[(\operatorname{trace} \boldsymbol{\varepsilon}(\mathbf{u}))^2 - \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) \right] & (1.52) \\
III &= \det \boldsymbol{\varepsilon}(\mathbf{u}) & (1.53)
\end{aligned}
$$

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

$$L\varphi = -(a_{ij}\varphi_{,j})_{,i} + (b_i\varphi)_{,i} + c\,\varphi = q \ . \tag{2.1}$$

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

$$\mathbf{v} \cdot (\mathbf{a}(\mathbf{x}) \cdot \mathbf{v}) = a_{ij}(\mathbf{x})\,v_i v_j \geq C\,\|\mathbf{v}\|^2 \qquad \forall\,\mathbf{x} \ \ \forall\,\mathbf{v} \ . \tag{2.2}$$

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

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

- 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

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

- 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

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

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

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

$$\simeq \frac{\frac{a_j + a_{j+1}}{2}\frac{\varphi(x_{j+1}) - \varphi(x_j)}{h_{j+1}} - \frac{a_{j-1} + a_j}{2}\frac{\varphi(x_j) - \varphi(x_{j-1})}{h_j}}{h_{j+\frac{1}{2}}} \,. \tag{2.15}$$

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 $J(\varphi, \varphi') = -a\,\varphi'$. 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

$$F_{j+\frac{1}{2}} = -\frac{a_j + a_{j+1}}{2}\,\frac{\varphi_{j+1} - \varphi_j}{h_{j+1}}\;.\tag{2.16}$$

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

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

Similarly, we have

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

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

$$F_{j+\frac{1}{2}} = F_{j,j+\frac{1}{2}} = -F_{j+1,j+\frac{1}{2}} \quad\Rightarrow\quad \varphi_{j+\frac{1}{2}} = \frac{a_j\varphi_j + a_{j+1}\varphi_{j+1}}{a_j + a_{j+1}}\;.\tag{2.19}$$

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 $a \equiv 1$, $f = 1$ 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

- <u>Mass</u>: 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

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

- <u>Momentum</u>: 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

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

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,

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

or

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

31

```
#-- 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*

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

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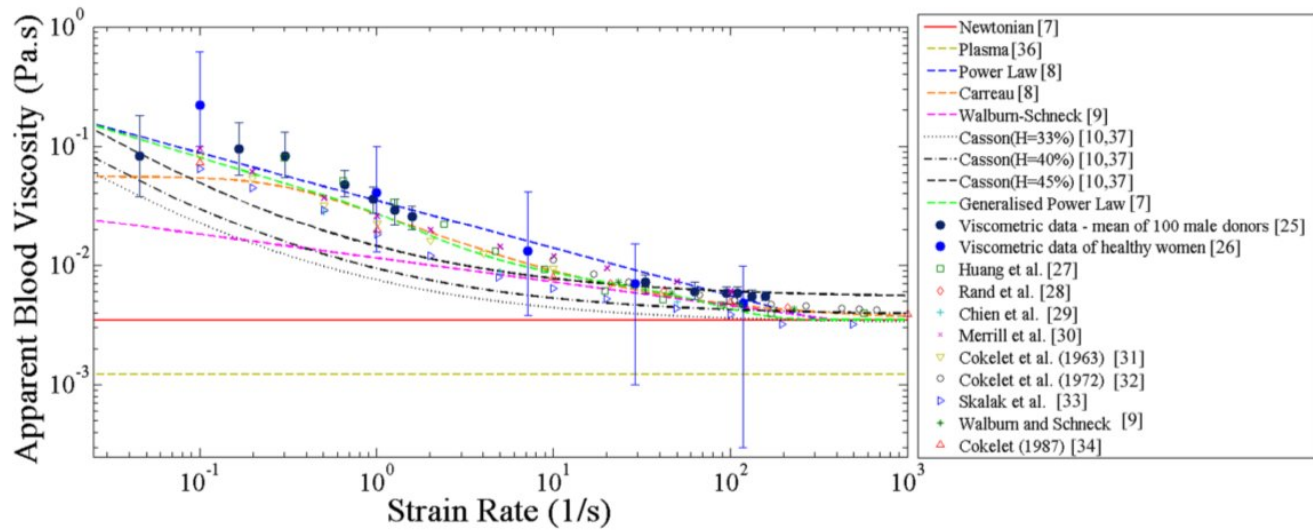
- <u>Quasi-newtonian fluid</u>: Viscosity may depend on the shear rate, for incompressible flows given by

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

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]	$\mu = 0.1 \left(\left[\sqrt{\eta} + \sqrt{\tau_y \left(\frac{1 - e^{-m|\dot{\gamma}|}}{|\dot{\gamma}|} \right)} \right] \right)^2$, $\tau_y = (0.625 H)3$, $\eta = \eta 0(1-H)^{-2.5}$, $\eta_0 = 0.012$, $H = 40\%$ (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]	$\mu = \lambda |\dot{\gamma}|^{n-1}$, $\lambda = \mu_{\infty G} + \Delta\mu exp\left[-\left(1 + \frac{|\dot{\gamma}|}{a}\right) exp\left(-\frac{b}{|\dot{\gamma}|}\right) \right]$, $n = n_\infty - \Delta n\ exp\left[-\left(1 + \frac{|\dot{\gamma}|}{c}\right) exp\left(-\frac{d}{|\dot{\gamma}|}\right) \right]$, $\mu_{\infty G} = 0.0035$, $n_\infty = 1.0$, $\Delta\mu = 0.025$, $\Delta n = 0.45$, $a = 50$, $b = 3$, $c = 50$, and $d = 4$

doi:10.1371/journal.pone.0128178.t001

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.*

37

- 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.

4 Flow in a long pipe: Turbulence

In this section we work out the following example: A long pipe conveys water between two reservoirs that are far apart. The inclination of the pipe is s (in meters of descent per meter of length) and its diameter D. Compute the velocity field in the pipe and the flow rate.

4.1 Why the flow cannot be laminar

Applying the general expression for conservation of momentum in fully developed flow (3.7) to the case in which ω is the circle of radius r and the flow steady we obtain

$$0 = -\mathcal{G}\,\pi\,r^2 + r \int_0^{2\pi} \tau(r,\theta)\,d\theta \tag{4.1}$$

where τ is the radial shear stress along x_3, given by $\boldsymbol{\tau} \cdot \check{\mathbf{e}}_r$. Because of the symmetry, τ does not depend on θ, which gives

$$\tau(r)\,2\pi\,r = \mathcal{G}\,\pi\,r^2 \; . \tag{4.2}$$

where σ_{rz} is the shear stress along z (the axial direction) on surfaces with normal $\check{\boldsymbol{\nu}} = \check{\mathbf{r}}$. The inclination generates the pressure gradient

$$\mathcal{G} = -s\,\rho\,g \; , \tag{4.3}$$

and from the Newtonian-like law

$$\tau(r) = \mu\,\frac{dw}{dr} \; . \tag{4.4}$$

Notice first that

$$\frac{1}{r}\frac{d}{dr}\left(\mu\, r\,\frac{dw}{dr}\right) = \mathcal{G} \tag{4.5}$$

in agreement with (3.12), since lhe left-hand side of (4.5) is $\nabla \cdot (\mu\,\nabla w)$ in cylindrical coordinates and we have assumed steady flow. This is the equation that determines w, with boundary condition $w(R) = 0$. The condition $w'(0) = 0$ is generally also imposed, but truly speaking $r = 0$ is not a boundary. Anyway, the governing equation is

$$\frac{dw}{dr}(r) = -\frac{s\,\rho\,g}{2}\frac{r}{\mu(r)} \tag{4.6}$$

which can be integrated with initial condition $w(r = 0) = w_{\text{max}}$ to yield

$$w(r) = w_{\text{max}} - \frac{s\,\rho\,g}{2}\int_0^r \frac{r'dr'}{\mu(r')}\ . \tag{4.7}$$

The unknown w_{max} can be computed from $w(R) = 0$, namely

$$w_{\text{max}} = \frac{s\,\rho\,g}{2}\int_0^R \frac{r'dr'}{\mu(r')}\ . \tag{4.8}$$

If the viscosity is constant one recovers the familiar parabolic Poiseuille profile

$$w(r) = w_{\text{max}} - \frac{s\,\rho\,g}{4\,\mu}\,r^2 \tag{4.9}$$

with

$$w_{\text{max}} = \frac{s\,\rho\,g}{16\,\mu}\,D^2\ . \tag{4.10}$$

Assuming $D = 0.5$ m and a gentle slope of $s = 10^{-2}$ (ten meters per kilometer), since $\mu = 10^{-3}$ Pa-s and $\rho = 1000$ kg/m^3 one gets

$$w_{\text{max}} = 1530 \text{ m/s} = 5512 \text{ km/h !!!!!} \tag{4.11}$$

Exo. 4.1 *Compute the flow rate (in m^3/s) of the laminar solution calculated above.*

Exo. 4.2 *Compute the velocity profile of the Carreau fluid of exercise 3.4.*

4.2 Turbulence

Anybody understands that this huge value of the velocity does not occur in reality. The parallel flow is indeed a solution of the conservation equations, but it is an *unstable* solution. Both mathematically and physically one observes a flow that is neither steady nor parallel, that is called *turbulent*.

- Turbulent flows are stochastic. They are described with the tools of statistical theory. Though the **instantaneous** values of velocity and pressure are randomic, the **mean** values of the variables are quite deterministic.

- These mean values (of velocity, of pressure, of force on solid surfaces, etc.) are in fact what engineers are most interested in. If the boundary conditions do not depend on time, the mean values also do not depend on time, as would be the case, in our pipe example, some seconds after the valve connecting the two reservoirs is opened.

- It is customary to decompose all variables into mean and fluctuating components, e.g.,

$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}', \qquad p = \bar{p} + p' \ . \tag{4.12}$$

Inserting this into the momentum balance equation and taking the mean, one arrives at

$$0 = \int_V \bar{\mathbf{f}} \ dV \ + \ \int_{\partial V} \left(-\bar{p} + \mu \left(\nabla \bar{\mathbf{u}} + \nabla \bar{\mathbf{u}}^T \right) - \rho \, \bar{\mathbf{u}} \otimes \bar{\mathbf{u}} - \rho \, \overline{\mathbf{u}' \otimes \mathbf{u}'} \right) \cdot \check{\mathbf{n}} \ dS \ . \tag{4.13}$$

Exo. 4.3 *Verify the previous assertion.*

We observe that *the averaged equation is the same as the original equation if the so-called Reynolds stress tensor is added to the average stresses:*

$$\boldsymbol{\sigma} \longleftarrow \boldsymbol{\sigma}(\nabla \bar{\mathbf{u}}, \bar{p}) + \boldsymbol{\sigma}^{\mathrm{Re}} \ , \qquad \text{with} \qquad \boldsymbol{\sigma}^{\mathrm{Re}} = -\rho \, \overline{\mathbf{u}' \otimes \mathbf{u}'} \ . \tag{4.14}$$

- Equation (4.2) then becomes

$$\left[\mu \, \partial_r \bar{w} - \rho \, \overline{u_r' u_z'} \right] 2\pi \, r = \mathcal{G} \, \pi \, r^2 \ . \tag{4.15}$$

Though u_r' and u_z' are rapidly fluctuating functions with zero mean, they are *correlated* and the mean of their product is not zero. Typically, velocity fluctuations that have $u_r' > 0$ (outwards from the center) also have $u_z' > 0$, because u_z is larger near the centerline.

Remark 4.1 *The Reynolds stress should not be thought as a "correction" or a "small perturbation" to an underlying laminar flow. Quite to the contrary, it is the term $\mu \partial_r \bar{w}$ that is negligible througout the flow, with the exception of a narrow layer near the walls.*

4.3 Turbulence models

- If one could express $\boldsymbol{\sigma}^{\mathrm{Re}}$ somehow in terms of $\bar{\mathbf{u}}$ and/or its derivatives, then one could substitute into (4.15) and solve for $\bar{w}(r)$. This is accomplished by the so-called *Boussinesq turbulent viscosity hypothesis.* It states that

$$\boldsymbol{\sigma}^{\mathrm{Re}} \simeq -\frac{2}{3}\,\rho\,k\,\mathbf{1} + \mu^{\mathrm{t}}\,(\nabla\bar{\mathbf{u}} + \nabla\bar{\mathbf{u}}^T) \tag{4.16}$$

where

$$k = \frac{1}{2}\,\overline{\|\mathbf{u}'\|^2} \tag{4.17}$$

is the *turbulent kinetic energy* (per unit mass) and μ^{t} is the *turbulent viscosity.* This hypothesis agrees with physical observations in many flows, especially if there are no large wakes and if the boundary layer is attached to the wall. The agreement is not perfect in general, but it is sufficient for engineering predictions.

- Prandtl (1904) produced a model for μ^{t} inspired in molecular models of gases. His *mixing length theory* leads to

$$\mu^{\mathrm{t}} = \rho\,\ell^2\,\|\nabla\bar{\mathbf{u}} + \nabla\bar{\mathbf{u}}^T\| \tag{4.18}$$

where ℓ is the so-called Prandtl's mixing length. Again particularizing to the pipe example, it leads to

$$\mu^{\mathrm{t}} = \rho\,\ell^2\,\left|\frac{d\bar{w}}{dr}\right|\,. \tag{4.19}$$

- If y is the distance to the wall, it is intuitive that the length scale of the turbulent vortices, and thus of the mixing, is y itself. In fact, it is fairly accurate that

$$\ell = \kappa\,y \tag{4.20}$$

where κ, the von Karman constant, turns out to be quite universal (all flows, pipes or planes). Beautiful theories have been built that explain this universality and other properties of turbulent flows, we suggest the interest reader to look for the books by Tennekes & Lumley and by Pope.

- We follow here the more pragmatic approach of Launder & Spalding (1972) in this first discussion about turbulence. A vast experience exists on steady flow in circular pipes, from which we can borrow Nikuradse's law:

$$\frac{\ell}{R} = 0.14 - 0.08 \left(1 - \frac{y}{R}\right)^2 - 0.06 \left(1 - \frac{y}{R}\right)^4 = 0.14 - 0.08 \left(\frac{r}{R}\right)^2 - 0.06 \left(\frac{r}{R}\right)^4 . \tag{4.21}$$

Exo. 4.4 *The final differential equation is then*

$$\frac{1}{r} \frac{d}{dr} \left((\mu + \mu^t) \, r \, \frac{d\bar{w}}{dr} \right) = \mathcal{G} \tag{4.22}$$

with $\mu^t = \rho \, \ell(r)^2 |d\bar{w}/dr|$ and $\ell(r)$ taken from (4.21).

Numerically solve this equation with boundary condition $\bar{w}(r = 0) = \bar{w}_{\max}$. Iteratively adjust $\bar{w}_{\max}$ until $\bar{w}(R) = 0$ is satisfied. Plot the resulting velocity profile.

4.4 Wall laws

- Nothing is simple in turbulence. Boundary conditions are no exception. The mean velocity field computed in Exo. 4.4 does not agree with experimental observation.

- The unrealistic prediction can be traced back to the boundary condition $\bar{\mathbf{u}} = 0$ at the wall. The averaged model we have presented so far, being a so-called *high-Reynolds-number* (or *high-Re*) model, is not physically realistic in the close vicinity of the wall, where viscous effects are comparable to (or larger than) turbulent ones. Essentially, we are imposing the boundary condition at a location where the differential equation is not valid.

- The idea is to replace the "natural" condition $\bar{w}(R) = 0$ by some condition at $\tilde{R} < R$, a point within the turbulent-dominated region where (4.22) is valid.

- A popular and frequently accurate boundary condition in CFD is the *logarithmic law of the wall*. Denoting by τ_w the shear stress at the wall, it is customary to define shear velocity $u^* = \sqrt{\tau_w/\rho}$ and then the wall variables (traditionally u is the longitudinal velocity)

$$u^+ = \frac{\bar{w}}{u^*} \,, \qquad y^+ = \frac{y}{\nu/u^*} \,. \tag{4.23}$$

It so happens that in many turbulent flows, between $y^+ = 20$ and $y^+ = 100$, the following relation holds:

$$u^+ = \frac{1}{\kappa} \ln \left(E \, y^+ \right) , \tag{4.24}$$

where $\kappa \simeq 0.4$ and $E \simeq 9$. How does this provide a boundary condition? A simple way is to *choose* $\tilde{R}$ as satisfying $y^+ = (R - \tilde{R})^+ = 30$. Normally this is a very small correction of the pipe radius, in the micrometer range. For the pipe we are considering, for example,

$$\tau_w = -\frac{s \, \rho \, g \, D}{4} = -12.25 Pa \qquad \Rightarrow \qquad u^* = \sqrt{\frac{|\tau_w|}{\rho}} = 0.11 \text{ m/s} \,. \tag{4.25}$$

As a consequence,

$$(R - \tilde{R})^+ = 30 \qquad \Rightarrow \qquad R - \tilde{R} = 30\frac{\nu}{u^*} = 2.72 \times 10^{-4} \text{ m} . \tag{4.26}$$

In the simplified treatment we are following here, we will take $\tilde{R} = R$ and exploit the wall law at $y^+ = 30$ which gives

$$\frac{\bar{w}}{\sqrt{|\tau_w|/\rho}} = \frac{1}{\kappa} \ln (E\, y^+) = 14 \tag{4.27}$$

so that

$$\left(\mu + \mu^{\mathrm{t}}\right) \frac{d\bar{w}}{dr} = -\frac{\rho}{196}\, \bar{w}^2 , \tag{4.28}$$

which is the boundary condition imposed at $r = R$.

• Notice that we impose a "drag law" and not simply $\left(\mu + \mu^{\mathrm{t}}\right) d\bar{w}/dr = \tau_w$, because it is only in very symmetric situations that we know the value of τ_w a priori.

Exo. 4.5 *Compute numerically the velocity profile produced by the model described above. Predict the flow in the pipe of the example, in particular the flow rate and the average velocity. Compute the Reynolds number. Compare to the prediction of the "Moody chart" (google me).*

5 Incompressible Navier-Stokes equations

- In the previous two sections we have applied the basic principles of fluid mechanics to *parallel flows.* Turbulence was discussed, also, under conditions leading to a *parallel mean flow.*

- In more general situations, one has to go back to the basic principles as introduced in section 1. They can be equivalently written in integral or differential form, and the latter can equivalently be conservative or non-conservative.

- In this section we particularize the basic principles for the case of an incompressible Newtonian fluid, arriving at the Navier-Stokes equations. We then discuss in general the treatment of turbulence for these equations.

5.1 Equations and fluxes

- When a Newtonian fluid flows with constant density and viscosity, a closed system of equations is obtained from just the mass and momentum conservation principles.

Exo. 5.1 *Deduce from Section 1 that the differential equations in non-conservative form are the*

Incompressible Navier-Stokes equations (non-conservative form):

$$\rho\,\partial_t \mathbf{u} + \rho\,(\mathbf{u} \cdot \nabla)\,\mathbf{u} - \nabla \cdot \left[\mu\,(\nabla\mathbf{u} + \nabla\mathbf{u}^T)\right] + \nabla p \;=\; \mathbf{f} \qquad (5.1)$$
$$\nabla \cdot \mathbf{u} \;=\; 0 \qquad (5.2)$$

The simplest form, when μ is constant, reads

$$\rho\, \partial_t \mathbf{u} + \rho\, (\mathbf{u} \cdot \nabla)\, \mathbf{u} - \mu\, \nabla^2 \mathbf{u} + \nabla p \;=\; \mathbf{f} \tag{5.3}$$

$$\nabla \cdot \mathbf{u} \;=\; 0 \tag{5.4}$$

Exo. 5.2 *Deduce from Section 1 that the differential equations in conservative form are the*

Incompressible Navier-Stokes equations (conservative form):

$$\rho\, \partial_t \mathbf{u} + \nabla \cdot \left[p\, \mathbb{I} - \mu\, (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \rho\, \mathbf{u} \otimes \mathbf{u} \right] \;=\; \mathbf{f} \tag{5.5}$$

$$\nabla \cdot \mathbf{u} \;=\; 0 \tag{5.6}$$

Exo. 5.3 *Deduce from Section 1 that the differential equations in conservative form are the*

Incompressible Navier-Stokes equations (integral form):

$$\int_V \rho\, \partial_t \mathbf{u}\; dV + \int_S \boldsymbol{\zeta} \cdot \check{\mathbf{n}}\; dS \;=\; \int_V \mathbf{f}\; dV \tag{5.7}$$

$$\int_S \mathbf{u} \cdot \check{\mathbf{n}}\; dS \;=\; 0 \tag{5.8}$$

where the momentum flux $\boldsymbol{\zeta}$ is

$$\boldsymbol{\zeta} = p\, \mathbb{I} - \mu\, (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \rho\, \mathbf{u} \otimes \mathbf{u} = -\boldsymbol{\sigma} + \rho\, \mathbf{u} \otimes \mathbf{u} \tag{5.9}$$

and the mass flux is $\rho\, \mathbf{u}$.

- In any of these forms, it is a closed system for the unknowns $\mathbf{u}$ and p.

- There are several types of possible boundary conditions:

  1. **Imposed velocity:** At rigid walls, if $\mathbf{u}_w$ is the velocity of the wall, set $\mathbf{u} = \mathbf{u}_w$.

  2. **Imposed force:** Used when the force $\mathbf{L}$ applied on the fluid (per unit surface) at some boundary is known. The condition reads
  $$\boldsymbol{\sigma} \cdot \check{\mathbf{n}} = \mathbf{L} \ . \tag{5.10}$$

  3. **Drag law:** This corresponds to
  $$\boldsymbol{\sigma} \cdot \check{\mathbf{n}} = -\mathbf{D}(\mathbf{u}) \ . \tag{5.11}$$

     An impermeable wall with drag would have the following condition:
  $$\mathbf{u} \cdot \check{\mathbf{n}} = 0 \ , \qquad (\boldsymbol{\sigma} \cdot \check{\mathbf{n}})_\tau = -\mathbf{D}(\mathbf{u}) \ , \tag{5.12}$$

     where $\mathbf{v}_\tau$ refers to the tangential component of a vector $\mathbf{v}$, i.e.,
  $$\mathbf{v}_\tau = \mathbf{v} - (\mathbf{v} \cdot \check{\mathbf{n}})\,\check{\mathbf{n}} \ . \tag{5.13}$$

  4. **Free surface with surface tension:**
  $$\boldsymbol{\sigma} \cdot \check{\mathbf{n}} = -\,\gamma\, H\, \check{\mathbf{n}} + (\nabla\,\gamma)_\tau \tag{5.14}$$

     where H is the mean curvature.

  5. **Outflow:** Some combination of the above that tries to minimize the upstream effect of domain truncation.

5.2 Some important variants

The incompressible Navier-Stokes equations as described above are an excellent model for several natural and industrial flows. It is worthwhile however to consider a couple of frequent variants.

5.2.1 Buoyancy-coupled flows

When thermal buoyancy effects are considered, the volume force $\mathbf{f}$ can be modeled by

$$\mathbf{f} = [\rho(T_0) - \rho(T_0)\,\beta\,(T - T_0)]\,\mathbf{g} = \rho_0\,[1 - \beta\,(T - T_0)]\,\mathbf{g} \tag{5.15}$$

in which β is the thermal expansion coefficient

$$\beta = -\frac{d\rho}{dT}(T_0)\,. \tag{5.16}$$

The closed set of equations is then approximated by

$$\rho_0\,\partial_t\mathbf{u} + \rho_0\,(\mathbf{u}\cdot\nabla)\,\mathbf{u} - \nabla\cdot\left[\mu(T)\,(\nabla\mathbf{u} + \nabla\mathbf{u}^T)\right] + \nabla p = \rho_0\,[1 - \beta\,(T - T_0)]\,\mathbf{g} \tag{5.17}$$

$$\nabla\cdot\mathbf{u} = 0 \tag{5.18}$$

$$\partial_t T + \mathbf{u}\cdot\nabla T = \alpha\,\nabla^2 T + q \tag{5.19}$$

where α is the thermal diffusivity ($\alpha = k_T/(\rho\,c_p)$, with k_T the thermal conductivity and c_p the specific heat) and $q = Q/(\rho\,c_p)$, with Q the volumetric heat source.

Notice that the left-hand side of (5.19) is DT/Dt. The model consists of a species that is source of buoyancy (the temperature) which is transported and diffused by the velocity field. Salinity is another important such species.

5.3   Reynolds-averaged Navier-Stokes equations

- In the modeling of incompressible turbulent flows, as we have seen, it is in most cases necessary to solve an averaged version of the Navier-Stokes equations.

- In the pipe-flow example we adopted Nikuradse's formula for the Prandtl's mixing length $\ell(y)$. Such formulae are however only available for some selected flows, in general situations the computation of μ^{t} requires the solution of additional equations.

- There exist 1-equation models, 2-equation models, and so on. Some of the popular ones are known as: Spalart-Allmaras model, $k-\epsilon$ model, $k-\omega$ model, algebraic stress model, stress transport model, etc. An excellent survey is provided by Wilcox (Turbulence modeling for CFD, 2006).

- To provide some insight into RANS modeling, we describe here the $k-\epsilon$ model, which is the most popular 2-equation model.

- Reynolds averaging (substituting $\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'$ in the Navier-Stokes equations and averaging) is the basis of all RANS models:

Exo. 5.4 *Deduce the RANS equations:*

$$\rho\,\partial_t\bar{\mathbf{u}} + \nabla \cdot \left[\bar{p}\,\mathbb{I} - \mu\left(\nabla\bar{\mathbf{u}} + \nabla\bar{\mathbf{u}}^T\right) + \rho\,\bar{\mathbf{u}}\otimes\bar{\mathbf{u}} + \rho\,\overline{\mathbf{u}'\otimes\mathbf{u}'}\right] = \mathbf{f} \tag{5.20}$$

$$\nabla\cdot\bar{\mathbf{u}} = 0 \tag{5.21}$$

The $k - \epsilon$ model

- The mass and momentum equations are as in the non-averaged case, only that **velocity and pressure variables are now averages** and **turbulent viscosity must be added to physical viscosity**. We drop here the bar to express averages for simplicity.

$$\rho \, \partial_t \mathbf{u} + \rho \, (\mathbf{u} \cdot \nabla) \, \mathbf{u} - \nabla \cdot \left[(\mu + \mu^{\mathrm{t}}) \, (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \right] + \nabla p \;\; = \;\; \mathbf{f} \tag{5.22}$$

$$\nabla \cdot \mathbf{u} \;\; = \;\; 0 \tag{5.23}$$

- The turbulent viscosity is given by

$$\mu^{\mathrm{t}} = \frac{c_\mu \, \rho \, k^2}{\epsilon} \; . \tag{5.24}$$

- The turbulent variable k is the **turbulent kinetic energy** per unit mass, the amount of kinetic energy that is contained by the **velocity fluctuations**:

$$k = \frac{1}{2} \, \overline{\|\mathbf{u}'\|^2} \tag{5.25}$$

- The turbulent dissipation ϵ is the **turbulent dissipation rate** per unit mass, the rate at which energy stored in the fluctuations is dissipated:

$$\epsilon = \frac{\mu}{\rho} \, \overline{(\nabla \mathbf{u}' + (\nabla \mathbf{u}')^T) : \nabla \mathbf{u}'} \tag{5.26}$$

- The model for k and ϵ consists of the convection-diffusion-reaction equations

$$\partial_t k + \mathbf{u} \cdot \nabla k - \nabla \cdot (D_k \nabla k) + \gamma_k\, k \;=\; F_k \tag{5.27}$$

$$\partial_t \epsilon + \mathbf{u} \cdot \nabla \epsilon - \nabla \cdot (D_\epsilon \nabla \epsilon) + \gamma_\epsilon\, \epsilon \;=\; F_\epsilon \tag{5.28}$$

where the diffusion coefficients are

$$D_k = \frac{1}{\rho}\left(\frac{\mu^{\mathrm{t}}}{\sigma_k} + \mu\right)\;, \qquad D_\epsilon = \frac{1}{\rho}\left(\frac{\mu^{\mathrm{t}}}{\sigma_\epsilon} + \mu\right)\;, \tag{5.29}$$

the reaction coefficients are

$$\gamma_k = \frac{\epsilon}{k}\;, \qquad \gamma_\epsilon = c_2\,\frac{\epsilon}{k}\;, \tag{5.30}$$

and the source terms are

$$F_k = \frac{\mu^{\mathrm{t}}}{2\rho}\,\|\nabla \mathbf{u} + \nabla \mathbf{u}^T\|^2 \;, \; F_\epsilon = \frac{c_1 k}{2}\,\|\nabla \mathbf{u} + \nabla \mathbf{u}^T\|^2 \;. \tag{5.31}$$

- The model constants have as standard values

$$c_\mu = 0.09\;, \qquad c_1 = 0.126\;, \qquad c_2 = 1.92\;, \qquad \sigma_k = 1.0\;, \qquad \sigma_\epsilon = 1.3\;. \tag{5.32}$$

- The closed system of equations of the $k-\epsilon$ model are (5.22), (5.23), (5.27) and (5.28). One vector equation and three scalar ones, for one vector unknown and three scalar unknown.

- The boundary conditions for this model can vary. Most frequent is the *logarithmic law of the wall* as described in Section 4.4. In the simplified treatment adopted there, they would read:

1. **At inflows:**

$$\mathbf{u} = \mathbf{u}_{\text{in}} \;, \qquad k = k_{\text{in}} \;, \qquad \epsilon = \epsilon_{\text{in}} \;. \tag{5.33}$$

2. **At planar walls:**

$$\mathbf{u} \cdot \check{\mathbf{n}} \;=\; 0 \;, \tag{5.34}$$

$$\left(\mu + \mu^{\text{t}}\right) \frac{\partial \mathbf{u}}{\partial n} \;=\; -\frac{\rho}{196} \, \|\mathbf{u}\|^2 \;, \tag{5.35}$$

$$k \;=\; \frac{u^{*2}}{\sqrt{c_\mu}} \;, \tag{5.36}$$

$$\epsilon \;=\; \frac{\rho \, u^{*4}}{12.3 \, \mu} \;. \tag{5.37}$$

3. **At outflows:** Several possibilities, zero applied forces and zero normal derivatives of k and ϵ for example.

- The equations for k and ϵ can be written in **conservation form**

$$\partial_t k + \nabla \cdot (\mathbf{u}\, k - D_k \, \nabla k) \;=\; F_k - \gamma_k \, k \;, \tag{5.38}$$

$$\partial_t \epsilon + \nabla \cdot (\mathbf{u}\, \epsilon - D_\epsilon \, \nabla \epsilon) \;=\; F_\epsilon - \gamma_\epsilon \, \epsilon \;, \tag{5.39}$$

the expressions in parentheses being the **fluxes**.

Exo. 5.5 *Write down the ODEs that arise from the $k - \epsilon$ model in the case of decaying homogeneous isotropic turbulence (google me).*

Exo. 5.6 *Write down the final differential system to compute $w(r,t)$, $k(r,t)$ and $\epsilon(r,t)$ in a long cylindrical pipe of circular cross section (transient fully developed flow).*

Exo. 5.7 *Read the supplementary material:*

- *A. Lew et al (2001), A note on the numerical treatment of the $k - \epsilon$ turbulence model (Int. J. of CFD).*

- *Chapters 1 and 2 of A. Prosperetti and G. Tryggvason (2007), Computational Methods for Multiphase Flow (Cambridge Univ. Press).*

Prepare a 7-minute summary of each.

- One observes that thermal effects, salinity effects, turbulence, among others, lead to systems which consist of two ingredients:

  – the incompressible Navier-Stokes equations,

  – one or several convection-diffusion-reaction equations.

  These ingredients are coupled through the effective viscosity and/or the volumetric force.

- In turn, the incompressible Navier-Stokes equations can be regarded as the sum of two sub-ingredients:

  – a (nonlinear) convection-diffusion equation for the velocity, assuming the pressure known,

  – the incompressibility constraint.

- The convection-diffusion-reaction equation is a classical topic of courses in numerical methods for PDEs. Readers unfamiliar with concepts such as convective fluxes, diffusive fluxes, upwind discretizations, Péclet number, discrete maximum principles, etc., are encourage to revise Chapters 4 and 5 of Wesseling, or Chapter 4 of Ferziger & Peric.

6 The MAC discretization method of the incompressible Navier-Stokes equations

6.1 Conservation in a rectangle

Consider a finite volume V which is a rectangle of sides h_x and h_y, and denote its edges by E, W, N and S, with exterior normals $(1,0)$, $(-1,0)$, $(0,1)$ and $(0,-1)$, respectively. Our aim here is to obtain explicit expressions for the mass and momentum conservation equations in this rectangle.

The mass flux vector $\rho\,\mathbf{u}$ must satisfy

$$\int_{\partial V} \rho\,\mathbf{u} \cdot \check{\mathbf{n}}\ dS = 0 \ . \tag{6.1}$$

The momentum flux vector

$$\boldsymbol{\zeta} = p\,\mathbb{I} - \mu\,(\nabla\mathbf{u} + \nabla\mathbf{u}^T) + \rho\,\mathbf{u} \otimes \mathbf{u} \tag{6.2}$$

consists of three terms, which we denote by *pressure*, *viscous* and *inertia* terms.

The momentum equation contains the integral of $\boldsymbol{\zeta} \cdot \check{\mathbf{n}}$ over the boundary of V, which is the only nontrivial part to calculate and is detailed below. In what follows we adopt the usual notation of (x, y) instead of (x_1, x_2), and (u, v) instead of (u_1, u_2).

6.1.1 Mass conservation

The discrete mass conservation equation reads

$$(u_E - u_W)\,h_y + (v_N - v_S)\,h_x = 0 \ . \tag{6.3}$$

The finite volumes for this equation are centered at pressure nodes and have as unknowns u_E, u_W, v_N and v_S, exactly as needed and thus requiring no interpolation.

In matrix form (ignoring for now boundary conditions),

$$\underline{\underline{D_x}}\,\underline{u} \ + \ \underline{\underline{D_y}}\,\underline{v} \ = \ 0 \tag{6.4}$$

6.1.2 Momentum along the x_1 direction

For the pressure term,

$$\int_E p\, n_x \, dS \;=\; p_E \, h_y \;, \tag{6.5}$$

$$\int_W p\, n_x \, dS \;=\; -p_W \, h_y \;, \tag{6.6}$$

$$\int_N p\, n_x \, dS \;=\; 0 \;, \tag{6.7}$$

$$\int_S p\, n_x \, dS \;=\; 0 \;. \tag{6.8}$$

For the viscous term, integrating edge by edge,

$$-\left(\int_E \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)\check{n}dS\right)_x = -\int_E 2\mu\, \partial_x u \; dy = -2\,\mu\, \partial_x u|_E \, h_y \;=\; (\mathrm{VE}) \;, \tag{6.9}$$

$$-\left(\int_W \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)\check{n}dS\right)_x = +\int_W 2\mu\, \partial_x u \; dy = 2\,\mu\, \partial_x u|_W \, h_y \;=\; (\mathrm{VW}) \;, \tag{6.10}$$

$$-\left(\int_N \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)\check{n}dS\right)_x = -\int_N \mu \left(\partial_y u + \partial_x v\right) \, dx = -\,\mu \left(\partial_y u + \partial_x v\right)|_N \, h_x \;=\; (\mathrm{VN}) \;, \tag{6.11}$$

$$-\left(\int_S \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)\check{n}dS\right)_x = +\int_S \mu \left(\partial_y u + \partial_x v\right) \, dx = \mu \left(\partial_y u + \partial_x v\right)|_N \, h_x \;=\; (\mathrm{VS}) \;. \tag{6.12}$$

For the inertia term, the x component being $\int_{\partial V} \rho\, u\, \mathbf{u} \cdot \check{\mathbf{n}}\, dS$,

$$\int_E \rho\, u\, \mathbf{u} \cdot \check{\mathbf{n}}\, dS \;=\; \rho\, u_E^2\, h_y \;, \tag{6.13}$$

$$\int_W \rho\, u\, \mathbf{u} \cdot \check{\mathbf{n}}\, dS \;=\; -\rho\, u_W^2\, h_y \;, \tag{6.14}$$

$$\int_N \rho\, u\, \mathbf{u} \cdot \check{\mathbf{n}}\, dS \;=\; \rho\, u_N\, v_N\, h_x \;, \tag{6.15}$$

$$\int_S \rho\, u\, \mathbf{u} \cdot \check{\mathbf{n}}\, dS \;=\; -\rho\, u_S\, v_S\, h_x \;. \tag{6.16}$$

Now we introduce the staggered arrangement of variables, in which the unknowns are:

- For pressure: p_E, p_W.

- For u: u_P, u_{EE}, u_{WW}, u_{NN}, u_{SS}.

- For v: v_{NE}, v_{NW}, v_{SE}, v_{SW}.

Then, the pressure term becomes

$$(\mathrm{P}) \;=\; \int_{\partial V} p\, n_x\, dS = (p_E - p_W)\, h_y \;. \tag{6.17}$$

or, in matrix form,

$$(\mathrm{P}) \;=\; h_x\, h_y\, \underline{\underline{G_x}}\, \underline{p} \;. \tag{6.18}$$

The viscous term becomes

- East face:
$$(\text{VE}) \; = \; -2\,\mu\,\frac{u_{EE} - u_P}{h_x}\,h_y \tag{6.19}$$

- West face:
$$(\text{VW}) \; = \; -2\,\mu\,\frac{u_{WW} - u_P}{h_x}\,h_y \tag{6.20}$$

- North face:
$$(\text{VN}) \; = \; -\,\mu\,\left(\frac{u_{NN} - u_P}{h_y} + \frac{v_{NE} - v_{NW}}{h_x}\right)h_x \tag{6.21}$$

- South face:
$$(\text{VS}) \; = \; -\,\mu\,\left(\frac{u_{SS} - u_P}{h_y} + \frac{v_{SW} - v_{SE}}{h_x}\right)h_x \tag{6.22}$$

Now one observes that, from the geometry of the cell and mass conservation,

$$(u_{EE} - u_P)\,h_y \; + \; (v_{NE} - v_{SE})\,h_x = 0 \; , \quad \text{and} \quad (u_P - u_{WW})\,h_y \; + \; (v_{NW} - v_{SW})\,h_x = 0 \; . \tag{6.23}$$

This cancels some of the terms above, so that the viscous contribution ends up being

$$(\text{VX}) \; = \; -\,\mu\,\left(\frac{u_{EE} - u_P}{h_x}\,h_y + \frac{u_{WW} - u_P}{h_x}\,h_y + \frac{u_{NN} - u_P}{h_y}\,h_x + \frac{u_{SS} - u_P}{h_y}\,h_x\right) \tag{6.24}$$

or

$$(\text{VX}) \; = \; -\,\mu\,h_x\,h_y\,\underline{\underline{L}}\,\underline{u} \; . \tag{6.25}$$

We will leave the inertia term in its original form

$$(\text{IX}) \;=\; \rho \left(u_E^2 - u_W^2 + u_N v_N - u_S v_S \right) \;, \tag{6.26}$$

complemented by a centered interpolation:

$$u_E = \frac{u_{EE} + u_P}{2} \;, \qquad u_W = \frac{u_{WW} + u_P}{2} \;, \tag{6.27}$$

$$u_N = \frac{u_{NN} + u_P}{2} \;, \qquad u_S = \frac{u_{SS} + u_P}{2} \;, \tag{6.28}$$

$$v_N = \frac{v_{NE} + v_{NW}}{2} \;, \qquad v_S = \frac{v_{SE} + v_{SW}}{2} \;. \tag{6.29}$$

Notice that the vector of values of u_E at all east faces of finite volumes centered in nodes of u can be built as $\underline{u_E} = \underline{\underline{A_{xu}^E}}\, \underline{u}$, where $\underline{\underline{A_{xu}^E}}$ is an interpolation matrix. Similar matrix operations can be devised for the other necessary quantities.

Adding up the three contributions, one arrives at (after dividing by $h_x h_y$)

$$\rho \frac{d}{dt} \underline{u} \;+\; \underline{\underline{G_x}}\, \underline{p} \;-\; \mu \underline{\underline{L}}\, \underline{u} + \; \text{IX}(\underline{u}, \underline{v}) \;=\; \underline{f_x} \;. \tag{6.30}$$

6.1.3 Momentum along the y direction

Exo. 6.1 *Perform the analogous set of calculations that lead to the discrete momentum equation along the y direction.*

One arrives, eventually, to

$$\rho \, \frac{d}{dt} \, \underline{v} \; + \; \underline{\underline{G_y}} \, \underline{p} \; - \; \mu \, \underline{\underline{L}} \, \underline{v} \; + \; \mathrm{IY}(\underline{u}, \underline{v}) = \underline{f_y} \tag{6.31}$$

6.2 Semi-discrete system

$$\rho \frac{d}{dt} \underline{u} \; + \; \underline{\underline{G_x}} \; \underline{p} \; - \; \mu \underline{\underline{L}} \underline{u} + \; \mathrm{IX}(\underline{u}, \underline{v}) \quad = \quad \underline{f_x} \tag{6.32}$$

$$\rho \frac{d}{dt} \underline{v} \; + \; \underline{\underline{G_y}} \underline{p} \; - \; \mu \underline{\underline{L}} \underline{v} \; + \; \mathrm{IY}(\underline{u}, \underline{v}) \quad = \quad \underline{f_y} \tag{6.33}$$

$$\underline{\underline{D_x}} \; \underline{u} \; + \; \underline{\underline{D_y}} \; \underline{v} \quad = \quad 0 \tag{6.34}$$

which can even be simplified to, with some additional quite natural notations,

$$\rho \frac{d}{dt} \underline{U} \; + \; \underline{\underline{G}} \; \underline{p} \; - \; \mu \underline{\underline{L}} \underline{U} + \; \mathrm{I}(\underline{U}) \quad = \quad \underline{f} \tag{6.35}$$

$$\underline{\underline{D}} \; \underline{U} \quad = \quad 0 \tag{6.36}$$

This is a so-called *differential-algebraic equation* (DAE) system.

6.3 Monolithic system

$$\rho \frac{\underline{U}^{n+1} - \underline{U}^n}{\Delta t} \; + \; \underline{\underline{G}} \; \underline{p}^{n+\theta} \; - \; \mu \underline{\underline{L}} \underline{U}^{n+\theta} + \; \mathrm{I}(\underline{U}^{n+\theta}) \quad = \quad \underline{f}^{n+\theta} \tag{6.37}$$

$$\underline{\underline{D}} \; \underline{U}^{n+1} \quad = \quad 0 \tag{6.38}$$

6.4 Projection method

Chorin's (1968) original projection method was defined as follows:

- **Momentum predictor**:

$$\rho \frac{\hat{\underline{U}}^{n+1} - \underline{U}^n}{\Delta t} - \mu \underline{\underline{L}}\, \underline{U}^n + \mathrm{I}(\underline{U}^n) = \underline{f}^n \tag{6.39}$$

  The resulting $\hat{\underline{U}}^{n+1}$ does not satisfy $\underline{\underline{D}}\, \hat{\underline{U}}^{n+1} = 0$, it has to be *projected back* on the discretely-incompressible space.

- **Pressure Poisson equation**:

$$\underline{\underline{D}}\, \underline{\underline{G}}\, \underline{p}^{n+1} = \frac{\rho}{\Delta t}\, \underline{\underline{D}}\, \hat{\underline{U}}^{n+1} \tag{6.40}$$

  The product $\underline{\underline{D}}\, \underline{\underline{G}}$ is a matrix that, leaving aside boundary conditions, coincides with $\underline{\underline{L}}$ (the discrete Laplacian matrix). This is a salient property of the MAC discretization.

- **Velocity correction**:

$$\underline{U}^{n+1} = \hat{\underline{U}}^{n+1} - \frac{\Delta t}{\rho}\, \underline{\underline{G}}\, \underline{p}^{n+1} \tag{6.41}$$

Eliminating $\hat{\underline{U}}^{n+1}$ one gets

$$\rho \frac{\underline{U}^{n+1} - \underline{U}^n}{\Delta t} + \underline{\underline{G}}\, \underline{p}^{n+1} - \mu \underline{\underline{L}}\, \underline{U}^n + \mathrm{I}(\underline{U}^n) = \underline{f}^n \tag{6.42}$$

$$\underline{\underline{D}}\, \underline{U}^{n+1} = 0 \tag{6.43}$$

which shows that the algorithm is consistent, but clearly of first order in Δt.

6.5   ABCN time discretization

The following combination of Adams-Bashforth scheme for time discretization of the inertia terms, combined with Crank-Nicholson scheme for the viscous term, is a popular method with formally second order accuracy in time.

- **Momentum predictor**:

$$\rho \frac{\hat{\underline{U}}^{n+1} - \underline{U}^n}{\Delta t} - \frac{\mu}{2} \underline{\underline{L}} \, (\hat{\underline{U}}^{n+1} + \underline{U}^n) + \frac{3}{2} \, \underline{\mathrm{I}}(\underline{U}^n) - \frac{1}{2} \, \underline{\mathrm{I}}(\underline{U}^{n-1}) = \underline{f}^{n+\frac{1}{2}} \tag{6.44}$$

- **Pressure Poisson equation**:

$$\underline{\underline{D}} \, \underline{\underline{G}} \, \underline{\phi}^{n+1} = \frac{\rho}{\Delta t} \, \underline{\underline{D}} \, \hat{\underline{U}}^{n+1} \tag{6.45}$$

- **Velocity correction**:

$$\underline{U}^{n+1} = \hat{\underline{U}}^{n+1} - \frac{\Delta t}{\rho} \, \underline{\underline{G}} \, \underline{\phi}^{n+1} \tag{6.46}$$

Exo. 6.2 *Read Chapter 7 of Wesseling.   Explain the necessity of pressure stabilization in the case of collocated discretization (all variables located at cell centers).* Hint: Show that in collocated discretization the stencil corresponding to $\underline{\underline{D}} \, \underline{\underline{G}} \, \underline{p}$ is

$$\frac{p_{i+2,j} - 2 \, p_{i,j} + p_{i-2,j}}{h_x^2} + \frac{p_{i,j+2} - 2 \, p_{i,j} + p_{i,j-2}}{h_y^2} \tag{6.47}$$

so that adjacent pressure unknowns are completely decoupled.

Exo. 6.3 *Read Sousa et al (2015) for more projection-like methods and a warning about the usage of projection methods for low inertia flows.*