Introduction to Computational Fluid Dynamics

Gustavo C. Buscaglia

Graduate course

ICMC-USP, São Carlos, Brasil
gustavo.buscaglia@gmail.com

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>

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

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

<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>

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

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

Double contraction:

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

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

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

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

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:

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

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

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.