Mathematical methods in fluid dynamics

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Contents

Introduction

This text represents lecture notes for the course **Mathematical methods in fluid dynamics** (01MMDY), taught at FNSPE CTU in Prague in the first year of the Master's degree "Mathematical Engineering" study program.

The first part deals with derivation of conservation laws and the problems for partial differential equations generally used describe fluid flow. There is a considerable overlap with classic continuum mechanics courses, with an emphasis on the study of flow. The second part is devoted to the mathematical analysis of the problem of incompressible flow. Great attention is paid to the explanation of all the mathematical terms and concepts used. The final part is focused more practically. It contains the formulation of problems and approaches in specific applications. These also include more complex phenomena and processes in which flow plays a central role. Students thus gain an overview of the various approaches used in mathematical modeling of processes in nature and industry. The course covers the following topics:

1. Formulation and brief derivation of conservation laws in a fluid (continuity equation, Navier-Stokes equations, energy equation)
2. Euler's equations, boundary conditions for viscous and inviscid flow problems.
3. Irrotational flow, potential equation.
4. Basic qualitative properties of the Navier-Stokes equations - strong and weak solutions, questions of existence and uniqueness in stationary and non-stationary cases.
5. Flow problems, formulation of flow equations in a lower dimension, boundary conditions in a lower dimension.
6. Turbulent flow and turbulence modeling, Reynolds-averaged NS equations and filtering.
7. Thermodynamics of fluids, heat transfer, radiation.
8. Reacting multicomponent flow, combustion modeling.
9. Multiphase flow, phase transitions.
10. Dimensionless numbers characterizing the flow.
11. Flow problems with a free boundary.

CHAPTER

1 Mathematical apparatus

1.1 Vectors

- A vector $\boldsymbol{x} \in \mathbb{R}^n$ is a column of real numbers

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = (x_1, x_2, \ldots, x_n)^{\mathrm{T}}.$$

  Vectors of the standard basis of $\mathbb{R}^n$ will be denoted by $\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_n$, with

$$\boldsymbol{e}_\ell = (\delta_{\ell 1}, \delta_{\ell 2}, \ldots, \delta_{\ell n})^{\mathrm{T}} \quad \forall \ell \in \hat{n}.$$

- For the *dot product* of two vectors $\boldsymbol{a} = (a_1, a_2, \ldots, a_n)$ and $\boldsymbol{b} = (b_1, b_2, \ldots, b_n)$, we will consider consistently the standard inner (scalar) product v $\mathbb{R}^n$ and write using the symbol $\cdot$ or matrix multiplication

$$\boldsymbol{a} \cdot \boldsymbol{b} = \boldsymbol{a}^{\mathrm{T}} \boldsymbol{b} = \sum_{i=1}^{n} a_i b_i.$$

  It applies

$$\boldsymbol{a} \cdot \boldsymbol{b} = \|\boldsymbol{a}\| \, \|\boldsymbol{b}\| \cos(\theta), \tag{1.1}$$

  where θ is the angle between the vectors $\boldsymbol{a}$ and $\boldsymbol{b}$.

- Euclidean norm of a vector $\boldsymbol{a} = (a_1, a_2, \ldots, a_n)$ induced by the standard inner product is

$$\|\boldsymbol{a}\| = |\boldsymbol{a} \cdot \boldsymbol{a}|^{\frac{1}{2}} = \left(\sum_{i=1}^{n} |a_i|^2 \right)^{\frac{1}{2}}.$$

- The cross (vector) product of two vectors $\boldsymbol{a} = (a_1, a_2, a_3)$ and $\boldsymbol{b} = (b_1, b_2, b_3)$ in $\mathbb{R}^3$ is an anticommutative operation defined by the relation

$$\boldsymbol{a} \times \boldsymbol{b} = \begin{vmatrix} \boldsymbol{e}_1 & \boldsymbol{e}_2 & \boldsymbol{e}_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} = \begin{pmatrix} a_2 b_3 - a_3 b_2 \\ a_3 b_1 - a_1 b_3 \\ a_1 b_2 - a_2 b_1 \end{pmatrix} = -\boldsymbol{b} \times \boldsymbol{a}.$$

The Lagrange identity holds for the magnitude (norm) of the cross product

$$\|\boldsymbol{a}\times\boldsymbol{b}\|^2 = \|\boldsymbol{a}\|^2\|\boldsymbol{b}\|^2 - |\boldsymbol{a}\cdot\boldsymbol{b}|^2 = \det\begin{pmatrix} \boldsymbol{a}\cdot\boldsymbol{a} & \boldsymbol{a}\cdot\boldsymbol{b} \\ \boldsymbol{b}\cdot\boldsymbol{a} & \boldsymbol{b}\cdot\boldsymbol{b} \end{pmatrix}, \tag{1.2}$$

where the determinant of the so-called Gram matrix (a Gramian) appears on the right-hand side. Note that the cross product can also be expressed using an angle θ between the vectors $\boldsymbol{a}$ and $\boldsymbol{b}$

$$\boldsymbol{a}\times\boldsymbol{b} = \|\boldsymbol{a}\|\,\|\boldsymbol{b}\|\sin(\theta)\,\boldsymbol{n},$$

where $\boldsymbol{n}$ is a unit vector perpendicular to the plane given by the vectors $\boldsymbol{a}$ and $\boldsymbol{b}$. If $\boldsymbol{a},\boldsymbol{b}$ are linearly dependent, $\boldsymbol{a}\times\boldsymbol{b} = \boldsymbol{0}$ holds.

1.2 Concept of a Tensor Field

In fluid dynamics, there are objects called *tensors*, but for our purposes, the general concept of a tensor can be greatly simplified. Nevertheless, we will advantageously use the notations that occur in the tensor algebra, and it is therefore beneficial to be aware of the connections.

1.2.1 What is a Tensor

Let V be a vector space of dimension n over the field T. Tensor $\mathbf{T}$ of type (p,q) $(p,q\in\mathbb{N}_0)$ and order $p+q$ is a multilinear form

$$\mathbf{T}: \underbrace{V^*\times V^*\times\cdots\times V^*}_{p\text{-times}}\times\underbrace{V\times V\times\cdots\times V}_{q\text{-times}}\to\mathbb{R},$$

or, alternatively, an element of the tensor product of spaces

$$\mathbf{T}\in\underbrace{V\otimes V\otimes\cdots\otimes V}_{p\text{-times}}\otimes\underbrace{V^*\otimes V^*\otimes\cdots\otimes V^*}_{q\text{-times}}.$$

For example, a $(1,0)$-tensor is by both these definitions

$$\boldsymbol{v}: V^*\to\mathbb{R},\ \text{or}\ \boldsymbol{v}\in V,$$

respectively, i.e. it is a vector. A unique correspondence between the two definitions is ensured by the Riesz theorem 1.7.2. Likewise, for a $(0,1)$-tensor, we have

$$\underline{\boldsymbol{w}}: V\to\mathbb{R},\ \text{or}\ \underline{\boldsymbol{w}}\in V^*,$$

i.e. it is a linear functional.

Definition of $\mathbf{T}$ is independent of the choice of basis. In a given basis $\mathscr{X}$, however, a tensor can be expressed by a $(p+q)$- dimensional table („matrix“) of numbers from T in the form

$$\lceil\mathbf{T}\rceil_{\mathscr{X}} \equiv \hat{\mathbf{T}} = \left(\tau^{j_1 j_2\cdots j_p}_{i_1 i_2\cdots i_q}\right)$$

A (p,q)-type tensor $\mathbf{T}$ where $p=0$ is called *covariant*. For $q=0$, $\mathbf{T}$ is *contravariant*. If $pq>0$, $\mathbf{T}$ is tensor of mixed type (q-covariant and p-contravariant).

1.2.2 Einstein's Summation Rule

In an term expressed in tensor elements, any index appearing twice implies summation over the respective index. For example

$$\rho^{i}_{klm} = \sigma^{ij}_{k\ell}\tau_{jm} := \sum_{j=1}^{n} \sigma^{ij}_{k\ell}\tau_{jm}. \tag{1.3}$$

Summation index (here j) appears once as a superscript and once as a subscript. If for example $\mathbf{T}$ is a 3rd order tensor of type $(1,2)$, by its application to the triplet $\left(\underline{\boldsymbol{u}}, \boldsymbol{v}, \boldsymbol{w}\right) \in V^* \times V^2$, we get

$$\mathbf{T}\left(\underline{\boldsymbol{u}}, \boldsymbol{v}, \boldsymbol{w}\right) = \tau^{i}_{jk} u_i v^j w^k.$$

1.2.3 Tensor Product and Inner Product

Let $\mathbf{S}, \mathbf{T}$ be two tensors with the representations (in the basis $\mathscr{X}$)

$$\hat{\mathbf{S}} = \left(\sigma^{k_1 k_2 \cdots k_r}_{\ell_1 \ell_2 \cdots \ell_s}\right), \hat{\mathbf{T}} = \left(\tau^{j_1 j_2 \cdots j_p}_{i_1 i_2 \cdots i_q}\right).$$

By the *tensor product* of these two tensors, we understand the $\mathbf{U} = \mathbf{S} \otimes \mathbf{T}$ with a representation

$$\hat{\mathbf{U}} = \left(\mu^{k_1 k_2 \cdots k_r j_1 j_2 \cdots j_p}_{\ell_1 \ell_2 \cdots \ell_s i_1 i_2 \cdots i_q}\right),$$

where

$$\mu^{k_1 k_2 \cdots k_r j_1 j_2 \cdots j_p}_{\ell_1 \ell_2 \cdots \ell_s i_1 i_2 \cdots i_q} = \sigma^{k_1 k_2 \cdots k_r}_{\ell_1 \ell_2 \cdots \ell_s} \tau^{j_1 j_2 \cdots j_p}_{i_1 i_2 \cdots i_q}.$$

The *inner (scalar) product* of two tensors of conjugate type (later from Sect 1.2.8 de facto of the same type)

$$\hat{\mathbf{S}} = \left(\sigma^{j_1 j_2 \cdots j_p}_{i_1 i_2 \cdots i_q}\right), \hat{\mathbf{T}} = \left(\tau^{i_1 i_2 \cdots i_q}_{j_1 j_2 \cdots j_p}\right)$$

is a scalar

$$\mathbf{S} \odot \mathbf{T} = \sigma^{j_1 j_2 \cdots j_p}_{i_1 i_2 \cdots i_q} \tau^{i_1 i_2 \cdots i_q}_{j_1 j_2 \cdots j_p}.$$

1.2.4 Covariance and Contravariance, Transformation of Basis

Let $\mathscr{X} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)$, $\mathscr{Y} = \left(\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n\right)$ be bases of the vector space V. Let $\boldsymbol{v} \in V$. Then

$$\boldsymbol{v} = \sum_{j=1}^{n} \underline{\boldsymbol{x}}^j(\boldsymbol{v})\, \boldsymbol{x}_j = \sum_{i=1}^{n} \underline{\boldsymbol{y}}^i(\boldsymbol{v})\, \boldsymbol{y}_i,$$

where $\underline{\boldsymbol{x}}^i, \underline{\boldsymbol{y}}^i$ denote the i-th coordinate functionals in the bases $\mathscr{X}, \mathscr{Y}$[1]. Next, let us denote the column vectors of the coordinates of the vector $\boldsymbol{v}$ in the bases $\mathscr{X}, \mathscr{Y}$, respectively, as $\lceil \boldsymbol{v} \rceil_{\mathscr{X}}, \lceil \boldsymbol{v} \rceil_{\mathscr{Y}}$. The i-th coordinate of the vector $\boldsymbol{v}$ in the basis $\mathscr{Y}$ can be obtained through the coordinates in the basis $\mathscr{X}$ according to

$$\underline{\boldsymbol{y}}^i(\boldsymbol{v}) = \underline{\boldsymbol{y}}^i\left(\sum_{j=1}^{n} \underline{\boldsymbol{x}}^j(\boldsymbol{v})\, \boldsymbol{x}_j\right) = \sum_{j=1}^{n} \underline{\boldsymbol{y}}^i\left(\boldsymbol{x}_j\right) \underline{\boldsymbol{x}}^j(\boldsymbol{v}),$$

or

$$\lceil \boldsymbol{v} \rceil_{\mathscr{Y}} = {}^{\mathscr{X}}\hat{\mathbf{P}}^{\mathscr{Y}} \lceil \boldsymbol{v} \rceil_{\mathscr{X}} = \left({}^{\mathscr{X}}\hat{\mathbf{P}}^{\mathscr{Y}}\right)^{-1} \lceil \boldsymbol{v} \rceil_{\mathscr{X}}, \tag{1.4}$$

where

$${}^{\mathscr{X}}\hat{\mathbf{P}}^{\mathscr{Y}} = \left(\boldsymbol{y}^i\left(\boldsymbol{x}_j\right)\right) = \left(\lceil \boldsymbol{x}_1 \rceil_{\mathscr{Y}} \ldots \lceil \boldsymbol{x}_n \rceil_{\mathscr{Y}}\right) \tag{1.5}$$

[1] We write the indices of the coordinate functionals at the top, just like the components of the vector in standard basis.

is the transition matrix[2] from the basis $\mathscr{X}$ to the base $\mathscr{Y}$. For the transition matrix from $\mathscr{Y}$ to $\mathscr{X}$, an analogous formula

$$ {}^{\mathscr{Y}}\hat{\mathbf{P}}^{\mathscr{X}} = \left(\boldsymbol{x}^i\left(\boldsymbol{y}_j\right)\right) = \left(\lceil \boldsymbol{y}_1 \rceil_{\mathscr{X}} \cdots \lceil \boldsymbol{y}_n \rceil_{\mathscr{X}}\right) $$

holds and from the relationship

$$ \lceil \boldsymbol{v} \rceil_{\mathscr{Y}} = {}^{\mathscr{X}}\hat{\mathbf{P}}^{\mathscr{Y}} \lceil \boldsymbol{v} \rceil_{\mathscr{X}} = {}^{\mathscr{X}}\hat{\mathbf{P}}^{\mathscr{Y}}\,{}^{\mathscr{Y}}\hat{\mathbf{P}}^{\mathscr{X}} \lceil \boldsymbol{v} \rceil_{\mathscr{Y}}, $$

it is obvious that ${}^{\mathscr{Y}}\hat{\mathbf{P}}^{\mathscr{X}} = \left({}^{\mathscr{X}}\hat{\mathbf{P}}^{\mathscr{Y}}\right)^{-1}$.

Now, let us specifically choose $V = \mathbb{R}^n$ and denote $\hat{\mathbf{X}} = (\boldsymbol{x}_1 \cdots \boldsymbol{x}_n)$, $\hat{\mathbf{Y}} = \left(\boldsymbol{y}_1 \cdots \boldsymbol{y}_n\right)$. Let there be a transformation relation between the bases in the form

$$ \hat{\mathbf{Y}} = \hat{\mathbf{X}}\hat{\mathbf{A}}, \tag{1.6} $$

where $\hat{\mathbf{A}} \in \mathbb{R}^{n\times n}$ is a regular matrix. Then for the vector $\boldsymbol{v} \in \mathbb{R}^n$, we have

$$ \hat{\mathbf{Y}} \lceil \boldsymbol{v} \rceil_{\mathscr{Y}} = \hat{\mathbf{X}}\hat{\mathbf{A}} \lceil \boldsymbol{v} \rceil_{\mathscr{Y}} = \hat{\mathbf{X}} \lceil \boldsymbol{v} \rceil_{\mathscr{X}}, $$

from which

$$ \lceil \boldsymbol{v} \rceil_{\mathscr{Y}} = \hat{\mathbf{A}}^{-1} \lceil \boldsymbol{v} \rceil_{\mathscr{X}}. \tag{1.7} $$

By comparing (1.4) a (1.7), we see that

$$ {}^{\mathscr{X}}\hat{\mathbf{P}}^{\mathscr{Y}} = \hat{\mathbf{A}}^{-1}, $$

and therefore also ${}^{\mathscr{Y}}\hat{\mathbf{P}}^{\mathscr{X}} = \hat{\mathbf{A}}$. When transforming the representation in the basis $\mathscr{X}$ to the basis $\mathscr{Y}$, the coordinates of the vector are transformed inversely (*contravariantly*, i.e., „against“) to the transformation of bases.

Next, let $\underline{\boldsymbol{w}} \in V^*$. Then

$$ \underline{\boldsymbol{w}}(\boldsymbol{v}) = \underline{\boldsymbol{w}}\left(\sum_{j=1}^{n} \underline{\boldsymbol{x}}^j(\boldsymbol{v})\,\boldsymbol{x}_j\right) = \sum_{j=1}^{n} \underline{\boldsymbol{x}}^j(\boldsymbol{v})\,\underline{\boldsymbol{w}}\left(\boldsymbol{x}_j\right) = \left(\sum_{j=1}^{n} \underline{\boldsymbol{w}}\left(\boldsymbol{x}_j\right)\underline{\boldsymbol{x}}^j\right)(\boldsymbol{v}), $$

i.e., the j-th coordinate of $\underline{\boldsymbol{w}}$ in the dual basis $\mathscr{X}^* = \left(\underline{\boldsymbol{x}}^1, \ldots, \underline{\boldsymbol{x}}^n\right)$ is equal to $\underline{\boldsymbol{w}}\left(\boldsymbol{x}_j\right)$. For coordinates in the basis $\mathscr{Y}^*$, the relationship

$$ \underline{\boldsymbol{w}}\left(\boldsymbol{y}_i\right) = \underline{\boldsymbol{w}}\left(\sum_{j=1}^{n} \underline{\boldsymbol{x}}^j\left(\boldsymbol{y}_i\right)\boldsymbol{x}_j\right) = \sum_{j=1}^{n} \underline{\boldsymbol{x}}^j\left(\boldsymbol{y}_i\right)\underline{\boldsymbol{w}}\left(\boldsymbol{x}_j\right) $$

holds. For $V = \mathbb{R}^n$, it can be expressed as

$$ \left\lceil \underline{\boldsymbol{w}} \right\rceil_{\mathscr{Y}^*} = \left({}^{\mathscr{Y}}\hat{\mathbf{P}}^{\mathscr{X}}\right)^{\mathrm{T}} \left\lceil \underline{\boldsymbol{w}} \right\rceil_{\mathscr{X}^*}, $$

and with the primary bases bound by (1.6), we get

$$ \begin{aligned} \left\lceil \underline{\boldsymbol{w}} \right\rceil_{\mathscr{Y}^*} &= \hat{\mathbf{A}}^{\mathrm{T}} \left\lceil \underline{\boldsymbol{w}} \right\rceil_{\mathscr{X}^*}, \\ \left\lceil \underline{\boldsymbol{w}} \right\rceil_{\mathscr{Y}^*}^{T} &= \left\lceil \underline{\boldsymbol{w}} \right\rceil_{\mathscr{X}^*}^{\mathrm{T}} \hat{\mathbf{A}}. \end{aligned} \tag{1.8} $$

Hence, when changing the representation in the basis $\mathscr{X}^*$ to the basis $\mathscr{Y}^*$, the coordinates of the linear functional are transformed in the same way (covariantly) as the bases. Linear functionals are therefore also called covariant vectors or *covectors*.

[2] also referred to as *change-of-basis matrix*

1.2.5 Covectors as „Darts“

In a finite-dimensional space V with the inner product $(\cdot,\cdot)$, every element $\underline{\boldsymbol{w}} \in V^*$ has unique representative $\boldsymbol{u} \in V$ such that

$$(\boldsymbol{v}, \boldsymbol{u}) = \underline{\boldsymbol{w}}(\boldsymbol{v}) \ \forall \boldsymbol{v} \in V,$$

as given by the Riesz theorem 1.7.2[3]. In particular, each dual basis $\mathscr{X}^* = \left(\underline{\boldsymbol{x}}^1, \ldots, \underline{\boldsymbol{x}}^n\right)$ has a corresponding linearly independent system of representative vectors $\mathscr{X}^{**} = \left(\boldsymbol{\chi}^1, \ldots, \boldsymbol{\chi}^n\right)$ which forms the so called *covariant basis* of V.

1.2.6 Contravariant and Covariant Vectors in Physics

In the following text, we will try to consistently use Einstein's summation rule (1.3), if it becomes clear through which coordinates the summation takes place.

- vector: position, velocity, momentum (units have the length unit in the numerator)
- covector: function gradient (units have length unit in the denominator)
  - from the relationship $\langle \nabla f(\boldsymbol{x}), \boldsymbol{v} \rangle = \mathrm{d}f(\boldsymbol{x})\,\boldsymbol{v}$ it can be seen that the gradient has the nature of a linear functional

1.2.7 Orthogonal Transformations of Tensors

Consider an orthonormal basis $\mathscr{X} = (\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$ of the space $\mathbb{R}^3$. In that case, the j-th coordinate of any vector $\boldsymbol{v} \in V$ in the basis $\mathscr{X}$ is given by the relation

$$\boldsymbol{x}_j \cdot \boldsymbol{v} = \boldsymbol{x}_j \cdot \left(\underline{\boldsymbol{x}}^i(\boldsymbol{v})\,\boldsymbol{x}_i\right) = \underline{\boldsymbol{x}}^i(\boldsymbol{v})\left(\boldsymbol{x}_j \cdot \boldsymbol{x}_i\right) = \underline{\boldsymbol{x}}^j(\boldsymbol{v}).$$

A representative of the covariant vector $\underline{\boldsymbol{x}}^j$ according to the Riesz theorem is therefore a vector $\boldsymbol{x}_j$ and the *covariant* basis $\mathscr{X}^{**}$ coincides with the original (contravariant) basis $\mathscr{X}$. Next, let $\hat{\mathbf{Q}} = \left(\alpha_{ij}\right) \in \mathbb{R}^{3\times 3}$ is an orthogonal transformation matrix that satisfies by definition

$$\hat{\mathbf{Q}}^{\mathrm{T}} = \hat{\mathbf{Q}}^{-1}, \tag{1.9}$$

i.e. covariant and contravariant vectors transform the same way according to (1.7) and (1.8), respectively. As we will stick to orthonormal (and preferably the standard) bases of $\mathbb{R}^3$, we will no longer distinguish between covariant and contravariant vectors and tensors, respectively, and only lower indices will be used.

Given a transformation $\mathbf{Q} = \left(q_{ij}\right)$ from the base $\mathscr{X}$ to the base $\mathscr{Y}$, a tensor $\mathbf{T}$ of order s transforms as

$$\begin{aligned} \hat{\mathbf{T}} &= \lceil \mathbf{T} \rceil_{\mathscr{X}} = \left(\tau_{i_1 \cdots i_s}\right), \\ \hat{\mathbf{T}}' &= \lceil \mathbf{T} \rceil_{\mathscr{Y}} = \left(\tau'_{i_1 \cdots i_s}\right), \end{aligned} \tag{1.10}$$

where

$$\tau'_{i_1 \cdots i_s} = q_{i_1 j_1} \cdots q_{i_s j_s} \tau_{j_1 \cdots j_s}. \tag{1.11}$$

Thanks to (1.9), the inverse transformation reads

$$\tau_{i_1 \cdots i_s} = q_{j_1 i_1} \cdots q_{j_s i_s} \tau'_{j_1 \cdots j_s}. \tag{1.12}$$

For order 2 tensors, we have

$$\tau'_{ij} = q_{iI} q_{jJ} \tau_{IJ}, \text{ i.e. } \mathbf{T}' = \mathbf{Q}^{\mathrm{T}} \mathbf{T} \mathbf{Q}. \tag{1.13}$$

[3] Theorem 1.7.2 is stated for arbitrary-dimensional Hilbert spaces. It can be proved easily for finite-dimensional inner product spaces, which are always complete (Definition 9), and thus Hilbert.

1.2.8 Tensors in Fluid Dynamics

For our purposes, we will consider only vectors and second-order tensors. We will unify the notation for tensor $\mathbf{T}$ and its representation in the standard basis $\hat{\mathbf{T}}$, i.e. in the following text, we will no longer write a hat over the symbols that represent matrices. If we work with the tensor representation $\mathbf{T}$ in the basis transformed by the orthogonal transformation $\mathbf{Q}$, we denote it as $\mathbf{T}'$, which corresponds to the notation in (1.10). Scalar, vector, and tensor physical quantities are dependent on time and on spatial coordinates. These quantities are therefore called scalar, vector, and tensor *fields*, respectively.

For tensors of 2nd order with representation in the standard basis, we define:

- *transpose* of the tensor $\mathbf{T} = (\tau_{ij})$ is a tensor $\mathbf{T}^{\mathrm{T}} = (\tau_{ji})$.
- tensor $\mathbf{E}$ is *symmetric* $\iff \mathbf{E} = \mathbf{E}^{\mathrm{T}}$,
- tensor $\mathbf{W}$ is *skew-symmetric* (also *antisymmetric*) $\iff \mathbf{W} = -\mathbf{W}^{\mathrm{T}}$

and for the uniformity of notation of some relations, we introduce in addition

- inner (scalar) product of tensors
$$\mathbf{S} \cdot \mathbf{T} = \mathbf{S} \odot \mathbf{T} = \sigma_{ij}\tau_{ij}$$
- *inner* (scalar) *product of a tensor and a vector*
$$\boldsymbol{v} \cdot \mathbf{T} = \mathbf{T} \cdot \boldsymbol{v} = \hat{\mathbf{T}}\boldsymbol{v} = (\tau_{ij} v_j), \tag{1.14}$$
i.e. a result of multiplication of a column vector by a matrix from the left (but thanks to this notation and due to the fact that we will usually use it with symmetric tensors, it is not necessary to distinguish column and row vectors).

The following obvious observations apply

- Every tensor $\mathbf{T}$ can be decomposed into a sum of symmetric and skew-symmetric tensor as
$$\mathbf{T} = \mathbf{E} + \mathbf{W} = \frac{1}{2}\left(\mathbf{T} + \mathbf{T}^{\mathrm{T}}\right) + \frac{1}{2}\left(\mathbf{T} - \mathbf{T}^{\mathrm{T}}\right). \tag{1.15}$$
- If $\mathbf{E} = \mathbf{E}^{\mathrm{T}}$ and $\mathbf{W} = -\mathbf{W}^{\mathrm{T}}$, then $\mathbf{E} \cdot \mathbf{W} = \mathbf{0}$.
- In $\mathbb{R}^3$, there is a vector $\boldsymbol{w}$ corresponding to each skew-symmetric tensor $\mathbf{W}$ such that
$$\left(\forall \boldsymbol{v} \in \mathbb{R}^3\right)(\mathbf{W} \cdot \boldsymbol{v} = \boldsymbol{w} \times \boldsymbol{v}). \tag{1.16}$$
Indeed, we have
$$\boldsymbol{w} = (w_i) \iff \mathbf{W} = \begin{pmatrix} 0 & -w_3 & w_2 \\ w_3 & 0 & -w_1 \\ -w_2 & w_1 & 0 \end{pmatrix}. \tag{1.17}$$

1.2.9 Useful Technical Tools and Relationships

We will use the standard symbols

- Kronecker symbol
$$\delta_{ij} = \begin{cases} 0 & i \neq j, \\ 1 & i = j, \end{cases}$$

- and the Levi-Civita symbol

$$\varepsilon_{ijk} = \begin{cases} 1 & \text{if } (i,j,k) \text{ is an even permutation of } (1,2,3), \\ -1 & \text{if } (i,j,k) \text{ is an odd permutation of } (1,2,3), \\ 0 & \text{otherwise.} \end{cases}$$

Using the symbol ε_{ijk}, the i-th component of the cross product $\boldsymbol{a} \times \boldsymbol{b}$ can be easily expressed as

$$(\boldsymbol{a} \times \boldsymbol{b})_i = \varepsilon_{ijk} a_j b_k$$

and the determinant of the matrix $\mathbf{A} = (\alpha_{ij}) \in \mathbb{R}^{3\times 3}$ as

$$\det \mathbf{A} = \varepsilon_{ijk}\alpha_{1i}\alpha_{2j}\alpha_{3k} = \frac{1}{3!}\varepsilon_{IJK}\varepsilon_{ijk}\alpha_{Ii}\alpha_{Jj}\alpha_{Kk}, \tag{1.18}$$

where the rightmost expression sums 6 (equal) values of the determinant $\mathbf{A}$ obtained by calculating determinants of matrices with permuted rows, multiplied by the correct sign.

Remark 1. According to Cramer's rule, it holds for a regular matrix $\mathbf{A} = (\alpha_{ij}) \in \mathbb{R}^{n\times n}$ that

$$\mathbf{A}\boldsymbol{x} = \boldsymbol{b} \iff x_i = \frac{1}{\det \mathbf{A}}\Delta_i, \forall i \in \{1,2,\ldots,n\},$$

where Δ_i is the determinant of the matrix that arises from $\mathbf{A}$ by replacing its i-th column by a vector $\boldsymbol{b}$. By applying Cramer's rule to the equality $\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$ where $\mathbf{A}^{-1} = (\tilde{\alpha}_{ij})$, we get

$$\tilde{\alpha}_{ij} = \frac{1}{\det \mathbf{A}}\Delta_{ji},$$

where Δ_{ji} is the determinant of the matrix $\mathbf{A}_{ji}$, which originated from $\mathbf{A}$ by replacing its i-th column by the j-th column of the unit matrix $\mathbf{I}$. Δ_{ij} (Not Δ_{ji}!) is called the algebraic complement (*cofactor*) of an element α_{ij}, because it appears in the expansion of the determinant $\mathbf{A}$ with respect to the i- th row line, or j-th column). Again, just for $n = 3$,

$$\Delta_{Ii} = \frac{1}{2}\varepsilon_{IJK}\varepsilon_{ijk}\alpha_{Jj}\alpha_{Kk}, \tag{1.19}$$

which includes a sum of two identical results obtained by expanding the determinant of the matrix $\mathbf{A}_{Ii}$ according to the I-th row and i-th column, respectively (hence the factor $\frac{1}{2}$).

1.2.10 Tensor Invariants

An *invariant* of a tensor $\mathbf{T} = (\tau_{ij})$ is a scalar function $\lambda(\mathbf{T})$, whose value is independent of the choice of the (orthonormal) basis of the space $V(= \mathbb{R}^3)$. That is,

$$\lambda\left(\left(\tau'_{ij}\right)\right) = \lambda\left(\left(q_{ik}q_{j\ell}\tau_{k\ell}\right)\right) = \lambda\left(\left(\tau_{ij}\right)\right)$$

for any orthogonal matrix $\mathbf{Q} = (q_{ij}) \in \mathbb{R}^{3\times 3}$.

- For example, the inner (scalar) product of tensors $\mathbf{S} = (\sigma_{ij})$ and $\mathbf{T} = (\tau_{ij})$ is an invariant. Indeed, on can easily show that

$$\sigma'_{ij}\tau'_{ij} = q_{ir}q_{js}\sigma_{rs}q_{ik}q_{j\ell}\tau_{k\ell} = \underbrace{q_{ir}q_{ik}}_{\delta_{rk}}\underbrace{q_{js}q_{j\ell}}_{\delta_{s\ell}}\sigma_{rs}\tau_{k\ell} = \delta_{rk}\delta_{s\ell}\sigma_{rs}\tau_{k\ell} = \sigma_{k\ell}\tau_{k\ell} = \mathbf{S}\cdot\mathbf{T}.$$

- Specially for $\mathbf{S}=\mathbf{I}$ we get the so-called *trace* of the tensor $\mathbf{T}$

$$\mathbf{I}\cdot\mathbf{T}=\delta_{ij}\tau_{ij}=\tau_{ii}=:\mathrm{Tr}\mathbf{T}.$$

Theorem 2. *(Cayley-Hamilton) Every square matrix* $\mathbf{A}\in\mathbb{R}^{n\times n}$ *is a root of its characteristic polynomial*

$$l(\lambda)=\det(\mathbf{A}-\lambda\mathbf{I}).$$

From the fact that

$$\det(\mathbf{BC})=\det\mathbf{B}\det\mathbf{C}$$

for any $\mathbf{B},\mathbf{C}\in\mathbb{R}^{n\times n}$ it follows that the characteristic polynomial obviously does not depend on the choice of basis, and its n of coefficients are called *principal invariants* of the matrix (tensor) $\mathbf{A}$. In $\mathbb{R}^3$, these principal invariants are [Ari62, Mar11]

$$\begin{aligned}{}_{\mathbf{A}}I_1&=\mathrm{Tr}\mathbf{A},\\ {}_{\mathbf{A}}I_2&=\frac{1}{2}\left((\mathrm{Tr}\mathbf{A})^2-\mathrm{Tr}\left(\mathbf{A}^2\right)\right),\\ {}_{\mathbf{A}}I_3&=\det\mathbf{A}.\end{aligned}$$

The tensor $\mathbf{A}$ may (and does) have other invariants, but from each set of invariants, it is possible to select at most three „independent“ ones (for example, these three principal ones), while each the rest can be expressed as a function of the three.

1.2.11 Isotropic Tensors and Tensor Functions

A tensor function $\mathbf{F}:\mathbb{R}^{3\times3}\to\mathbb{R}^{3\times3}$ is called *isotropic*, iff for each orthogonal transformation $\mathbf{Q}$ and each argument $\mathbf{T}$

$$\mathbf{F}'(\mathbf{T})=\mathbf{F}\left(\mathbf{T}'\right),$$

i.e. according to (1.13)

$$\mathbf{Q}^{\mathrm{T}}\mathbf{F}(\mathbf{T})\,\mathbf{Q}\overset{!}{=}\mathbf{F}\left(\mathbf{Q}^{\mathrm{T}}\mathbf{T}\mathbf{Q}\right). \tag{1.20}$$

Component-wise, (1.20) can be interpreted according to the transformation relation (1.11) as

$$\mathbf{F}'\left((\tau_{IJ})\right)_{ij}=q_{ir}q_{js}\mathbf{F}\left((\tau_{IJ})\right)_{rs}\overset{!}{=}\mathbf{F}\left((q_{Ir}q_{Js}\tau_{rs})\right)_{ij}=\mathbf{F}\left((\tau'_{IJ})\right)_{ij}, \tag{1.21}$$

i.e. the map $\mathbf{F}$ performs the same operations over the components of the tensor $\mathbf{T}$, independent of the choice of basis. For a particular choice of basis, the result is always the same tensor.

Now assume a linear function $\mathbf{F}(\mathbf{T})_{ij}=\alpha_{ijk\ell}\tau_{k\ell}+\beta_{ij}$, where $\mathbf{A}=(\varphi_{ijk\ell})$ is a 4th order tensor a $\mathbf{B}$ is a 2nd order tensor. Substituting $\mathbf{F}$ into (1.21), the left-hand side can be written using the inverse transformation relation (1.12) as

$$\begin{aligned}\mathbf{F}'\left((\tau_{IJ})\right)_{ij}&=q_{ir}q_{js}\left(\alpha_{rsk\ell}\tau_{k\ell}+\beta_{rs}\right)=q_{ir}q_{js}\underbrace{q_{Rr}q_{Ss}q_{Kk}q_{L\ell}\alpha'_{RSKL}}_{\alpha_{rsk\ell}}\underbrace{q_{Mk}q_{N\ell}\tau'_{MN}}_{\tau_{k\ell}}+\beta'_{ij}\\ &=\delta_{iR}\delta_{jS}\delta_{KM}\delta_{LN}\alpha'_{RSKL}\tau'_{MN}+\beta'_{ij}=\alpha'_{ijKL}\tau'_{KL}+\beta'_{ij}=\alpha'_{ijk\ell}\tau'_{k\ell}+\beta'_{ij}.\end{aligned}$$

On the right side, we then have

$$\mathbf{F}\left((\tau'_{IJ})\right)_{ij}=\alpha_{ijk\ell}\tau'_{k\ell}+\beta_{ij}.$$

It comes out by comparison that

$$\begin{aligned}\alpha'_{ijk\ell}&=\alpha_{ijk\ell},\\ \beta'_{ij}&=\beta_{ij}.\end{aligned}$$

This means that all components of tensors $\mathbf{A},\mathbf{B}$ must be invariants. We say that tensors $\mathbf{A},\mathbf{B}$ are *isotropic* (i.e. this is different from the isotropy of the tensor function). For example, isotropic tensors are

$$\begin{aligned}\mathbf{I} &= \left(\delta_{ij}\right),\\ &\left(\varepsilon_{ijk}\right),\\ \mathbf{I}\otimes\mathbf{I} &= \left(\delta_{ij}\delta_{k\ell}\right).\end{aligned}$$

It can be shown that the general isotropic tensor must have the form:

- $a\left(\delta_{ij}\right)$ for a tensor of order 2,
- $b\left(\varepsilon_{ijk}\right)$ for a tensor of order 3,
- $a\left(\delta_{ij}\delta_{k\ell}\right)+b\left(\delta_{ik}\delta_{j\ell}\right)+c\left(\delta_{i\ell}\delta_{jk}\right)$ for a tensor of order 4,

where $a,b,c\in\mathbb{R}$.

1.3 Asymptotic Behavior of Functions

We will use Landau symbols o,O with the following meaning. Let $f,g:\mathbb{R}^n\to\mathbb{R}$. Then we write

$$\begin{aligned}f(\boldsymbol{x}) = O\left(g(\boldsymbol{x})\right) &\iff (\exists\delta>0)\,(\exists K>0)\,(\forall x\in\mathbb{R})\left(|x|<\delta \implies \left|f(x)\right|\le K\left|g(x)\right|\right),\\ f(\boldsymbol{x}) = o\left(g(\boldsymbol{x})\right) &\iff \lim_{\boldsymbol{x}\to 0}\frac{f(\boldsymbol{x})}{g(\boldsymbol{x})}=0.\end{aligned}$$

For vector functions $\boldsymbol{f},\boldsymbol{g}:\mathbb{R}^n\to\mathbb{R}^m$ in addition

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{o}\left(\boldsymbol{g}(\boldsymbol{x})\right) \iff (\forall i\in\{1,2,\ldots,m\})\left(\lim_{\boldsymbol{x}\to 0}\frac{f_i(\boldsymbol{x})}{g_i(\boldsymbol{x})}=0\right).$$

1.4 Differential Multivariate Calculus

- Function $\boldsymbol{f}:\mathbb{R}^n\to\mathbb{R}^m$ is a vector of scalar functions $f_\ell:\mathbb{R}^n\to\mathbb{R}$

$$\boldsymbol{f}(\boldsymbol{x}) = \left(f_1(\boldsymbol{x}),\ldots,f_m(\boldsymbol{x})\right)^{\mathrm{T}}.$$

- The *derivative* (total derivative, *total differential*) of a function of n variables $\boldsymbol{f}:\mathbb{R}^n\to\mathbb{R}^m$ at the point $\boldsymbol{x}_0$ will be denoted as $\boldsymbol{f}'(\boldsymbol{x}_0)$ or alternatively $\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}}$.
- *derivative* of a function of multiple variables $\boldsymbol{f}:\mathbb{R}^n\to\mathbb{R}^m$ *with respect to the vector* $\boldsymbol{v}$ at the point $\boldsymbol{x}_0$ is a vector

$$\frac{\partial\boldsymbol{f}}{\partial\boldsymbol{v}}(\boldsymbol{x}_0) := \lim_{h\to 0}\frac{1}{h}\left(\boldsymbol{f}(\boldsymbol{x}_0+h\boldsymbol{v})-\boldsymbol{f}(\boldsymbol{x}_0)\right)$$

and if the total derivative $\boldsymbol{f}'(\boldsymbol{x}_0)$ exists,

$$\frac{\partial\boldsymbol{f}}{\partial\boldsymbol{v}}(\boldsymbol{x}_0) = \boldsymbol{f}'(\boldsymbol{x}_0)\,\boldsymbol{v}$$

holds. If $\boldsymbol{v}$ is a unit vector, we call $\frac{\partial\boldsymbol{f}}{\partial\boldsymbol{v}}(\boldsymbol{x}_0)$ the derivative of a function $\boldsymbol{f}$ *in the direction* $\boldsymbol{v}$ at point $\boldsymbol{x}_0$.

Remark 3. The definition of the total derivative can be restricted to a certain subset of variables. Let there be a given function $\boldsymbol{f} : \mathbb{R}^{n_1+n_2} \to \mathbb{R}^m$, $\boldsymbol{f} = \boldsymbol{f}\left(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}\right)$ where $\boldsymbol{x}^{(1)} \in \mathbb{R}^{n_1}$, $\boldsymbol{x}^{(2)} \in \mathbb{R}^{n_2}$. Then the total derivative of the function $\boldsymbol{f}$ with respect to the vector of variables $\boldsymbol{x}^{(1)}$ at point $\left(\boldsymbol{x}_0^{(1)}, \boldsymbol{x}_0^{(2)}\right)$ is a linear map $\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}^{(1)}}\left(\boldsymbol{x}_0^{(1)}, \boldsymbol{x}_0^{(2)}\right) : \mathbb{R}^{n_1} \to \mathbb{R}^m$ such that

$$\lim_{\boldsymbol{h}\to\boldsymbol{0}} \frac{1}{||\boldsymbol{h}||}\left(\boldsymbol{f}(\boldsymbol{x}_0^{(1)} + \boldsymbol{h}, \boldsymbol{x}_0^{(2)}) - \boldsymbol{f}(\boldsymbol{x}_0^{(1)}, \boldsymbol{x}_0^{(2)}) - \frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}^{(1)}}\left(\boldsymbol{x}_0^{(1)}, \boldsymbol{x}_0^{(2)}\right)\boldsymbol{h}\right) = \boldsymbol{0}. \tag{1.22}$$

This definition can be extended in a straightforward manner to any permutation of components of vectors $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}$ in the argument of $\boldsymbol{f}$. Two different approaches to notation of the total derivative need to be noted here according to one set of variables. Given that the selected set of variables $\boldsymbol{x}^{(1)}$ is only composed of a single component, the notation $\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}^{(1)}}\left(\boldsymbol{x}_0^{(1)}, \boldsymbol{x}_0^{(2)}\right)$ coincides with the partial derivative of the function $\boldsymbol{f}$ with respect to $\boldsymbol{x}^{(1)}$. Therefore, it is also possible to denote the total derivative by a set of variables $\boldsymbol{x}^{(1)} = \left(x_1^{(1)}, \ldots, x_{n_1}^{(1)}\right)^{\mathrm{T}}$ by the symbol $\frac{\partial f}{\partial\left(x_1^{(1)}, \ldots, x_{n_1}^{(1)}\right)}\left(\boldsymbol{x}_0^{(1)}, \boldsymbol{x}_0^{(2)}\right)$.

- *Partial derivatives* of a function $\boldsymbol{f}$ at the point $\boldsymbol{x}_0$ are derivatives in the direction of the standard basis vectors. They are denoted

$$\frac{\partial \boldsymbol{f}}{\partial x_\ell}(\boldsymbol{x}_0) = \partial_{x_\ell}\boldsymbol{f}(\boldsymbol{x}_0) = \partial_\ell \boldsymbol{f}(\boldsymbol{x}_0) := \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{e}_\ell}(\boldsymbol{x}_0). \tag{1.23}$$

- The matrix representing the linear map $\boldsymbol{f}'(\boldsymbol{x}_0)$ in standard bases of the spaces $\mathbb{R}^n$ and $\mathbb{R}^m$ is called the Jacobi matrix and denoted b

$$\mathbf{J}_{\boldsymbol{f}}(\boldsymbol{x}_0) = \begin{pmatrix} \partial_1\boldsymbol{f}(\boldsymbol{x}_0) & \partial_2\boldsymbol{f}(\boldsymbol{x_0}) & \ldots & \partial_n\boldsymbol{f}(\boldsymbol{x_0}) \end{pmatrix} = \begin{pmatrix} \partial_1 f_1(\boldsymbol{x}_0) & \partial_2 f_1(\boldsymbol{x}_0) & \ldots & \partial_n f_1(\boldsymbol{x}_0) \\ \partial_1 f_2(\boldsymbol{x}_0) & \partial_2 f_2(\boldsymbol{x}_0) & \ldots & \partial_n f_2(\boldsymbol{x}_0) \\ \vdots & \vdots & \ddots & \vdots \\ \partial_1 f_m(\boldsymbol{x}_0) & \ldots & \ldots & \partial_n f_m(\boldsymbol{x}_0) \end{pmatrix}.$$

- Derivative of a function composition $\boldsymbol{f} \circ \boldsymbol{g} : \mathbb{R}^n \to \mathbb{R}^m$, where $\boldsymbol{g} : \mathbb{R}^n \to \mathbb{R}^s$ and $\boldsymbol{f} : \mathbb{R}^s \to \mathbb{R}^m$, is under the assumption of the existence of total derivatives $\boldsymbol{f}'(\boldsymbol{g}(\boldsymbol{x}_0))$ and $\boldsymbol{g}'(\boldsymbol{x}_0)$ given by the expression

$$\left(\boldsymbol{f} \circ \boldsymbol{g}\right)'(\boldsymbol{x}_0) = \boldsymbol{f}'\left(\boldsymbol{g}(\boldsymbol{x}_0)\right)\boldsymbol{g}'(\boldsymbol{x}_0), \tag{1.24}$$

where on the right-hand side of (1.24). there is a composition of the two linear maps $\boldsymbol{f}'$ and $\boldsymbol{g}'$. For the Jacobi matrix of the composite linear map, we therefore have

$$\mathbf{J}_{\boldsymbol{f}\circ\boldsymbol{g}}(\boldsymbol{x}_0) = \mathbf{J}_{\boldsymbol{f}}(\boldsymbol{g}(\boldsymbol{x}_0))\mathbf{J}_{\boldsymbol{g}}(\boldsymbol{x}_0).$$

The rule for calculating the partial derivatives of a function composition follows from the definition of matrix multiplication. The derivative of the i-th component of the function $f \circ g$ with respect to the ℓ-th variable is calculated as

$$\mathbf{J}_{\boldsymbol{f}\circ\boldsymbol{g}}(\boldsymbol{x}_0)_{i\ell} = \frac{\partial(\boldsymbol{f}\circ\boldsymbol{g})_i}{\partial x_\ell}(\boldsymbol{x}_0) = \sum_{k=1}^{s} \frac{\partial f_i(\boldsymbol{g}(\boldsymbol{x}_0))}{\partial y_k}\frac{\partial g_k(\boldsymbol{x}_0)}{\partial x_\ell}, \tag{1.25}$$

where y_k indicate the components of the function argument $\boldsymbol{f} = \boldsymbol{f}(\boldsymbol{y})$.

- To represent derivatives of a function of several variables, the Del (nabla) operator ∇ is commonly introduced, which can be represented as a vector of partial derivatives $\nabla = (\partial_1, \partial_2, \dots, \partial_n)^{\mathrm{T}} = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \dots, \frac{\partial}{\partial x_n}\right)^{\mathrm{T}}$. The (total) derivative of a scalar function $f : \mathbb{R}^n \to \mathbb{R}$ can be represented by its gradient, since

$$\frac{\partial f}{\partial \boldsymbol{v}}(\boldsymbol{x}_0) = f'(\boldsymbol{x}_0)\boldsymbol{v} = \nabla f(\boldsymbol{x}_0) \cdot \boldsymbol{v} = \left(\partial_1 f, \partial_2 f, \dots, \partial_n f\right)^{\mathrm{T}} \cdot \boldsymbol{v}.$$

- Partial derivatives of the second order (and higher orders) will be abbreviated according to the scheme

$$\partial_{ij} f(\boldsymbol{x}_0) = \partial_j \partial_i f(\boldsymbol{x}_0) = \frac{\partial^2 f}{\partial x_i \partial x_j}(\boldsymbol{x}_0) = \frac{\partial}{\partial x_j}\left(\frac{\partial f}{\partial x_i}\right)\Big|_{\boldsymbol{x}_0}.$$

1.5 Integral Calculus of Functions of Several Variables

- Integral of a scalar function $f : \mathbb{R}^n \to \mathbb{R}$ over a *measurable*[4] set $V \subset \mathbb{R}^n$ is denoted by

$$\int_V f(\boldsymbol{x})\,\mathrm{d}\mu(\boldsymbol{x}) = \int_V f(\boldsymbol{x})\,\mathrm{d}V = \int_V f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x},$$

  where $\mu = \mu_n$ denotes the n-dimensional Lebesgue measure on $\mathbb{R}^n$. The set of all (Lebesgue) integrable functions on the set V is denoted by $\mathrm{L}(V)$, see Definition 31.

- We say that a map $\boldsymbol{\varphi} : \mathbb{R}^n \to \mathbb{R}^n$ is *regular* on an open set $M \subset \mathbb{R}^n$, if the elements of the matrix $\mathbf{J}_{\boldsymbol{\varphi}}$ are continuous on M and $\det \mathbf{J}_{\boldsymbol{\varphi}}(\boldsymbol{x}) \neq 0$ for each $\boldsymbol{x} \in M$.

Theorem. (on substitution in a multidimensional integral) *Let $\boldsymbol{\varphi} : \mathbb{R}^n \to \mathbb{R}^n$ be a simple regular mapping defined on an open set A. Then for each measurable subset $V \subset A$, it holds that*

$$\int_V f\left(\boldsymbol{\varphi}(\boldsymbol{\xi})\right)\left|\det \mathbf{J}_{\boldsymbol{\varphi}}(\boldsymbol{\xi})\right|\mathrm{d}\boldsymbol{\xi} = \int_{\boldsymbol{\varphi}(V)} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x},$$

and, alternatively, we have

$$\int_W f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int_{\boldsymbol{\varphi}^{-1}(W)} f\left(\boldsymbol{\varphi}(\boldsymbol{\xi})\right)\left|\det \mathbf{J}_{\boldsymbol{\varphi}}(\boldsymbol{\xi})\right|\mathrm{d}\boldsymbol{\xi}$$

for any measurable $W \subset \boldsymbol{\varphi}(A)$.

Theorem. (Fubini) *Let $n, m \in \mathbb{N}$, $V \subset \mathbb{R}^{n+m}$. Consider a function $f \in \mathrm{L}(V)$, $f = f(\boldsymbol{x})$, $\boldsymbol{x} = \left(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}\right)^{\mathrm{T}}$ where $\boldsymbol{x}^{(1)} \in \mathbb{R}^n$, $\boldsymbol{x}^{(2)} \in \mathbb{R}^m$. Let us denote*

$$A_{\boldsymbol{x}^{(1)}} = \left\{\boldsymbol{x}^{(2)} \subset \mathbb{R}^m \,\middle|\, \left(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}\right) \in V\right\},$$
$$B = \left\{\boldsymbol{x}^{(1)} \in \mathbb{R}^n \,\middle|\, A_{\boldsymbol{x}^{(1)}} \neq \emptyset\right\}.$$

Then

$$\int_V f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int_B \left(\int_{A_{\boldsymbol{x}^{(1)}}} f\left(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}\right)\mathrm{d}\boldsymbol{x}^{(2)}\right)\mathrm{d}\boldsymbol{x}^{(1)} =: \int_B \mathrm{d}\boldsymbol{x}^{(1)} \int_{A_{\boldsymbol{x}^{(1)}}} \mathrm{d}\boldsymbol{x}^{(2)} f\left(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}\right)$$

holds.

[4] The concepts of *measurable function* and *measurable set* are not introduced in this course. These terms appear in the theory of the Lebesgue integral, which can be constructed in a classical way based on measure theory or by using the alternative Daniell's construction, which does not need the prior development of measure theory. For our purposes, every imaginable set will be measurable, as well as every imaginable function defined on such a set. However, for the sake of correctness, we state the assumption of measurability in the wording of the theorems.

1.5.1 Interchange of Derivative and Integral

Theorem 4. (on the derivative of integral with respect to a parameter) *Let $I \subset \mathbb{R}$ be an open interval and V be a measurable set. Let $f : V \times I \to \mathbb{R}$ meet the following requirements:*

1. *Integral $F(\alpha) := \int_V f(\boldsymbol{x}, \alpha)\,\mathrm{d}\boldsymbol{x}$ converges (is finite) for at least one $\alpha \in I$, i.e. shortly*

$$(\exists \alpha \in I)\left(f(\cdot, \alpha) \in \mathrm{L}(V)\right).$$

2. *For each $\alpha \in I$, $f(\cdot, \alpha)$ is a function measurable on V.*

3. *Function $f(\boldsymbol{x}, \cdot)$ is differentiable on I for almost all*[5] *$\boldsymbol{x} \in V$.*

4. *$\frac{\partial f}{\partial \alpha}$ is dominated by an integrable function $g \in \mathrm{L}(V)$, i.e. for almost all $\boldsymbol{x} \in V$ and for all $\alpha \in I$*

$$\left|\frac{\partial f(\boldsymbol{x}, \alpha)}{\partial \alpha}\right| \leq g(\boldsymbol{x})$$

holds.

Then for all $\alpha \in I$, the integral $F(\alpha)$ converges and

$$\frac{\mathrm{d}F}{\mathrm{d}\alpha} = \int_V \frac{\partial f(\boldsymbol{x}, \alpha)}{\partial \alpha}\mathrm{d}\boldsymbol{x}.$$

1.6 Integration over Manifolds

1.6.1 Line integral

Definition. Under the term *curve in* $\mathbb{R}^n$, we understand any continuous function $\boldsymbol{\varphi} : [a, b] \to \mathbb{R}^n$. If $\boldsymbol{\varphi}$ is injective on (a, b), the curve $\boldsymbol{\varphi}$ is called *simple*. If $\boldsymbol{\varphi}(a) = \boldsymbol{\varphi}(b)$, the curve is *closed*, otherwise the curve is *open*. The set $\varphi = \langle \boldsymbol{\varphi} \rangle = \boldsymbol{\varphi}([a, b])$ is called a *path* or the *geometric image of the curve* $\boldsymbol{\varphi}$ in $\mathbb{R}^n$. In turn, the map $\boldsymbol{\varphi}$ is called a *parameterization* of a the path φ.

Definition. Let $\varphi : [a, b] \to \mathbb{R}^n$ be a path and let $(\forall t \in (a, b))\left(\exists \dot{\varphi}(t)\right)$. By a *line integral (path integral, curve integral) of the first kind* of a function $f : \mathbb{R}^n \to \mathbb{R}$ along the path φ, we understand the integral

$$\int_\varphi f(\boldsymbol{x})\,\mathrm{d}l = \int_a^b f\left(\boldsymbol{\varphi}(t)\right)\left\|\dot{\boldsymbol{\varphi}}(t)\right\|\mathrm{d}t. \tag{1.26}$$

Definition. By a *line integral of the second kind* of a vector field (function) $\boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^n$, we understand the integral

$$\int_\varphi \boldsymbol{f}(\boldsymbol{x}) \cdot \mathrm{d}\boldsymbol{l} = \int_a^b \boldsymbol{f}\left(\boldsymbol{\varphi}(t)\right) \cdot \dot{\boldsymbol{\varphi}}(t)\,\mathrm{d}t = \int_a^b f_i\left(\boldsymbol{\varphi}(t)\right)\dot{\varphi}_i(t)\,\mathrm{d}t, \tag{1.27}$$

where the orientation of the path is given by its parameterization.

[5] The given statement $A(x)$ holds *almost everywhere* on V, if there is a set $N \subset V$ with a zero measure $\mu(N) = 0$ such that statement $A(x)$ holds $\forall x \in V \setminus N$.

Remark. Components of the vector $\dot{\varphi}_i(t)\,\mathrm{d}t$ correspond to the components of the displacement of the point $\boldsymbol{x} = \boldsymbol{\varphi}(t)$ along the path in the directions of the coordinate axes, i.e. standard basis vectors $\boldsymbol{e}_1, \ldots, \boldsymbol{e}_n$. That's why the integral (1.27) is sometimes also written as

$$\int_{\varphi} \boldsymbol{f}(\boldsymbol{x}) \cdot \mathrm{d}\boldsymbol{l} = \int_{\varphi} \boldsymbol{f}(\boldsymbol{x}) \cdot \mathrm{d}\boldsymbol{x} = \int_{\varphi} f_k(\boldsymbol{x})\,\mathrm{d}x_k. \tag{1.28}$$

Remark. Let φ be a path with parameterization $\boldsymbol{\varphi} : [a,b] \to \mathbb{R}^n$. A *path oriented in the direction opposite* to the path φ is the path $-\varphi$ given by the parameterization

$$\tilde{\boldsymbol{\varphi}}(t) = \boldsymbol{\varphi}(a+b-t).$$

For the line integral of the second kind,

$$\int_{-\varphi} \boldsymbol{f}\,\mathrm{d}\boldsymbol{l} = -\int_{\varphi} \boldsymbol{f}\,\mathrm{d}\boldsymbol{l}$$

holds.

1.6.2 Surface integral

Although it is possible, with a certain degree of abstraction, to generally introduce integration on arbitrary m-dimensional manifolds in n-dimensional space ($m < n$), we focus on the definition of surface integrals only for surfaces in $\mathbb{R}^3$.

Definition. Each map $\boldsymbol{S} : M \to \mathbb{R}^3$ where $M \subset \mathbb{R}^2$ is a domain is called a *surface parameterization.* A set

$$S = \langle \boldsymbol{S} \rangle = \boldsymbol{S}(M)$$

is called a *surface* or a *geometric image* of the map $\boldsymbol{S}$. If the map $\boldsymbol{S}$ is injective, we call S a simple surface. If in addition $\boldsymbol{S} \in \mathrm{C}^1(M)$ and

$$\frac{\partial \boldsymbol{S}}{\partial u}(u,v) \times \frac{\partial \boldsymbol{S}}{\partial v}(u,v) \neq \boldsymbol{0}\ \forall\,(u,v) \in M,$$

we speak about a *simple regular surface.*

Remark. A simple regular surface has a uniquely defined normal vector at every point $\boldsymbol{x} \in S$ that is equal to

$$\boldsymbol{n}(\boldsymbol{x}) = \frac{\frac{\partial \boldsymbol{S}}{\partial u}(u,v) \times \frac{\partial \boldsymbol{S}}{\partial v}(u,v)}{\left\| \frac{\partial \boldsymbol{S}}{\partial u}(u,v) \times \frac{\partial \boldsymbol{S}}{\partial v}(u,v) \right\|},$$

where $(u,v) = \boldsymbol{S}^{-1}(\boldsymbol{x})$.

Definition. *A surface integral of the first kind* of a scalar function $f : \mathbb{R}^3 \to \mathbb{R}$ over a simple regular surface S is defined as

$$\int_S f(\boldsymbol{x})\,\mathrm{d}S = \int_M f(\boldsymbol{S}(u,v)) \left\| \frac{\partial \boldsymbol{S}}{\partial u}(u,v) \times \frac{\partial \boldsymbol{S}}{\partial v}(u,v) \right\| \mathrm{d}(u,v). \tag{1.29}$$

Remark. Expression $\mathrm{d}S = \left\| \frac{\partial \boldsymbol{S}}{\partial u}(u,v) \times \frac{\partial \boldsymbol{S}}{\partial v}(u,v) \right\| \mathrm{d}(u,v)$ has the sense of the area of the infinitesimal parallelogram given by the vectors $\frac{\partial \boldsymbol{S}}{\partial u}\mathrm{d}u$ and $\frac{\partial \boldsymbol{S}}{\partial v}\mathrm{d}v$. The area of S is therefore given by the surface integral of unity

$$\mu_2(S) = \int_S \mathrm{d}S.$$

Remark. For calculation of $\mathrm{d}S$, one can use the Lagrange identity (1.2).

Definition. *A surface integral of the second kind* of a vector field $\boldsymbol{f}:\mathbb{R}^3\to\mathbb{R}^3$ over a simple smooth regular surface S is defined as

$$\int_S \boldsymbol{f}(\boldsymbol{x})\cdot\mathrm{d}\boldsymbol{S}=\int_S \boldsymbol{f}(\boldsymbol{x})\cdot\boldsymbol{n}\mathrm{d}S=\int_M f(\boldsymbol{S}(u,v))\cdot\left(\frac{\partial\boldsymbol{S}}{\partial u}(u,v)\times\frac{\partial\boldsymbol{S}}{\partial v}(u,v)\right)\mathrm{d}(u,v). \tag{1.30}$$

Remark. It holds that

$$\mathrm{d}\boldsymbol{S}=\boldsymbol{n}\mathrm{d}S=\frac{\partial\boldsymbol{S}}{\partial u}(u,v)\times\frac{\partial\boldsymbol{S}}{\partial v}(u,v)\,\mathrm{d}(u,v),$$

where $\boldsymbol{n}$ is the unit normal vector to the surface S at the point $\boldsymbol{S}(u,v)$. Depending on the parameterization, it can point to one side or the other, which affects the sign of the integral. In the following chapters, we will generally consider closed surfaces forming the boundary of connected sets $V\subset\mathbb{R}^3$, i.e. $S=\partial V$. The vector $\boldsymbol{n}$ will always point outward from the volume V. Under these assumptions, the sign of the surface integral is uniquely determined.

Remark. The integrand of the surface integral of the second kind is the projection of the vector field $\boldsymbol{f}$ to the direction normal to the surface S.

Remark. Formal notation of the surface integral of 2nd kind is also

$$\int_S \boldsymbol{f}(\boldsymbol{x})\cdot\mathrm{d}\boldsymbol{S}=\int_S f_1(\boldsymbol{x})\,\mathrm{d}x_2\mathrm{d}x_3+f_2(\boldsymbol{x})\,\mathrm{d}x_1\mathrm{d}x_3+f_3(\boldsymbol{x})\,\mathrm{d}x_1\mathrm{d}x_2.$$

1.6.3 Green's formula

The following theorems are a generalization of integration by parts.

Theorem 5. (Green's formula) *Let $n\in\{2,3\}$, $V\subset\mathbb{R}^n$ be a domain, let $f,g\in\mathrm{C}^1(V)$ and $f,g\in\mathrm{C}(\partial V)$. Then*

$$\int_V \frac{\partial f(\boldsymbol{x})}{\partial x_k}g(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}=-\int_V f(\boldsymbol{x})\frac{\partial g(\boldsymbol{x})}{\partial x_k}\mathrm{d}\boldsymbol{x}+\int_{\partial V} f(\boldsymbol{x})\,g(\boldsymbol{x})\,n_k\mathrm{d}S$$

holds, where n_k is k-th component of the vector of the outward pointing normal vector to the boundary of the domain V.

Theorem 6. (Green's theorem). *Let $S\subset\mathbb{R}^2$ be a domain and ∂S be a closed, piecewise smooth curve. Let $\boldsymbol{f}:\mathbb{R}^2\to\mathbb{R}^2$ be a vector field continuously differentiable on S and continuous on ∂S. Then*

$$\int_{\partial S}\boldsymbol{f}(\boldsymbol{x})\cdot\mathrm{d}\boldsymbol{l}=\int_S\left(\frac{\partial f_2}{\partial x_1}-\frac{\partial f_1}{\partial x_2}\right)\mathrm{d}\boldsymbol{x},$$

where the curve ∂S is considered positively (counter-clockwise) oriented.

Theorem 7. (Gauss-Ostrogradsky theorem) *Let $\boldsymbol{f}\in\mathrm{C}^1\left(\mathbb{R}^3\right)$ be a vector field, $V\subset\mathbb{R}^3$ be a domain. Then*

$$\int_V\nabla\cdot\boldsymbol{f}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}=\int_{\partial V}\boldsymbol{f}(\boldsymbol{x})\cdot\mathrm{d}\boldsymbol{S}$$

holds, where $\mathrm{d}\boldsymbol{S}$ points outof the volume V.

1.7 Concepts from functional analysis

In this section, we summarize the definitions of function spaces and recall the related statements used in the theory of partial differential equations [Eva98], which is applied in sections 4.3 and 4.4. In these parts, we will further extend our theoretical knowledge, but only in the narrow context of the studied problem. Suitable sources for a more comprehensive study of functional analysis and functional theory spaces are e.g. [Con90, BEH08, KJF77, Maz85].

1.7.1 Elementary concepts

Definition 8. We say that the sequence of vectors $(\boldsymbol{x}_n)_{n\in\mathbb{N}} \subset \mathscr{M}$ in a metric space $\mathscr{M}$ with metric ρ is *Cauchy*, iff

$$(\forall \varepsilon > 0)\,(\exists n_0 \in \mathbb{N})\,(\forall m, n > n_0)\left(\rho\left(\boldsymbol{x}_n, \boldsymbol{x}_m\right) < \varepsilon\right).$$

Definition 9. We say that a metric space V is *complete* iff every Cauchy sequence $(\boldsymbol{x}_n)_{n\in\mathbb{N}} \subset V$ is convergent in it, i.e. there exists $\boldsymbol{x} \in V$ such that

$$\lim_{n\to+\infty} \boldsymbol{x}_n = \boldsymbol{x}.$$

A complete normed space is called a *Banach space*. A complete space endowed with an inner product is called a *Hilbert space*.[6]

Definition 10. An orthogonal system of vectors $(\boldsymbol{x}_\alpha)_{\alpha\in M}$ in a Hilbert space $\mathscr{H}$ is called *maximal*, *complete*, or *a basis of* $\mathscr{H}$, if and only if it is not a proper subset of another orthogonal system.

Remark. The set of indexes M in Definition (10) can be finite, countable or uncountable. Discussion of properties of uncountable bases and uncountable sums (using a generalization of sequences to the so-called „networks“) is beyond the scope of this mathematical introduction and can be found e.g. in [BEH08, Con90].

Theorem 11. *All bases of $\mathscr{H}$ have the same cardinality, which we call the dimension of the space $\mathscr{H}$.*

Definition 12. A set M is dense in a topological space $\mathscr{X}$ if and only if $\bar{M} = \mathscr{X}$.

Definition 13. A topological space $\mathscr{X}$ is called separable if and only if it contains a countable set dense in $\mathscr{X}$.

Theorem 14. *A Hilbert space $\mathscr{H}$ is separable if and only if it has a countable basis.*

1.7.2 Properties of Banach and Hilbert spaces

Definition 15. Let $\mathscr{B}_1, \mathscr{B}_2$ be Banach spaces. We say that a linear operator $A : \mathscr{B}_1 \to \mathscr{B}_2$ is *bounded*, iff there is a constant $K \geq 0$ such that

$$(\forall \boldsymbol{v} \in \mathscr{B}_1)\left(\|A\boldsymbol{v}\|_{\mathscr{B}_2} \leq K\,\|\boldsymbol{v}\|_{\mathscr{B}_1}\right).$$

We say the operator A is *continuous*, iff

$$(\forall \varepsilon > 0)\,(\exists \delta > 0)\,(\forall \boldsymbol{u}, \boldsymbol{v} \in \mathscr{B}_1)\left(\|\boldsymbol{u} - \boldsymbol{v}\|_{\mathscr{B}_1} < \delta \implies \|A\boldsymbol{u} - A\boldsymbol{v}\|_{\mathscr{B}_2} < \varepsilon\right).$$

Remark. The notion of continuity can be generalized to metric spaces. In Banach spaces, however, the above two conditions are obviously equivalent.

[6] A general vector space with an inner product is called simply an *inner product space* or, more rarely, a *pre-Hilbert space*.

Definition 16. Let $\mathscr{B}$ be a Banach space. The space of all linear functionals on $\mathscr{B}$ is called the *algebraic dual space* and is marked $\mathscr{B}^*$. The space of all *continuous* linear functionals on $\mathscr{B}$ is called a (continuous) *dual space* and is denoted $\mathscr{B}'$.

Remark. If $\dim \mathscr{B} < +\infty$, we have $\mathscr{B}' = \mathscr{B}^*$.

Definition 17. Let $\mathscr{B}$ be a Banach space with the norm $\|\cdot\|_{\mathscr{B}}$. The *dual norm* on the dual space $\mathscr{B}'$ is given by the relation

$$\left\|\underline{\boldsymbol{w}}\right\|_{\mathscr{B}'} = \sup_{\boldsymbol{v}\in\mathscr{B}\setminus\{\boldsymbol{0}\}} \frac{\left|\underline{\boldsymbol{w}}(\boldsymbol{v})\right|}{\|\boldsymbol{v}\|_{\mathscr{B}}} = \sup_{\boldsymbol{v}\in\mathscr{B},\|\boldsymbol{v}\|_{\mathscr{B}}=1} \left|\underline{\boldsymbol{w}}(\boldsymbol{v})\right|$$

for each $\underline{\boldsymbol{w}} \in \mathscr{B}'$.

Theorem. (Riesz representation theorem) *Let $\mathscr{H}$ be a Hilbert space with an inner product $(\cdot,\cdot)$. Then for each element $\underline{\boldsymbol{w}} \in \mathscr{H}'$ there is exactly one element $\boldsymbol{u} \in \mathscr{H}$ such that*

$$(\boldsymbol{v},\boldsymbol{u}) = \underline{\boldsymbol{w}}(\boldsymbol{v}) \;\forall \boldsymbol{v} \in \mathscr{H}.$$

Moreover,

$$\|\boldsymbol{v}\|_{\mathscr{H}} = \left\|\underline{\boldsymbol{w}}\right\|_{\mathscr{H}'}$$

holds.

Remark 18. Riesz theorem proves the existence of the isomorphism (linear bijective mapping)

$$I : \mathscr{H}' \to \mathscr{H}$$

defined as

$$I\underline{\boldsymbol{w}} = \boldsymbol{u},$$

which in addition preserves the „size“ of the elements (in the norms $\|\cdot\|_{\mathscr{H}}$ and $\|\cdot\|_{\mathscr{H}'}$, respectively). Therefore, $\mathscr{H}$ and $\mathscr{H}'$ can be considered de facto equal (they have the same properties in terms of linear algebra and functional analysis - see in particular the concepts in Section 1.7.10). Dual space $\mathscr{H}'$ is also Hilbert, with an induced inner product

$$\left(\underline{\boldsymbol{w}}_1,\underline{\boldsymbol{w}}_2\right)_{\mathscr{H}'} = \left(I\underline{\boldsymbol{w}}_1, I\underline{\boldsymbol{w}}_2\right)_{\mathscr{H}}.$$

Linear functionals can be represented not only by means of an inner product, but also using any bilinear form that has „nice-enough“ properties, as shown by the following lemma:

Lemma 19. (Lax-Milgram) *Let $\mathscr{H}$ be a Hilbert space with an inner product $(\cdot,\cdot)_{\mathscr{H}}$, let $B : \mathscr{H}\times\mathscr{H} \to \mathbb{R}$ be a bilinear form for which the constants $K, L > 0$ exist such that for each $\boldsymbol{u},\boldsymbol{v} \in \mathscr{H}$, the following properties hold:*

1. *continuity, or boundedness of B: $|B(\boldsymbol{u},\boldsymbol{v})| \le K\|\boldsymbol{u}\|_{\mathscr{H}}\|\boldsymbol{v}\|_{\mathscr{H}}$,*
2. *coercivity (or also „V-ellipticity“) B: $B(\boldsymbol{u},\boldsymbol{u}) \ge L\|\boldsymbol{u}\|^2_{\mathscr{H}}$.*

Then for every continuous linear functional $\underline{\boldsymbol{w}} \in \mathscr{H}'$ there is exactly one $\boldsymbol{u} \in \mathscr{H}$ so that

$$\underline{\boldsymbol{w}}(\boldsymbol{v}) = B(\boldsymbol{u},\boldsymbol{v}),$$

where

$$\|\boldsymbol{u}\|_{\mathscr{H}} \le \frac{1}{L}\left\|\underline{\boldsymbol{w}}\right\|_{\mathscr{H}'}.$$

Proof. See [Eva98, Chapter 6]. □

Remark. The inner product itself satisfies both conditions in the Lax-Milgram lemma 19 with constants $K = 1$ (Schwarz inequality) and $L = 1$ (apparently), and for them we get the Riesz theorem 1.7.2 directly .

Definition. Let $\mathscr{B}$be a Banach space and $v \in \mathscr{B}$. Then the map

$$\underline{\underline{\boldsymbol{v}}} : \mathscr{B}' \to \mathbb{R}$$

defined by the relation

$$\underline{\underline{\boldsymbol{v}}}\left(\underline{\boldsymbol{w}}\right) = \underline{\boldsymbol{w}}\left(\boldsymbol{v}\right)$$

is a continuous linear functional on $\mathscr{B}'$, i.e. $\underline{\underline{\boldsymbol{v}}} \in \mathscr{B}''$. The map

$$J = \left(\boldsymbol{v} \mapsto \underline{\underline{\boldsymbol{v}}}\right)$$

is called a *canonical evaluation map.* The space $\mathscr{B}$ is called *reflexive*, iff the canonical evaluation map $J : \mathscr{B} \to \mathscr{B}''$ is an isomorphism (i.e. a bijective and linear map, preserving linear relations between elements $\mathscr{B}$ and $\mathscr{B}''$, i.e. the „structure“ of the space $\mathscr{B}$).

Remark 20. Every Hilbert space is reflexive.

Proof. According to the Riesz representation theorem 1.7.2 and remark 18, $\mathscr{H}$ (over $\mathbb{R}$) is isomorphic with $\mathscr{H}'$ (and in turn, $\mathscr{H}'$ is also a Hilbert space, isomorphic with $\mathscr{H}''$). □

Definition 21. Let $\mathscr{B}$ be a Banach space. We say that a sequence $(\boldsymbol{u}_n)$ in space $\mathscr{B}$ *converges weakly* to the element $\boldsymbol{u} \in \mathscr{B}$ and we denote $\boldsymbol{u}_n \rightharpoonup \boldsymbol{u}$, iff

$$\lim_{n\to\infty} \underline{\boldsymbol{w}}\left(\boldsymbol{u}_n\right) = \underline{\boldsymbol{w}}\left(\boldsymbol{u}\right) \,, \ \forall \underline{\boldsymbol{w}} \in \mathscr{B}'.$$

Remark 22. Let $\mathscr{H}$ be a Hilbert space with an inner product $(\cdot,\cdot)_{\mathscr{H}}$. According to the Riesz theorem 1.7.2, the definition of weak convergence can be formulated as

$$\boldsymbol{u}_n \rightharpoonup \boldsymbol{u} \iff (\forall \boldsymbol{v} \in \mathscr{H}) \left(\lim_{n\to\infty} (\boldsymbol{u}_n, \boldsymbol{v})_{\mathscr{H}} = (\boldsymbol{u}, \boldsymbol{v})_{\mathscr{H}} \right).$$

Theorem 23. *A Banach space $\mathscr{B}$ is reflexive if and only if from every sequence $(\boldsymbol{u}_n)$ bounded in $\mathscr{B}$, a subsequence weakly convergent in $\mathscr{B}$ can be selected.*

1.7.3 Self-adjoint operators on Hilbert spaces

Theorem 24. *Let $\mathscr{H}$ be a Hilbert space with an inner product $(\cdot,\cdot)$. Let $A : \mathscr{H} \to \mathscr{H}$ be a bounded linear operator on $\mathscr{H}$ (we denote $A \in \mathfrak{B}(\mathscr{H})$). Then there is exactly one linear operator $A^* \in \mathfrak{B}(\mathscr{H})$ such that for all $\boldsymbol{u}, \boldsymbol{v} \in \mathscr{H}$,*

$$(A\boldsymbol{u}, \boldsymbol{v}) = \left(\boldsymbol{u}, A^* \boldsymbol{v}\right)$$

holds.

Proof. For a fixed $\boldsymbol{v} \in \mathscr{H}$, $\boldsymbol{u} \mapsto (A\boldsymbol{u}, \boldsymbol{v})$ is a continuous linear functional, so from the Riesz theorem 1.7.2, there is exactly one $\boldsymbol{z} \in \mathscr{H}$ such that

$$(A\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{u}, \boldsymbol{z}) \,.$$

The map $\boldsymbol{v} \mapsto \boldsymbol{z}$ is, however, a linear operator, which we denote A^*. □

Definition 25. Operator A^* from Theorem 24 is called the *adjoint* operator to the operator A.

- Operator A is called *normal*, iff $AA^* = A^* A$.
- Operator A is called *self-adjoint* , iff $A^* = A$.

1.7.4 Function spaces C^m and L_p

Definition 26. Let $\Omega \subset \mathbb{R}^n$ for a general $n \in \mathbb{N}$. The space $\mathrm{C}(\Omega)$ is the linear space of all functions $u : \Omega \to \mathbb{R}$ continuous on Ω with commonly defined vector operations[7]. Space $\mathrm{C}(\bar{\Omega})$ is the linear space of all functions from $\mathrm{C}(\Omega)$, which are in addition *uniformly continuous*[8] on Ω (i.e. we are not speaking about the closure $\bar{\Omega}$ here).

Definition 27. Let $m \in N_0$. We define the function spaces

$$\mathrm{C}^m(\Omega) = \left\{u \in \mathrm{C}(\Omega) \,|\, (\forall \alpha, |\alpha| \leq m)\left(\mathrm{D}^\alpha u \in \mathrm{C}(\Omega)\right)\right\},$$
$$\mathrm{C}^m(\bar{\Omega}) = \left\{u \in \mathrm{C}(\Omega) \,|\, (\forall \alpha, |\alpha| \leq m)\left(\mathrm{D}^\alpha u \in \mathrm{C}(\bar{\Omega})\right)\right\}$$

and

$$\mathrm{C}^\infty(\Omega) = \bigcap_{k\in\mathbb{N}} \mathrm{C}^k(\Omega),$$
$$\mathrm{C}^\infty(\bar{\Omega}) = \bigcap_{k\in\mathbb{N}} \mathrm{C}^k(\bar{\Omega}).$$

Remark. By definition 27, it follows that $\mathrm{C}^0(\Omega) = \mathrm{C}(\Omega)$.

Definition 28. We say that the function $\boldsymbol{f} : \mathbb{R}^m \to \mathbb{R}^n$ is *Lipschitz-continuous*, iff

$$(\exists K > 0)\left(\forall \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^m\right)\left(\left\|\boldsymbol{f}\left(\boldsymbol{y}\right) - \boldsymbol{f}\left(\boldsymbol{x}\right)\right\| < K\left\|\boldsymbol{y} - \boldsymbol{x}\right\|\right).$$

Definition 29. We say that $\Omega \subset \mathbb{R}^n$ is a *domain with a continuous* (or *Lipschitz*) *boundary*, if there exist m ($m \in \mathbb{N}$) Cartesian coordinate systems in $\mathbb{R}^n$ marked $(x_1^r, x_2^r, ..., x_{n-1}^r, x_n^r)$, m numbers $\Delta^r > 0$ and m continuous (or Lipschitz continuous) functions a^r ($r \in \hat{m}$) of $(n-1)$ variables such that

1. $(\forall A \in \partial\Omega)\,(\exists r \in \hat{m})\left(\exists \tilde{\boldsymbol{x}}^r = \left(x_1^r, x_2^r, ..., x_{n-1}^r\right)\right)\left(\left\|\tilde{\boldsymbol{x}}^r\right\| < \Delta^r \wedge A = \left[\tilde{\boldsymbol{x}}^r, a^r\left(\tilde{x}^r\right)\right]\right)$,
2. $(\exists \varepsilon_0 > 0)\,(\forall \varepsilon \in (0, \varepsilon_0))\,(\forall r \in \hat{m})$ the following holds:
   a) $U_+^r = \left\{\left[\tilde{\boldsymbol{x}}^r, x_n^r\right] \middle| \left\|\tilde{\boldsymbol{x}}^r\right\| < \Delta^r \wedge a^r\left(\tilde{\boldsymbol{x}}^r\right) < x_n^r < a^r\left(\tilde{\boldsymbol{x}}^r\right) + \varepsilon\right\} \subset \mathbb{R}^n \backslash \Omega$,
   b) $U_-^r = \left\{\left[\tilde{\boldsymbol{x}}^r, x_n^r\right] \middle| \left\|\tilde{\boldsymbol{x}}^r\right\| < \Delta^r \wedge a^r\left(\tilde{\boldsymbol{x}}^r\right) - \varepsilon < x_n^r < a^r\left(\tilde{\boldsymbol{x}}^r\right)\right\} \subset \Omega$.

Remark 30. $\tilde{x}^r$ denotes the first $n-1$ coordinates in the basis of the local coordinate system. The first point of the definition means that the boundary $\partial\Omega$ can be expressed as the union of a finite number of function graphs of the given type, which are oriented in space using appropriately chosen coordinate systems. Condition $|\tilde{x}^r| < \Delta^r$ expresses that individual functions are defined on bounded $(n-1)$-dimensional domains and because Lipschitz-continuous and continuous functions on bounded domains are also bounded, this condition essentially implies the boundedness of the domain Ω. The second point of the definition says that the domain is only on one side of its boundary.

Definition 31. Let $p \geq 1$. Then we define the space $\mathrm{L}_p(\Omega)$ of functions $u : \Omega \to \mathbb{R}$ as[9]

$$\mathrm{L}_p(\Omega) = \left\{ u \text{ measurable on } \Omega \middle| \int_\Omega |u(x)|^p \,\mathrm{d}x < +\infty \right\}.$$

[7] We should consider to match the definitions in some literature $u : \Omega \to \mathbb{C}$, but we will not encounter complex functions.
[8] $(\forall \varepsilon > 0)\,(\exists \delta > 0)\left(\forall \boldsymbol{x}, \boldsymbol{y} \in \Omega\right)\left(\left\|\boldsymbol{x} - \boldsymbol{y}\right\| < \delta \implies \left|u\left(\boldsymbol{x}\right) - u\left(\boldsymbol{y}\right)\right| < \varepsilon\right)$
[9] $\mathrm{L}_p(\Omega)$ is sometimes marked with an index p above, i.e. as $\mathrm{L}^p(\Omega)$.

Remark. It holds that $\mathrm{L}_1(\Omega) = \mathrm{L}(\Omega)$. The space $\mathrm{L}_2(\Omega)$ is a Hilbert space with the inner product

$$(u, v) = \int_\Omega u(\boldsymbol{x})\, v(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}$$

and the induced norm

$$\|u\|_{\mathrm{L}_2(\Omega)} = \left(\int_\Omega |u(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} \right)^{\frac{1}{2}}.$$

For $p \neq 2$, $\mathrm{L}_p(\Omega)$ is a Banach space with the norm

$$\|u\|_{\mathrm{L}_p(\Omega)} = \left(\int_\Omega |u(\boldsymbol{x})|^p \, \mathrm{d}\boldsymbol{x} \right)^{\frac{1}{p}}.$$

To prove the fact that this is indeed a norm, we need to show that the triangle inequality holds. For the norm on $\mathrm{L}_p(\Omega)$, the triangle inequality is known as the Minkowski inequality (Theorem 52).

1.7.5 Generalized functions and weak derivatives

The following concepts are based on [Sch66] and [Eva98].

Definition 32. A measurable function f is *locally integrable* on the set Ω iff it is integrable on every compact subset of Ω. The space of locally integrable functions in p-th power is denoted by $\mathrm{L}_{p,\mathrm{loc}}(\Omega)$.

Definition 33. Let $\alpha = (\alpha_1, \ldots, \alpha_n)$ where $\alpha_i \in \mathbb{N}_0$ and let us denote $|\alpha| = \sum_{i=1}^{n} \alpha_i$. The n-tuple α is called a *multiindex*. We define the differential operator

$$\mathrm{D}^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \ldots \partial x_n^{\alpha_n}} = \partial_1^{\alpha_1} \partial_2^{\alpha_2} \cdots \partial_n^{\alpha_n}.$$

Remark. For $|\alpha| = 0$, D^α is the identical operator, i.e. $\mathrm{D}^\alpha u = u$.

Definition 34. The vector space $\mathrm{C}_0^\infty(\Omega) \subset \mathrm{C}^\infty(\bar{\Omega})$, containing only functions with *compact support*[10] is called the *space of test functions* on Ω and also denoted by $\mathscr{D}(\Omega)$. By a *distribution* (or *generalized function*) ,we mean a continuous[11] linear functional $T : \mathscr{D}(\Omega) \to \mathbb{R}$. For $\varphi \in \mathscr{D}(\Omega)$, we denote

$$\langle T, \varphi \rangle := T(\varphi).$$

Remark. The set $\mathscr{D}'(\Omega)$ of all distributions on $\mathscr{D}(\Omega)$ is a (continuous) dual space to $\mathscr{D}(\Omega)$, which is a subset of the (algebraic) dual space $\mathscr{D}^*(\Omega)$.

Remark. Functions from $\mathrm{C}_0^\infty(\Omega)$ satisfy the *homogeneous Dirichlet boundary condition* on $\partial\Omega$ (they are equal to zero on $\partial\Omega$).

[10] The *support*, or more precisely the *closed support* of a function $\varphi \in \mathrm{C}^\infty(\Omega)$ is the subset of the domain of φ

$$\operatorname{supp} \varphi = \overline{\{\boldsymbol{x} \in \Omega | \varphi(\boldsymbol{x}) \neq 0\}}.$$

A set in $\mathbb{R}^3$ is compact (see section 1.7.10) iff it is bounded and closed. The closure in the definition is important, because e.g. continuous functions in $\mathbb{R}^n$ can only be nonzero on an open set.

[11] Continuity is understood in the usual way, but with respect to topology in space $\mathscr{D}(\Omega)$.

Definition 35. We say that the distribution T is *regular*, iff there exists a function $u \in \mathrm{L}_{1,\mathrm{loc}}(\Omega)$ such that $\forall \varphi \in \mathscr{D}(\Omega)$,

$$\langle T, \varphi \rangle = (u, \varphi) \equiv \int_\Omega u(\boldsymbol{x})\varphi(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \tag{1.31}$$

holds. We then label the distribution by T_u or we identify it directly with a function u.

Remark. Obviously, in Definition 35, it is enough to have $u \in \mathrm{L}_{1,\mathrm{loc}}(\Omega)$ and not $u \in \mathrm{L}_1(\Omega)$, because the integral (1.31) is actually taken over $\operatorname{supp}\varphi$, which is a compact set.

Definition 36. By the i-th *partial derivative of a distribution* T, we understand the distribution $\partial_i T$ defined by the relation

$$\langle \partial_i T, \varphi \rangle = -\langle T, \partial_i \varphi \rangle \ \forall \varphi \in \mathscr{D}(\Omega). \tag{1.32}$$

Remark. If T is regular (defined by a function u according to (1.31)) and $u \in \mathrm{C}^1(\Omega)$, then $\partial_i T$ is also regular and is defined by a function $\partial_i u$. If α is an arbitrary multiindex, it follows from multiple use of the relation (1.32) that

$$\langle \mathrm{D}^\alpha T, \varphi \rangle = (-1)^{|\alpha|} \langle T, \mathrm{D}^\alpha \varphi \rangle \ \forall \varphi \in \mathscr{D}(\Omega). \tag{1.33}$$

Any distribution T therefore has derivatives of all orders and if it is defined by a function u according to the relation (1.31), the distribution $\mathrm{D}^\alpha T$ is defined by a function $\mathrm{D}^\alpha u$, as long as this (classical, strong) derivative in the sense of calculus exists (see Green's formula 5). If not, we say that a function u has a *derivative in the sense of distributions*. By this derivative, we mean the distribution $\mathrm{D}^\alpha T_u$. An example is the Heaviside function $Y(x) = \chi_{(0,+\infty)}(x)$, whose first derivative is the Dirac „function" δ.

Definition 37. We say that the function $u \in \mathrm{L}_{1,\mathrm{loc}}(\Omega)$ has a *weak derivative* w.r.t some multi-index α iff the distribution $\mathrm{D}^\alpha T_u$ is regular. A function $v \in \mathrm{L}_{1,\mathrm{loc}}(\Omega)$ defined according to (1.31) is denoted as

$$v = \mathrm{D}^\alpha u. \tag{1.34}$$

Remark. For the weak derivative according to (1.31) and (1.33),

$$(\mathrm{D}^\alpha u, \varphi) = (-1)^{|\alpha|} (u, \mathrm{D}^\alpha \varphi) \ \forall \varphi \in \mathscr{D}(\Omega)$$

holds. If $f \in \mathrm{C}^{|\alpha|}(\Omega)$, then of course this relation also satisfies the definition of the classical (strong) derivative in the sense calculus, which we also denote $\mathrm{D}^\alpha u$. However, unlike the weak derivative, it must be defined at each point $\boldsymbol{x} \in \Omega$. The weak derivative is given uniquely in $\mathrm{L}_{1,\mathrm{loc}}(\Omega)$, i.e. if v, w are weak derivatives of u with respect to to α, then $v(x) = w(x)$ almost everywhere in Ω.

1.7.6 Sobolev spaces

Sobolev spaces [Maz85, Bre10, Kin23] are spaces of functions whose derivatives (of different orders) are from the space $\mathrm{L}_p(\Omega)$ (see note 40)

Definition 38. Let $m \in \mathbb{N}$. In space $\mathrm{C}^\infty(\bar{\Omega})$, we define the inner product

$$(u, v)_{\mathrm{H}^m(\Omega)} = \sum_{|\alpha| \le m} \int_\Omega \mathrm{D}^\alpha u \mathrm{D}^\alpha v \mathrm{d}\boldsymbol{x},$$

which induces the norm [Kin23, p. 11]

$$\|u\|_{\mathrm{H}^m(\Omega)} = \sqrt{\sum_{|\alpha| \le m} \int_\Omega |\mathrm{D}^\alpha u|^2 \, \mathrm{d}\boldsymbol{x}}.$$

By *Sobolev space* $\mathrm{H}^m(\Omega)$, we understand the completion (closure) of a set $\mathrm{C}^\infty(\bar{\Omega})$ with respect to the norm $\|\cdot\|_{\mathrm{H}^m(\Omega)}$. By $\mathrm{H}_0^m(\Omega)$, we understand the completion (closure) of $\mathrm{C}_0^\infty(\Omega)$ in $\mathrm{H}^m(\Omega)$.

Remark 39. (Completion procedure) Obviously $\mathrm{C}^\infty\left(\bar{\Omega}\right) \subset \mathrm{L}_2(\Omega)$ and in addition for each $u \in \mathrm{C}^\infty\left(\bar{\Omega}\right)$, we have $\|u\|_{\mathrm{H}^m(\Omega)} \leq \|u\|_{\mathrm{L}_2(\Omega)}$ by Definition 38. Each sequence $(v_n) \subset \mathrm{C}^\infty\left(\bar{\Omega}\right)$, which is Cauchy in the norm $\|\cdot\|_{\mathrm{H}^m(\Omega)}$, is therefore Cauchy in $\mathrm{L}_2(\Omega)$ and because $\mathrm{L}_2(\Omega)$ is a complete space, the limit of this sequence v exists in it. If the sequence (v_n) also has a limit in $\mathrm{C}^\infty\left(\bar{\Omega}\right)$, then these limits are equal. If this limit v does not exist in $\mathrm{C}^\infty\left(\bar{\Omega}\right)$, we will add it there. Carrying out this procedure for all Cauchy sequences, we obtain a complete space - space $\mathrm{H}^m(\Omega)$.

Remark. Space $\mathrm{H}^m(\Omega)$ is Hilbert (complete and with inner product). Specifically for $m = 1$ and $\Omega \in \mathbb{R}^2$, we have (for real functions)

$$(u, v)_{\mathrm{H}^1(\Omega)} = \int_\Omega (uv + \partial_1 u \partial_1 v + \partial_2 u \partial_2 v)\,\mathrm{d}\boldsymbol{x}, \tag{1.35}$$

$$\|u\|_{\mathrm{H}^1(\Omega)} = \sqrt{\int_\Omega \left(|u|^2 + |\partial_1 u|^2 + |\partial_2 u|^2\right)\mathrm{d}\boldsymbol{x}}. \tag{1.36}$$

Remark. Spaces $\mathrm{H}^m(\Omega)$ and $\mathrm{H}_0^m(\Omega)$, respectively, are also referred to in the literature as $\mathrm{W}^{m,2}(\Omega)$ and $\mathrm{W}_0^{m,2}(\Omega)$. Sobolev spaces are sometimes defined even more generally as closures of $\mathrm{C}^m(\bar{\Omega})$ relative to the norm

$$\|u\|_{\mathrm{W}^{m,p}(\Omega)} = \sqrt[p]{\sum_{|\alpha|\leq m} \int_\Omega |\mathrm{D}^\alpha u|^p\,\mathrm{d}\boldsymbol{x}}$$

and are denoted by $\mathrm{W}^{m,p}(\Omega)$. Generally, $\mathrm{W}^{m,p}(\Omega) \subset \mathrm{L}_p(\Omega)$. For $p \neq 2$, they are only Banach (and not Hilbert) spaces. The completion procedure is analogous to the one in Remark 39.

Remark 40. For our theory, the relationship

$$\mathrm{W}^{m,p}(\Omega) = \left\{ u : \Omega \mapsto \mathbb{R} \,|\, (\forall \alpha, |\alpha| \leq m) \left(\mathrm{D}^\alpha u \in \mathrm{L}_p(\Omega)\right)\right\}$$

is suitable, where the existence of derivatives $\mathrm{D}^\alpha u$ is considered in a weak sense, i.e. in terms of definition 37.

Theorem 41. (about traces) *There is continuous map* $T : \mathrm{H}^1(\Omega) \to \mathrm{L}_2(\partial\Omega)$ *such that for each* $u \in \mathrm{C}^\infty\left(\bar{\Omega}\right)$,

$$Tu = u|_{\partial\Omega}$$

holds.

Remark. By definition, $\mathrm{C}^\infty\left(\bar{\Omega}\right)$ is dense in $\mathrm{H}^1(\Omega)$. Theorem (41) says that not only smooth functions on $\bar{\Omega}$, but also the limits of sequences of such functions can be „restricted“ (or better, defined) on the boundary $\partial\Omega$. Such functions do not in principle need to be defined $\partial\Omega$ at all, i.e. they cannot be restricted in the classical sense of the word). Operator T is called the *trace operator*.

1.7.7 Properties of functions from Sobolev space $\mathrm{H}^1(\Omega)$

In the following section, we will get an idea of how much „wild“ can the functions from the Sobolev space $\mathrm{H}^1(\Omega)$ be.

Definition 42. We will say that the function $u : [a, b] \to \mathbb{R}$ is *absolutely continuous* on its domain, iff for each $\varepsilon > 0$, there is $\delta > 0$ such that for each interval distribution $[a, b]$ in the form

$$a = x_1 < y_1 \leq x_2 < y_2 \leq \cdots \leq x_m < y_m = b,$$

for which

$$\sum_{i=1}^{m} \left(y_i - x_i\right) < \delta,$$

it holds that

$$\sum_{i=1}^{m} \left|u\left(y_i\right) - u\left(x_i\right)\right| < \varepsilon.$$

Remark. On $[a,b]$, the following implications apply:

$$\text{Lipschitz property} \implies \text{absolute continuity} \implies \text{uniform continuity} \implies \text{continuity}.$$

Theorem 43. *Function $u : [a,b] \to \mathbb{R}$ is absolutely continuous if and only if there exists $v \in \mathrm{L}_1((a,b))$ so that for each $x \in (a,b)$, we have*

$$u(x) = u(a) + \int_{(a,x)} v(\xi)\,\mathrm{d}\xi. \tag{1.37}$$

Remark. Absolutely continuous functions are those for which the Fundamental Theorem of Calculus holds (relation 1.37). At the same time,

$$u'(x) = v(x)$$

almost everywhere on (a,b).

Definition 44. Let $\Omega \subset \mathbb{R}^n$ be a domain. We say that the function $u : \Omega \to \mathbb{R}$ is *absolutely continuous on a straight line* $p = \{\, t\boldsymbol{k} + \boldsymbol{P} \mid t \in \mathbb{R}\}$, if the function

$$f(t) = u(t\boldsymbol{k} + \boldsymbol{P})$$

is absolutely continuous on every interval $[a,b]$ such that

$$\{\, t\boldsymbol{k} + \boldsymbol{P} \mid t \in [a,b]\} \subset \Omega.$$

Theorem 45. (characterization of space $\mathrm{H}^1(\Omega)$ using absolute continuity) *Let $u \in \mathrm{H}^1(\Omega)$. Then there is a function $\tilde{u} \in \mathrm{H}^1(\Omega)$ such that $\tilde{u} = u$ almost everywhere in Ω and $\tilde{u}$ is absolutely continuous on almost all lines in Ω parallel to one of the coordinate axes. Classical partial derivatives $\tilde{u}$ exist almost everywhere in Ω and coincide with weak derivatives of $\tilde{u}$.*

Remark. Theorem 45 is formulated in accordance with the literature [Maz85, Kin23], but its statement should be analyzed in more detail.

- Every line parallel to one of the coordinate axes that has a non-empty intersection with Ω, passes through exactly one point of the projection of Ω to $(n-1)$- dimensional hyperplane that is perpendicular to the relevant axis. This projection has a certain $(n-1)$-dimensional Lebesgue measure. Claim „for almost all straight lines“ means „for straight lines passing through almost all points of the said projection in terms of the said measure“.

- For $\Omega = (a,b) \subset \mathbb{R}$, we get that the functions from $\mathrm{H}^1((a,b))$ are absolutely continuous on every compact subinterval of (a,b) and are differentiable almost everywhere in (a,b). This includes functions that are equal to a certain differentiable function almost everywhere, or functions that have a derivative almost everywhere, such as $u(x) = |x|$ on $(-1,1)$. Functions that have a jump-type discontinuity are not contained in $\mathrm{H}^1((a,b))$.

- The statement also applies analogously to the space $\mathrm{W}^{1,p}(\Omega)$, $p \geq 1$.

Theorem 46. *Let $u \in L_2(\Omega)$ have classical partial derivatives in $L_2(\Omega)$ and in addition, let it be absolutely continuous on lines parallel to the coordinate axes. Then the classical derivatives of u coincide with its weak derivatives, and thus $u \in H^1(\Omega)$.*

Remark. Theorem46 is the opposite implication to Theorem 46. It can be seen that a function from $L_2(\Omega)$, which has classical partial derivatives defined almost everywhere (and therefore also in $L_2(\Omega)$), does not yet have to lie in $H^1(\Omega)$. If that were the case, then e.g. step functions that have jumps would lie in $H^1(\Omega)$.

1.7.8 Bochner spaces

Let $\mathcal{J} = (0, t_{\max})$ bethe time interval and $u : \mathcal{J} \times \Omega \to \mathbb{R}$ be a function dependent on both time and spatial coordinates. However, the same function can be understood as a function of one variable $u : \mathcal{J} \to \mathcal{X}$, where $\mathcal{X} = \{w | w : \Omega \to \mathbb{R}\}$. Then $u(t) \in \mathcal{X}$ and the original notation of the value of the function at a point can now be expressed in another way: $u(t) = u(t)(\boldsymbol{x})$. The following definition is in this spirit.

Definition 47. Let $\mathcal{X}$ be either a Banach or Hilbert space, $\mathcal{J} = (a, b)$ be bounded open interval and let $p \in \mathbb{N}$. Then we define the *Bochner space*

$$L_p(\mathcal{J}; \mathcal{X}) = \left\{ u : \mathcal{J} \to \mathcal{X} \,\middle|\, \int_{\mathcal{J}} \|u(t)\|_{\mathcal{X}}^p \,\mathrm{d}t < +\infty \right\}$$

with the norm given by the *Bochner integral*

$$\|u\|_{L_p(\mathcal{J},\mathcal{X})} = \sqrt[p]{\int_{\mathcal{J}} \|u(t)\|_{\mathcal{X}}^p \,\mathrm{d}t} = \| \|u(t)\|_{\mathcal{X}} \|_{L_p(\mathcal{J})}. \tag{1.38}$$

Remark 48. If $\mathcal{X}$ is Banach, so is $L_p(\mathcal{J}; \mathcal{X})$. If $\mathcal{X}$ is Hilbert, then the space $L_2(\mathcal{J}; \mathcal{X})$ is Hilbert with the inner product given by

$$(u, v)_{L_2(\mathcal{J};\mathcal{X})} = \int_{\mathcal{J}} (u(t), v(t))_{\mathcal{X}} \,\mathrm{d}t.$$

For the formal introduction of the Bochner integral and the theorem that justifies Definition 47, we refer the reader e.g. to the book [AB06].

1.7.9 Useful inequalities

Theorem 49. (Cauchy-Schwarz inequality). *Let $\mathcal{H}$ be a linear space with an inner product $(\cdot, \cdot)$ and the induced norm $\|\cdot\|$. Then $\forall u, v \in \mathcal{H}$*

$$(u, v) \le \|u\| \, \|v\|$$

holds.

Theorem 50. (Young's inequality). *Let it $a, b \in \mathbb{R}$. Then $ab \le \frac{1}{2}a^2 + \frac{1}{2}b^2$.*

Remark 51. Let it $\nu > 0$. Then, by substituting into Young's inequality, we obtain its more general form

$$ab = \frac{a}{\sqrt{\nu}} \sqrt{\nu} b \le \frac{1}{2\nu} a^2 + \frac{1}{2} \nu b^2.$$

Theorem 52. (Minkowski inequality)
Let it $u, v \in \mathrm{L}_p(\Omega)$. Then

$$\left(\int_\Omega |u(\boldsymbol{x}) + v(\boldsymbol{x})|^p \,\mathrm{d}\boldsymbol{x}\right)^{\frac{1}{p}} \leq \left(\int_\Omega |u(\boldsymbol{x})|^p \,\mathrm{d}\boldsymbol{x}\right)^{\frac{1}{p}} + \left(\int_\Omega |v(\boldsymbol{x})|^p \,\mathrm{d}\boldsymbol{x}\right)^{\frac{1}{p}}.$$

Remark. The Minkowski inequality is a triangle inequality for the norm $\|\cdot\|_{\mathrm{L}_p(\Omega)}$. With its help, it is also proven that $\|\cdot\|_{\mathrm{L}_p(\Omega)}$ is a norm on $\mathrm{L}_p(\Omega)$.

Theorem 53. (Hölder's inequality)
Let $p, q \in [1, +\infty)$ such that $\frac{1}{p} + \frac{1}{q} = 1$. Then

- *for $u \in \mathrm{L}_p(\Omega)$, $v \in \mathrm{L}_q(\Omega)$*

$$\int_\Omega |u(\boldsymbol{x})\, v(\boldsymbol{x})| \,\mathrm{d}\boldsymbol{x} \leq \left(\int_\Omega |u(\boldsymbol{x})|^p \,\mathrm{d}\boldsymbol{x}\right)^{\frac{1}{p}} \left(\int_\Omega |v(\boldsymbol{x})|^q \,\mathrm{d}\boldsymbol{x}\right)^{\frac{1}{q}},$$

- *for $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^n$*

$$\sum_{i=1}^n |u_i\, v_i| \leq \left(\sum_{i=1}^n |u_i|^p\right)^{\frac{1}{p}} \left(\sum_{i=1}^n |v_i|^q\right)^{\frac{1}{q}},$$

Corollary 54. *For vector functions $\boldsymbol{u} \in \mathrm{L}_p(\Omega)^n$, $\boldsymbol{v} \in \mathrm{L}_q(\Omega)^n$ we find by combining both previous cases*

$$\int_\Omega |\boldsymbol{u} \cdot \boldsymbol{v}| \,\mathrm{d}\boldsymbol{x} = \int_\Omega \left|\sum_i u_i\, v_i\right| \mathrm{d}\boldsymbol{x} \leq \int_\Omega \left(\sum_{i=1}^n |u_i|^p\right)^{\frac{1}{p}} \left(\sum_{i=1}^n |v_i|^q\right)^{\frac{1}{q}} \mathrm{d}\boldsymbol{x} \leq \left(\int_\Omega \sum_{i=1}^n |u_i|^p \,\mathrm{d}\boldsymbol{x}\right)^{\frac{1}{p}} \left(\int_\Omega \sum_{i=1}^n |v_i|^q \,\mathrm{d}\boldsymbol{x}\right)^{\frac{1}{q}}$$

and specifically for $p = q = \frac{1}{2}$

$$\int_\Omega |\boldsymbol{u} \cdot \boldsymbol{v}| \,\mathrm{d}\boldsymbol{x} = \left(\int_\Omega \|\boldsymbol{u}\|^2 \,\mathrm{d}\boldsymbol{x}\right)^{\frac{1}{2}} \left(\int_\Omega \|\boldsymbol{v}\|^2 \,\mathrm{d}\boldsymbol{x}\right)^{\frac{1}{2}}.$$

Theorem 55. (Friedrichs inequality) *Let $\Omega \subset \mathbb{R}^n$ be a domain a Lipschitz boundary $\partial\Omega$. Let $\Gamma \subset \partial\Omega$ such that $(n-1)$-dimensional Lebesgue measure $m_{n-1}(\Gamma) > 0$. Then there exists $k > 0$ dependent only on Ω and Γ such that $\forall\, u \in \mathrm{H}^1(\Omega)$*

$$\|u\|^2_{\mathrm{H}^1(\Omega)} \leq k\left(\sum_{j=1}^n \int_\Omega \left|\partial_j u\right|^2 \mathrm{d}\boldsymbol{x} + \int_\Gamma u^2(s)\mathrm{d}S\right).$$

Remark. An intuitive interpretation of Friedrichs inequality is as follows. If a function has bounded derivatives in Ω, then in order to also have values bounded in Ω (i.e. $\|u\|^2_{\mathrm{L}_2(\Omega)} = \int_\Omega u^2 \mathrm{d}\boldsymbol{x} < .$), it is enough if these values are bounded at the boundary of Ω, or even only on a "large enough" portion of it ($\Gamma \subset \Omega$).

Corollary. (Poincaré's inequality) *Let $\Omega \subset \mathbb{R}^n$ be a domain a Lipschitz boundary $\partial\Omega$. Then there exists $k > 0$ dependent only on Ω such that for $\forall\, u \in \mathrm{H}^1_0(\Omega)$*

$$\|u\|^2_{\mathrm{H}^1_0(\Omega)} \leq k \sum_{j=1}^n \int_\Omega \left|\partial_j u\right|^2 \mathrm{d}\boldsymbol{x}.$$

Proof. This is directly the Friedrichs inequality for any admissible choice Γ, for example $\Gamma = \partial\Omega$. From the definition of space $\mathrm{H}_0^1(\Omega)$, we have $\int_{\partial\Omega} u^2(s)\mathrm{d}S = 0$. □

Corollary 56. *Because generally for $\Omega \subset \mathbb{R}^n$, the norm on $\mathrm{H}_0^1(\Omega)$ is defined as*

$$\|u\|_{\mathrm{H}_0^1(\Omega)} = \sqrt{\int_\Omega \left(|u|^2 + \sum_{j=1}^n \left|\partial_j u\right|^2 \right) \mathrm{d}\boldsymbol{x}},$$

the converse inequality holds trivially with the choice of constant of proportionality $K = 1$. It can be shown that

$$\|u\|'_{\mathrm{H}_0^1(\Omega)} = \sqrt{\int_\Omega \sum_{j=1}^n \left|\partial_j u\right|^2 \mathrm{d}\boldsymbol{x}}$$

is also a norm on $\mathrm{H}_0^1(\Omega)$. From Poincaré's inequality, we get the equivalence of norms $\|\cdot\|_{\mathrm{H}_0^1(\Omega)}$ and $\|\cdot\|'_{\mathrm{H}_0^1(\Omega)}$ on $\mathrm{H}_0^1(\Omega)$, i.e. the relationship

$$(\exists k, K > 0)\left(\forall u \in \mathrm{H}_0^1(\Omega)\right)\left(K\|u\|'_{\mathrm{H}_0^1(\Omega)} \le \|u\|_{\mathrm{H}_0^1(\Omega)} \le k\|u\|'_{\mathrm{H}_0^1(\Omega)}\right).$$

Remark. Norm equivalence means that both norms induce the same topology in the given space: the set is open, the sequence is convergent, etc. in one norm as well as in the other, and therefore both norms need not be distinguished from each other. On a finite-dimensional space, all norms are equivalent, but on Sobolev spaces, the equivalence of norms $\|\cdot\|_{\mathrm{H}_0^1(\Omega)}$ and $\|\cdot\|'_{\mathrm{H}_0^1(\Omega)}$ is a non-trivial result.

Remark 57. Poincaré's inequality in $\mathrm{H}_0^1(\Omega)$ de facto allows to estimate the L_2-norm of the function by the sum L_2-norms of its derivatives. Obviously, the same cannot apply to $\mathrm{H}^1(\Omega)$, i.e. without the compact support condition. As a counterexample, any constant but non-zero function can be considered.

The following theorem shows the possibility to estimate from above a function that is bounded by an integral of itself.

Theorem 58. (Grönwall's lemma) *Let $u : [t_0, t_1] \mapsto \mathbb{R}_0^+$ be continuous, let $\alpha > 0, \beta \ge 0$. Let*

$$(\forall\, t \in [t_0, t_1])\left(u(t) \le \int_{t_0}^{t_1} \left(\alpha u(\tau) + \beta\right)\mathrm{d}t \right).$$

Then

$$u(t) \le \frac{\beta}{\alpha}\left(\mathrm{e}^{\alpha(t-t_0)} - 1\right).$$

1.7.10 Compactness and embedding theorems

The following definitions, statements, and theorems can be found e.g. in [KJF77].

Definition 59. Let A, B are sets satisfying $A \subset B$. The identity map $\iota : A \to B$ defined as

$$\iota(x) = x \;\forall x \in A$$

is called the *inclusion operator*.

Remark. In the case of Hilbert spaces, isomorphism with the dual space can also be used as an inclusion operator according to note 18, i.e. $\mathscr{H}_1 \subset \mathscr{H}_2$ and $\iota : \mathscr{H}_1 \to \mathscr{H}_2'$.

Definition 60. Let $\mathscr{B}_1, \mathscr{B}_2$ be Banach spaces. A linear operator $T : \mathscr{B}_1 \mapsto \mathscr{B}_2$ is called *completely continuous*, if for every weakly convergent sequence $(\boldsymbol{u}_n)$ in $\mathscr{B}_1$, $\boldsymbol{u}_n \rightharpoonup \boldsymbol{u}$, the strong convergence $T\boldsymbol{u}_n \to T\boldsymbol{u}$ holds in $\mathscr{B}_2$.

Theorem 61. *Every completely continuous operator on a reflexive Banach space is also continuous (i.e. bounded - see Definition 15).*

Proof. Let $\mathscr{B}_1, \mathscr{B}_2$ be Banach spaces, $\mathscr{B}_1$ is reflexive and $T : \mathscr{B}_1 \mapsto \mathscr{B}_2$ is completely continuous. Let us consider

$$U = \left\{ \boldsymbol{v} \in \mathscr{B}_1 \,|\, \|\boldsymbol{v}\|_{\mathscr{B}_1} = 1 \right\}.$$

If T is not bounded, then a sequence $\boldsymbol{v}_n \in U$ exists such that

$$\lim_{n \to +\infty} \|T\boldsymbol{v}_n\|_{\mathscr{B}_2} = +\infty.$$

But as the sequence $\boldsymbol{v}_n$ is bounded, a weakly convergent subsequence $\boldsymbol{v}_{k_n}$ can be selected from it. Thanks to complete continuity of T, $T\boldsymbol{v}_{k_n}$ strongly converges in $\mathscr{B}_2$, which is a contradiction. □

Definition 62. A set A in topological space $\mathscr{X}$ is called compact if from every open cover of the set A, i.e. from the system of open sets $\mathscr{C}$ such that

$$A \subset \bigcup_{B \in \mathscr{C}} B,$$

finite subcover can be selected $\mathscr{C}_f$, i.e. $\exists \mathscr{C}_f \subset \mathscr{C}$, $\left|\mathscr{C}_f\right| \in \mathbb{N}$ such that

$$A \subset \bigcup_{B \in \mathscr{C}_f} B.$$

Definition 63. A set A in topological space $\mathscr{X}$ is called *sequentially compact* if for each sequence of elements of A there exists a subsequence that has a limit in A.

Remark. In metric spaces, compactness and sequential compactness are equivalent.

Definition 64. A set A in a metric space $\mathscr{X}$ is called *relatively compact*[12], if $\bar{A}$ is compact in $\mathscr{X}$.

Definition 65. A linear operator $T : \mathscr{B}_1 \mapsto \mathscr{B}_2$ is called *compact* if the image $T(A)$ of every bounded set $A \subset \mathscr{B}_1$ is relatively compact in $\mathscr{B}_2$, i.e. $\overline{T(A)}$ is compact.

Remark 66. Compact and completely continuous operators can also be defined on more general (topological vector) spaces. On Banach spaces, every compact operator is also completely continuous. On reflexive Banach spaces, the operator is compact if and only if it is completely continuous.

Theorem 67. *Let $\mathscr{H}$ be a Hilbert space an A be a compact self-adjoint operator on $\mathscr{H}$. Then there is a sequence of (repeating eigenvalues of the operator A) (μ_n) and a (countable) orthonormal basis $(\boldsymbol{x}_n)$ of the space*

$$\ker A^{\perp} = \{\boldsymbol{x} \in \mathscr{H} \,|\, A\boldsymbol{x} = \boldsymbol{0}\}^{\perp}$$

such that for every $\boldsymbol{v} \in \mathscr{H}$, we have

$$A\boldsymbol{v} = \sum_{n=1}^{+\infty} \mu_n(\boldsymbol{v}, \boldsymbol{x}_n)\, \boldsymbol{x}_n.$$

[12] Relatively compact sets are sometimes also called *precompact*. However, the same term also refers to totally bounded sets, i.e. sets that can for any $\varepsilon > 0$ be covered by finite union of open spheres of radius ε (or equivalently, there is a so-called finite ε- net, i.e. set of open spheres of radius ε with centers at mutual distance at least ε). In a complete metric space, relative compactness is equivalent to total boundedness, thereby removing the ambiguity of the definition of the term "precompact set".

Proof. See [Con90, chapter II], [Bre10], [Eva98, Appendix E]. □

Definition 68. We say that a Banach space $\mathscr{B}_1$ is *continuously embedded* into a Banach space $\mathscr{B}_2$ and denote by $\mathscr{B}_1 \hookrightarrow \mathscr{B}_2$, if the inclusion operator $\iota : \mathscr{B}_1 \mapsto \mathscr{B}_2$ is continuous, or (see definition 15), there exists $K > 0$ so that

$$\|\boldsymbol{v}\|_{\mathscr{B}_2} \leq K \|\boldsymbol{v}\|_{\mathscr{B}_1} \ \forall \boldsymbol{v} \in \mathscr{B}_1.$$

Space $\mathscr{B}_1$ is *compactly embedded* into space $\mathscr{B}_2$ (denoted by $\mathscr{B}_1 \hookrightarrow\hookrightarrow \mathscr{B}_2$) if the inclusion operator $\iota : \mathscr{B}_1 \mapsto \mathscr{B}_2$ is compact.

Remark 69. According to the note 66 and Theorem 61, the implication

$$\mathscr{B}_1 \hookrightarrow\hookrightarrow \mathscr{B}_2 \implies \mathscr{B}_1 \hookrightarrow \mathscr{B}_2$$

holds.

Theorem 70. *Let $\mathscr{B}_1 \hookrightarrow \mathscr{B}_2$ hold for two Banach spaces . Then $\mathscr{B}_2' \hookrightarrow \mathscr{B}_1'$.*

Proof. Obviously $\mathscr{B}_2' \subset \mathscr{B}_1'$. We want to prove that there exists $K > 0$ so that for each $\underline{\boldsymbol{w}} \in \mathscr{B}_2'$,

$$\left\|\underline{\boldsymbol{w}}\right\|_{\mathscr{B}_1'} \leq K \left\|\underline{\boldsymbol{w}}\right\|_{\mathscr{B}_2'}$$

holds. We know that by definition of continuous embedding, there exists K such that

$$\|\boldsymbol{v}\|_{\mathscr{B}_2} \leq K \|\boldsymbol{v}\|_{\mathscr{B}_1},$$

so if $\|\boldsymbol{v}\|_{\mathscr{B}_1} \leq 1$, then surely $\frac{1}{K}\|\boldsymbol{v}\|_{\mathscr{B}_2} \leq 1$. The following holds:

$$\begin{aligned}\left\|\underline{\boldsymbol{w}}\right\|_{\mathscr{B}_1'} &= \sup_{\substack{\boldsymbol{v}\in\mathscr{B}_1 \\ \|\boldsymbol{v}\|_{\mathscr{B}_1}=1}} \left|\underline{\boldsymbol{w}}(\boldsymbol{v})\right| = \sup_{\substack{\boldsymbol{v}\in\mathscr{B}_1 \\ \|\boldsymbol{v}\|_{\mathscr{B}_1}\leq 1}} \left|\underline{\boldsymbol{w}}(\boldsymbol{v})\right| \leq \sup_{\substack{\boldsymbol{v}\in\mathscr{B}_1 \\ \frac{1}{K}\|\boldsymbol{v}\|_{\mathscr{B}_2}\leq 1}} \left|\underline{\boldsymbol{w}}(\boldsymbol{v})\right| \\ &= K \sup_{\substack{\boldsymbol{v}\in\mathscr{B}_1 \\ \|\boldsymbol{v}\|_{\mathscr{B}_2}\leq 1}} \left|\underline{\boldsymbol{w}}(\boldsymbol{v})\right| \leq K \sup_{\substack{\boldsymbol{v}\in\mathscr{B}_2 \\ \|\boldsymbol{v}\|_{\mathscr{B}_2}\leq 1}} \left|\underline{\boldsymbol{w}}(\boldsymbol{v})\right| = K \left\|\underline{\boldsymbol{w}}\right\|_{\mathscr{B}_2'}.\end{aligned}$$

Note that inequalities occur in places where the supremum is taken over the ever larger set of vectors (in terms of inclusion). □

Theorem 71. *Let $\mathscr{H}_1, \mathscr{H}_2$ be Hilbert spaces for which $\mathscr{H}_1 \hookrightarrow\hookrightarrow \mathscr{H}_2$. Let A be a bounded linear operator $A : \mathscr{H}_1 \to \mathscr{H}_2$. Then, if there exists an inverse operator A^{-1}, it is compact.*

Lemma 72. (Rellich–Kondrachov compact embedding theorem) *Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with a Lipschitz boundary. Then for each $p > 1$ and q fulfilling*

$$q \in \begin{cases} \left[1, \frac{np}{n-p}\right) & \text{pro } n > p, \\ [p, +\infty) & \text{pro } n = p, \end{cases}$$

it holds that

$$\mathrm{W}^{1,p}(\Omega) \hookrightarrow\hookrightarrow \mathrm{L}_q(\Omega).$$

For $q = \frac{np}{n-p}$, we only have

$$\mathrm{W}^{1,p}(\Omega) \hookrightarrow \mathrm{L}_q(\Omega).$$

Proof. See [Eva98, Chapter 5], [Bre10, Chapter 9]. □

Corollary. *Specifically for $n \in \{2,3\}$ and $p = 2$,*

$$\mathrm{H}^1(\Omega) \hookrightarrow\hookrightarrow \mathrm{L}_2(\Omega)$$

holds.

Lemma 73. (Lions–Aubin) *Let $\mathscr{B}_0 \hookrightarrow\hookrightarrow \mathscr{B} \hookrightarrow \mathscr{B}_1$ be Banach spaces where $\mathscr{B}_0, \mathscr{B}_1$ are reflexive. Let $p_0, p_1 \in (1, +\infty)$. Let us define a function space*

$$\mathscr{Y} = \left\{ u \in \mathrm{L}_{p_0}(\mathscr{J}; \mathscr{B}_0) \middle| \frac{\partial u}{\partial t} \in \mathrm{L}_{p_1}(\mathscr{J}; \mathscr{B}_1) \right\}$$

with the norm

$$\|u\|_{\mathscr{Y}} = \|u\|_{\mathrm{L}_{p_0}(\mathscr{J};\mathscr{B}_0)} + \left\| \frac{\partial u}{\partial t} \right\|_{\mathrm{L}_{p_1}(\mathscr{J};\mathscr{B}_1)}$$

for each $u \in \mathscr{Y}$. Then

$$\mathscr{Y} \hookrightarrow\hookrightarrow \mathrm{L}_{p_0}(\mathscr{J}; \mathscr{B}).$$

Proof. Can be found e.g. in [Pok20a].

□

CHAPTER

2 Kinematics of fluids

2.1 Material body

The subject of study is the *material body*, which occupies a certain connected set $V \subset \mathbb{R}^3$. Without further assumptions, it is possible to discuss the mathematical tools that describe the transformation of the elements of this set in time.

2.2 Reference and current configuration of the material body

Consider an affine space $\left(\mathbb{R}^3, \boldsymbol{o}\right)$ and a coordinate system with the origin at a point $\boldsymbol{o}$, which does not move with respect to the observer. For simplicity and without loss of generality, let us choose a standard basis of the space

$$\begin{aligned} \boldsymbol{e_1} &= (1,0,0)^{\mathrm{T}}, \\ \boldsymbol{e_2} &= (0,1,0)^{\mathrm{T}}, \\ \boldsymbol{e_3} &= (0,0,1)^{\mathrm{T}} \end{aligned}$$

and the origin $\boldsymbol{o} = \boldsymbol{0}$, so every point $\boldsymbol{p} \in \left(\mathbb{R}^3, \boldsymbol{o}\right)$ has coordinates identical to the components of the vector $\boldsymbol{p} - \boldsymbol{o} \in \mathbb{R}^3$. From the mathematical point of view, we will identify the affine space $\left(\mathbb{R}^3, \boldsymbol{o}\right)$, whose elements are points, and the vector space $\mathbb{R}^3$, which contains vectors. Next, let us consider a time interval $\mathscr{J} = (0, t_{\max})$.

The initial subject of study for us will be the temporal evolution of the material body from time $t = 0$ to time $t = t_{\max}$. At time $t = 0$, the body is in its initial *(reference)* state and occupies the volume $V_0 \subset \mathbb{R}^3$ with the boundary ∂V_0. Every point $\boldsymbol{X} \in V_0$, $\boldsymbol{X} = (X, Y, Z)^{\mathrm{T}} = (X_1, X_2, X_3)^{\mathrm{T}}$ will be referred to as the *material point*. We will use capital letters to denote material points. Due to the physical processes of deformation (e.g. under the action of external forces), translation or rotation, the shape and/or the size of the material body changes so that at time t, it occupies the volume $V(t)$. Generally, the position of the individual material points changes over time. This brings the material body into a new, *current* state, which we describe using spatial coordinates $\boldsymbol{x} = \left(x, y, z\right)^{\mathrm{T}} = (x_1, x_2, x_3)^{\mathrm{T}}$ (see Fig. 2.1). Our goal is to find the relationship between the initial (reference) and the current the state of the material body.

Consider the material point $\boldsymbol{X}$ and denote as $\boldsymbol{x}(t, \boldsymbol{X})$ its position at time t. At time $t = 0$, we have $\boldsymbol{x}(0, \boldsymbol{X}) = \boldsymbol{X}$. The value of the function

$$\boldsymbol{x} : \mathscr{J} \times V_0 \to \mathbb{R}^3 \tag{2.1}$$

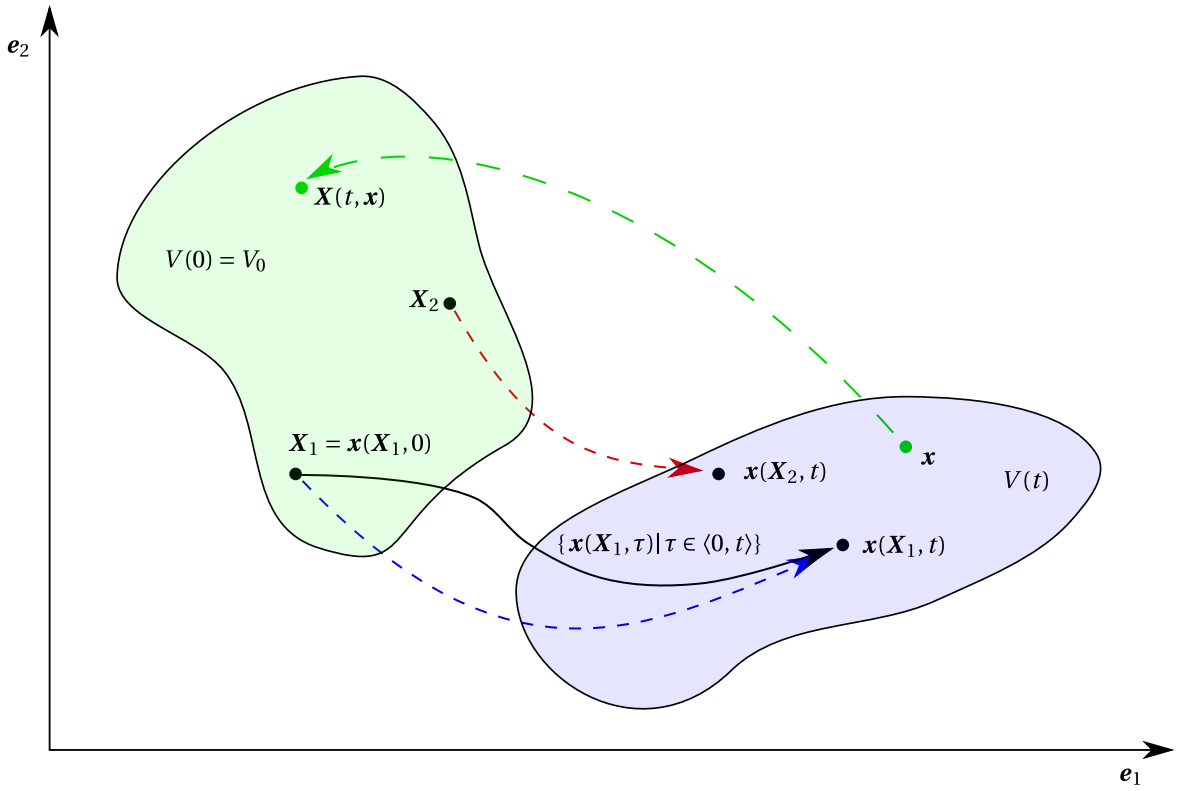

Figure 2.1: Reference and current configuration of the material body.

for a fixed $\boldsymbol{X} \in V_0$ can be imagined as follows. At time $t = 0$, we draw a cross on the material body at the point $\boldsymbol{X}$ cross and watch where this cross moves over time. If the continuum is a liquid, we can put a small ball to the point $\boldsymbol{X}$ watch it be carried away by the current.

Analogously, it is possible to define the velocity of a fixed material point $\boldsymbol{X} \in V_0$ as the time derivative of its position, i.e.

$$\boldsymbol{v}(t, \boldsymbol{X}) = \frac{\partial \boldsymbol{x}}{\partial t}(t, \boldsymbol{X}), \tag{2.2}$$

2.2.1 Transition between reference and spatial coordinates

The physical properties of a material body guarantee that two material points can never meet in one point of space and at the same time, one material point cannot be in two different places at the same time. In mathematical terms, the map (2.1) is an injection, i.e.,

$$\boldsymbol{x}(t, \boldsymbol{X}_1) = \boldsymbol{x}(t, \boldsymbol{X}_2) \iff \boldsymbol{X}_1 = \boldsymbol{X}_2.$$

Furthermore, two distinct material points can neither come infinitely close to each other nor infinitely distant from each other, which means that the Jacobian

$$\left|\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}}\right| = \begin{vmatrix} \frac{\partial x_1}{\partial X_1} & \frac{\partial x_1}{\partial X_2} & \frac{\partial x_1}{\partial X_3} \\ \frac{\partial x_2}{\partial X_1} & \frac{\partial x_2}{\partial X_2} & \frac{\partial x_2}{\partial X_3} \\ \frac{\partial x_3}{\partial X_1} & \frac{\partial x_3}{\partial X_2} & \frac{\partial x_3}{\partial X_3} \end{vmatrix} \neq 0. \tag{2.3}$$

Under these assumptions, the implicit function theorem holds that at every moment in time t, it guarantees the existence of the inverse mapping

$$\boldsymbol{X}(t, \cdot) : V(t) \to V_0,$$

which, for each point from the current configuration $\boldsymbol{x} \in V(t)$, determines the material point $\boldsymbol{X}(t,\boldsymbol{x})$ currently located at the position $\boldsymbol{x}$.

The velocity of a material point that passes through a fixed point in space $\boldsymbol{x} \in \mathbb{R}^3$ at time t is given by

$$\boldsymbol{V}(t,\boldsymbol{x}) = \boldsymbol{v}(t,\boldsymbol{X}(t,\boldsymbol{x})). \tag{2.4}$$

Thus, we find that the velocity can be bound by the relation (2.2) with a fixed material point $\boldsymbol{X}$, or by the relation (2.4) with a fixed point in space $\boldsymbol{x}$. The same applies to any other quantity (e.g. density, pressure, temperature, concentration...). If we are interested in the laws that govern how physical quantities change at the material point $\boldsymbol{X}$ (or in a small volume $\mathrm{d}\mathcal{V}$ which surrounds it), we exercise the so-called *Lagrangian* approach. If, on the other hand, we focus on a fixed point in space $\boldsymbol{x}$, we use the *Eulerian* approach. The outcome of both approaches is identical, although the resulting equations have a different form. We will discuss both approaches in detail in Chapter 3.

2.3 Deformation gradient

The change (deformation) of the configuration of the material in the vicinity of a material point $\boldsymbol{X}$, which is located (at the time t) at the coordinates $\boldsymbol{x} = \boldsymbol{x}(t,\boldsymbol{X})$, is described by a tensor $\mathbf{F}$ defined as

$$\mathbf{F}(t,\boldsymbol{X}) = \nabla \boldsymbol{x}(t,\boldsymbol{X}) = \left(\frac{\partial x^i}{\partial X^j}(t,\boldsymbol{X})\right), \tag{2.5}$$

which is called the *deformation gradient*. From the point of view of the theory of transformation of variables in differential expressions, it is the Jacobi tensor (matrix) of the transformation from the material coordinates $\boldsymbol{X}$ to spatial coordinates $\boldsymbol{x}$. Since we assume regularity of the transformation between the coordinates $\boldsymbol{X}$ and $\boldsymbol{x}$, there is also an inverse tensor $\mathbf{F}^{-1}$, which can be written

$$\mathbf{F}^{-1}(t,\boldsymbol{X}) = \left(\frac{\partial X^i}{\partial x^j}(t,\boldsymbol{X})\right), \tag{2.6}$$

and which expresses the Jacobi tensor of the coordinate transformation from $\boldsymbol{x}$ to $\boldsymbol{X}$.

The deformation gradient is a fundamental tool for the mathematical description of deformation.

2.4 Integrals and derivatives of vector and tensor fields

Let $\mathcal{J} = (0, t_{\max})$ be a time interval and $\Omega \subset \mathbb{R}^3$ be a domain. Let

$$\begin{aligned} f &: \mathcal{J} \times \Omega \to \mathbb{R}, \\ \boldsymbol{g} &: \mathcal{J} \times \Omega \to \mathbb{R}^3, \\ \mathbf{T} &: \mathcal{J} \times \Omega \to \mathbb{R}^{3\times 3}, \end{aligned}$$

be a scalar, vector, and tensor field, respectively. We will use the following formalism:

- The *nabla* (*del*) operator only works with spatial coordinates

$$\nabla = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\right) = (\partial_1, \partial_2, \partial_3) = (\partial_i)$$

  i.e., in accordance with Remark 3, the gradient of a function is given by the expression

$$\nabla f(t,\boldsymbol{x}) = \left(\frac{\partial f}{\partial x_1}(t,\boldsymbol{x}), \frac{\partial f}{\partial x_2}(t,\boldsymbol{x}), \frac{\partial f}{\partial x_3}(t,\boldsymbol{x})\right)^{\mathrm{T}} = \left(\partial_i f\right).$$

- Gradient of a vector field $\boldsymbol{g}$ is applied component-wise, i.e.

$$\nabla \boldsymbol{g} = \left(\partial_j g_i\right) = \left(\nabla \otimes \boldsymbol{g}\right)^{\mathrm{T}}.$$

- The divergence of a vector field is

$$\operatorname{div} \boldsymbol{g} = \nabla \cdot g = \partial_i g_i.$$

- Divergence of a tensor field: the divergence operator $\nabla\cdot$ is applied to a formal row vector composed of tensor columns $\mathbf{T}$, i.e.

$$\operatorname{div} \mathbf{T} = \nabla \cdot (\boldsymbol{T}_1, \boldsymbol{T}_2, \boldsymbol{T}_3) = \sum_{j=1}^{3} \frac{\partial \boldsymbol{T}_j}{\partial x_j} = \left(\partial_j \tau_{ij}\right).$$

- Curl of a vector field is given by

$$\operatorname{curl} \boldsymbol{g} = \nabla \times \boldsymbol{g} = \varepsilon_{ijk} \partial_k g_l.$$

Theorem. *(**Helmholtz**) Let $\Omega \subset \mathbb{R}^3$ be a bounded domain and $\boldsymbol{f} \in \mathrm{C}^2(\Omega)^2$ is a twice differentiable vector field defined on Ω. Then there is a scalar field Φ and vector field $\boldsymbol{A}$ such that*

$$\boldsymbol{f} = \nabla\Phi + \nabla \times \boldsymbol{A}.$$

Remark. Helmholtz's theorem states that every vector field can be decomposed into a sum of *potential* (*faithless, irrotational*) part $\nabla\Phi$ fulfilling $\nabla \times (\nabla\Phi) = \mathbf{0}$ and a *solenoidal* (*sourceless, divergence-free*) parts $\nabla \times \boldsymbol{A}$ fulfilling $\nabla \cdot (\nabla \times \boldsymbol{A}) = 0$. The scalar field Φ is called *scalar potential* and $\boldsymbol{A}$ is called *vector potential*. The proof of the theorem consists in finding a formula for both of these potentials in integral form.

- Laplace operator Δ (Laplacian) applicable to both scalar and vector quantities

$$\Delta f(t, \boldsymbol{x}) = \nabla \cdot \nabla f(t, \boldsymbol{x}) = \sum_{i=1}^{3} \frac{\partial^2 f}{\partial x_i^2}(t, \boldsymbol{x}) = \partial_{ii} f(t, \boldsymbol{x}),$$

$$\Delta \boldsymbol{g}(t, \boldsymbol{x}) = \left(\nabla \cdot \nabla \boldsymbol{g}(t, \boldsymbol{x})\right) = \sum_{i=1}^{3} \frac{\partial^2 \boldsymbol{g}}{\partial x_i^2}(t, \boldsymbol{x}) = \partial_{ii} \boldsymbol{g}(t, \boldsymbol{x}).$$

- Integral of a vector or tensor field over a spatial domain Ω is understood component-wise and its result is again a vector or tensor, respectively.

2.5 Material derivative

Consider any quantity w, whose value at material point $\boldsymbol{X}$ and time T is equal to $w(T, \boldsymbol{X})$. At a fixed point $\boldsymbol{x} \in \mathbb{R}^3$ and time t, its value is $W(t, \boldsymbol{x})$. For the sake of correctness, we will denote time as an argument of the function w by the capital letter T and time as argument of W by a lowercase letter t. Quantity increment w per unit of time at a fixed material point $\boldsymbol{X}$ (at the point that we marked on the body with a cross and which moves in the course of time) is equal to the partial derivative of the function w with respect to time, i.e.,

$$\frac{\partial w}{\partial T}(T, \boldsymbol{X}).$$

Similarly, the increment of this quantity per unit of time at a fixed point v space $\boldsymbol{x}$, which does not move, is equal to the partial derivative of the function W w.r.t. time, i.e.

$$\frac{\partial W}{\partial t}(t, \boldsymbol{x}).$$

Obviously, these are two generally different values. Let us now see how they are related.

Let us choose a fixed material point $\boldsymbol{X}$. Its position at time T is $\boldsymbol{x}(T,\boldsymbol{X})$, and therefore

$$w(T,\boldsymbol{X}) = W(t(T,\boldsymbol{X}),\boldsymbol{x}(t,\boldsymbol{X})) = W(\boldsymbol{\Phi}(T,\boldsymbol{X})),$$

where the inner function $\boldsymbol{\Phi} : \mathscr{J} \times V_0 \to \mathscr{J} \times \mathbb{R}^3$ has the form

$$\boldsymbol{\Phi}(T,\boldsymbol{X}) = (t(T,\boldsymbol{X}), x_1(T,\boldsymbol{X}), x_2(T,\boldsymbol{X}), x_3(T,\boldsymbol{X})) = (T, x_1(T,\boldsymbol{X}), x_2(T,\boldsymbol{X}), x_3(T,\boldsymbol{X})).$$

It can be seen that the first component of the map $\boldsymbol{\Phi}$ is a function t, whose value is based on the assumption that the passage of time is independent of the choice of coordinates, i.e.,

$$t(T,\boldsymbol{X}) = T.$$

Using different symbols for the components of the argument $\boldsymbol{\Phi}$ and components of $\boldsymbol{\Phi}$ itself will allow us to correctly apply the chain rule for differentiation of composite functions. It yields

$$\begin{aligned}
\frac{\partial w}{\partial T}(T,\boldsymbol{X}) &= \sum_{k=1}^{4} \frac{\partial W}{\partial \Phi_k}(\boldsymbol{\Phi}(T,\boldsymbol{X})) \frac{\partial \Phi_k}{\partial T}(T,\boldsymbol{X}) \\
&= \frac{\partial W}{\partial t}(t(T,\boldsymbol{X}),\boldsymbol{x}(T,\boldsymbol{X})) \frac{\partial t}{\partial T}(T,\boldsymbol{X}) + \sum_{k=1}^{3} \frac{\partial W}{\partial x_k}(t(T,\boldsymbol{X}),\boldsymbol{x}(T,\boldsymbol{X})) v_k(T,\boldsymbol{X}) \\
&= \frac{\partial W}{\partial t}(T,\boldsymbol{x}(T,\boldsymbol{X})) + \boldsymbol{v}(T,\boldsymbol{X}) \cdot \nabla W(T,\boldsymbol{x}(T,\boldsymbol{X})) \\
&= \frac{\partial W}{\partial t}(T,\boldsymbol{x}(T,\boldsymbol{X})) + \boldsymbol{V}(T,\boldsymbol{x}(T,\boldsymbol{X})) \cdot \nabla W(T,\boldsymbol{x}(T,\boldsymbol{X})).
\end{aligned} \tag{2.7}$$

After the last modification, all the functions on the right side of (2.7) are expressed using the same argument - the point $(t,\boldsymbol{x}) = (T,\boldsymbol{x}(T,\boldsymbol{X}))$. Therefore, one can rewrite (2.7) in operator form

$$\frac{\partial w}{\partial T}(T,\boldsymbol{X}) = \left(\frac{\partial}{\partial t} + \boldsymbol{V}\cdot\nabla\right) W \Big|_{T,\boldsymbol{x}(t,\boldsymbol{X})} =: \frac{\mathrm{D}W}{\mathrm{D}t}(T,\boldsymbol{x}(T,\boldsymbol{X})), \tag{2.8}$$

where the last relation is defined by the so-called *material derivative* operator

$$\frac{\mathrm{D}}{\mathrm{D}t} := \frac{\partial}{\partial t} + \boldsymbol{V}\cdot\nabla = \frac{\partial}{\partial t} + V_i\partial_i.$$

For vector quantities, we define the material derivative operator component-wise. In particular, for the functions

$$\begin{aligned}
\boldsymbol{w} &= (w_1, w_2, w_3) : \mathscr{J} \times V_0 \to \mathbb{R}^3, \\
\boldsymbol{W} &= (W_1, W_2, W_3) : \mathscr{J} \times \mathbb{R}^3 \to \mathbb{R}^3,
\end{aligned}$$

we define

$$\left(\frac{\mathrm{D}\boldsymbol{W}}{\mathrm{D}t}\right)_i = \frac{\mathrm{D}W_i}{\mathrm{D}t}$$

and if

$$\boldsymbol{w}(T,\boldsymbol{X}) = \boldsymbol{W}(T,\boldsymbol{x}(T,\boldsymbol{X})),$$

then

$$\frac{\partial \boldsymbol{w}}{\partial T}(T,\boldsymbol{X}) = \frac{\mathrm{D}\boldsymbol{W}}{\mathrm{D}t}(T,\boldsymbol{x}(T,\boldsymbol{X})).$$

2.6 Acceleration of a material point

Material point acceleration $\boldsymbol{a}\,[LT^{-2}]$ is defined as the time derivative of its velocity, as in the mechanics of point particles. In the material description, the acceleration is therefore given by the relation

$$\boldsymbol{a}(T,\boldsymbol{X}) = \frac{\partial \boldsymbol{v}}{\partial T}(T,\boldsymbol{X}) = \frac{\partial^2 \boldsymbol{x}}{\partial T^2}(T,\boldsymbol{X}). \tag{2.9}$$

Using the material derivative defined by the relation (2.8), it can be written as

$$\boldsymbol{a}\,(T,\boldsymbol{X}) = \frac{\partial \boldsymbol{v}}{\partial T}\,(T,\boldsymbol{X}) = \frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t}\,(T,\boldsymbol{x}\,(T,\boldsymbol{X}))\,.$$

After applying the inverse transformation $\boldsymbol{X} = \boldsymbol{X}\,(t,\boldsymbol{x})$, $T = T\,(t,\boldsymbol{x}) = t$, we get

$$\boldsymbol{a}\,(t,\boldsymbol{X}\,(t,\boldsymbol{x})) = \frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t}\,(t,\boldsymbol{x})\,. \tag{2.10}$$

By equality (2.10) , the function $\frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t}$ represents the acceleration of the material point $\boldsymbol{X}$, which passes through the site $\boldsymbol{x}$ at time t. However, that is the definition of a function A, which returns the acceleration value in spatial coordinates $t,\boldsymbol{x}$. Thus

$$\boldsymbol{A}\,(t,\boldsymbol{x}) = \frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t}\,(t,\boldsymbol{x})\,.$$

Remark. This result can also be formulated in general terms. If the quantity $\tilde{\boldsymbol{w}}$ described in the material coordinates by a function $\tilde{\boldsymbol{w}}\,(T,\boldsymbol{X})$ is related to the quantity $\boldsymbol{w}$ by the relationship

$$\tilde{\boldsymbol{w}}\,(T,\boldsymbol{X}) = \frac{\partial \boldsymbol{w}}{\partial T}\,(T,\boldsymbol{X})\,,$$

then the same quantity is described in spatial coordinates by means of the functions $\tilde{\boldsymbol{W}}, \boldsymbol{W}$ related by

$$\tilde{\boldsymbol{W}}\,(t,\boldsymbol{x}) = \frac{\mathrm{D}\boldsymbol{W}}{\mathrm{D}t}\,(t,\boldsymbol{x})\,.$$

2.7 Streamlines and trajectories

At the given time $t \in \mathscr{J}$, the velocity field defined in the domain $V\,(t)$ is a function

$$\boldsymbol{V}\,(t,\cdot) : V\,(t) \to R^3.$$

A curve that is at time t tangent to the velocity field at every point $\boldsymbol{V}$ is called a *streamline*. Let us pick a point $\boldsymbol{x}_0 \in V\,(t)$ and consider a curve φ described parametrically using a map

$$\boldsymbol{\varphi} = \left(s \mapsto \boldsymbol{\varphi}\,(s)\right) : \mathbb{R} \to \mathbb{R}^3.$$

Then if $\boldsymbol{\varphi}$ is the solution of the Cauchy problem (ODE system with an initial condition)

$$\frac{\mathrm{d}\boldsymbol{\varphi}}{\mathrm{d}s} = \boldsymbol{V}\left(t,\boldsymbol{\varphi}\right), \tag{2.11}$$

$$\boldsymbol{\varphi}\,(0) = \boldsymbol{x}_0, \tag{2.12}$$

then φ is the streamline passing through the point $\boldsymbol{x}_0$. In the equation (2.11), t is a fixed parameter.

Remark. The parameterization is not given uniquely, and therefore one can substitute $s = h\,(\tilde{s})$ and find other ODE systems whose solution describes the same curve φ.

Now let us choose a point $\boldsymbol{X}_0 \in V_0$. A curve describing its movement over time

$$\tilde{\varphi} = \left\{ \boldsymbol{x}(t, \boldsymbol{X}_0) \middle| \, t \in \mathscr{J} \right\}$$

is called a *trajectory* of the point $\boldsymbol{X}_0$ and its (natural) parameterization

$$\tilde{\boldsymbol{\varphi}} = (t \mapsto \boldsymbol{x}(t, \boldsymbol{X}_0)) : \mathscr{J} \to \mathbb{R}^3$$

satisfies the Cauchy problem (see (2.2) and (2.4))

$$\frac{\mathrm{d}\tilde{\boldsymbol{\varphi}}}{\mathrm{d}t} = \boldsymbol{V}\left(t, \tilde{\boldsymbol{\varphi}}\right) = \boldsymbol{v}(t, \boldsymbol{X}_0), \tag{2.13}$$

$$\boldsymbol{\varphi}(0) = \boldsymbol{X}_0. \tag{2.14}$$

Unlike in (2.11), t appears in the equation (2.13) as an independent variable. Therefore, streamlines and trajectories (curves φ and $\tilde{\varphi}$) are generally different. Only if the velocity field is $\boldsymbol{V}$ independent of time, streamlines and trajectories coincide. In that case, we speak about *stationary (steady) flow*.

2.8 Continuum hypothesis

Let us consider on $\mathbb{R}^3$ the classical Lebesgue measure m_3 and let there exist another measure M. The material body V is considered a *continuum* [RG14, Chapter 1], if for each (m_3-measurable) subset $A \subset V$

$$m_3(A) = 0 \implies M(A) = 0$$

holds (i.e. the measure M is continuous with respect to m_3) and the number $M(A)$ has a physical meaning of mass of the set A. Next, let Ψ and $\boldsymbol{\Psi}$, respectively, be the measure (and vector measure) such that for each point $\boldsymbol{x} \in V^0$, there exist the limits

$$\psi(\boldsymbol{x}) = \lim_{R \to 0+} \frac{\Psi(B_R(\boldsymbol{x}))}{M(B_R(\boldsymbol{x}))},$$

and

$$\boldsymbol{\psi}(\boldsymbol{x}) = \lim_{R \to 0+} \frac{\boldsymbol{\Psi}(B_R(\boldsymbol{x}))}{M(B_R(\boldsymbol{x}))},$$

respectively, where

$$B_R(\boldsymbol{x}) = \left\{ \boldsymbol{v} \in \mathbb{R}^3 \middle| \, |\boldsymbol{v} - \boldsymbol{x}| < R \right\}.$$

The function Ψ (and $\boldsymbol{\Psi}$) is then called an *extensive scalar (or vector) physical quantity*. For any $\mathcal{V} \subset V$, it then holds that

$$\Psi(\mathcal{V}_0) = \int_{\mathcal{V}_0} \psi(\boldsymbol{x}) \, \mathrm{d}M = \int_{\mathcal{V}_0} \psi(\boldsymbol{x}) \varrho(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x},$$

$$\boldsymbol{\Psi}(\mathcal{V}_0) = \int_{\mathcal{V}_0} \boldsymbol{\psi}(\boldsymbol{x}) \, \mathrm{d}M = \int_{\mathcal{V}_0} \boldsymbol{\psi}(\boldsymbol{x}) \varrho(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x},$$

where

$$\varrho(\boldsymbol{x}) = \lim_{R \to 0+} \frac{M(B_R(\boldsymbol{x}))}{\frac{4}{3}\pi R^3}$$

is the mass density.

Remark.

$$\psi = \frac{\mathrm{d}\Psi}{\mathrm{d}M}, \quad \text{and } \boldsymbol{\psi} = \frac{\mathrm{d}\boldsymbol{\Psi}}{\mathrm{d}M}$$

are the Radon-Nikodym derivatives of the measures Ψ and $\boldsymbol{\Psi}$, respectively.

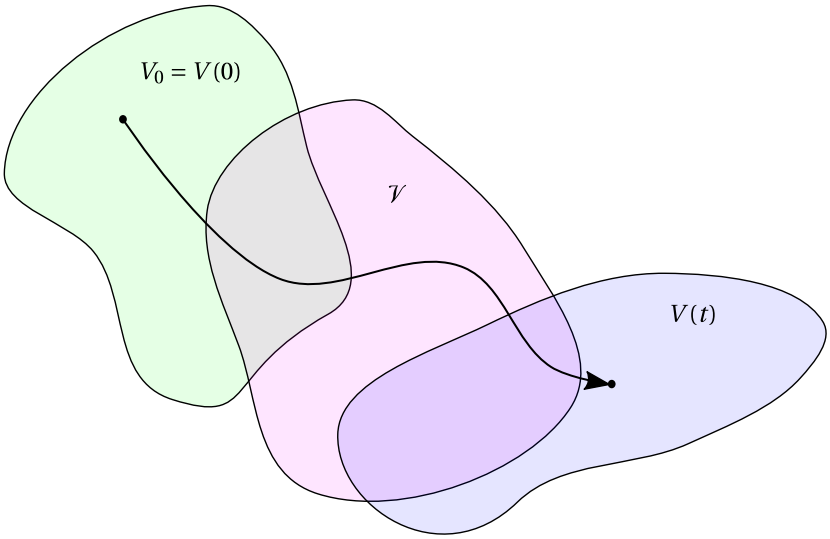

Figure 2.2: Euler's approach: fixed volume $\mathcal{V}$ and material body $V(t)$ moving through time.

For example, for a vector measure expressing the linear momentum $\boldsymbol{P}$, we obtain the „specific momentum", i.e., the velocity at a point $\boldsymbol{x}$ defined as

$$\boldsymbol{V}(\boldsymbol{x}) = \lim_{R \to 0+} \frac{\boldsymbol{P}(B_R(\boldsymbol{x}))}{M(B_R(\boldsymbol{x}))}.$$

2.9 Conservation of mass

We first derive the mathematical representation of the law of conservation of mass. We will show here several approaches with the help of which the result can be obtained, and at the same time we verify that they all lead to the same conclusion.

2.9.1 Euler's approach using a finite volume

As we have already outlined in Section 2.2.1, *Euler's approach* to describing the dynamics of the continuum consists in describing the laws that govern the development of physical quantities at a fixed point in space $\boldsymbol{x}$, or, respectively, in a fixed volume $\mathcal{V} \subset \mathbb{R}^3$ with a boundary $\partial\mathcal{V}$ (see Figure 2.2). Law of conservation of mass in the volume $\mathcal{V}$ can be formulated as

mass loss in the volume $\mathcal{V}$ is equal to the mass flux across the boundary $\partial\mathcal{V}$ in the direction out of $\mathcal{V}$.

If $\varrho(t,\boldsymbol{x})$ [kg $\cdot$ m^{-3}] is a function describing the density of the material at a spatial point $\boldsymbol{x}$ and at time t , then the total mass M [kg] contained in the volume $\mathcal{V}$ is

$$M(t) = \int_{\mathcal{V}} \varrho(t,\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}$$

and its *decrease* per unit time is equal to

$$-\frac{\mathrm{d}M}{\mathrm{d}t}(t). \tag{2.15}$$

Now consider an infinitesimally small surface $\mathrm{d}S \subset \partial\mathcal{V}$ with a normal $\boldsymbol{n}$, pointing out of the volume $\mathcal{V}$ (Figure 2.3). For all points $\boldsymbol{x} \in \mathrm{d}S$, we consider the same velocity $\boldsymbol{V}(t,\boldsymbol{x})$. The projection of velocity

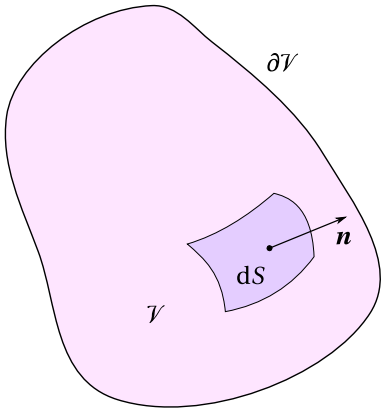

Figure 2.3: Euler's approach: fixed volume $\mathcal{V}$ with a boundary $\partial\mathcal{V}$, surface $\mathrm{d}S$ with the outward pointing normal $\boldsymbol{n}$.

into the direction perpendicular to $\mathrm{d}S$ is then $\boldsymbol{V}\cdot\boldsymbol{n}$ and the mass that passes through the surface $\mathrm{d}S$ per unit time is equal to

$$\varrho\boldsymbol{V}\cdot\boldsymbol{n}\mathrm{d}S.$$

The total mass flow out of the volume $\mathcal{V}$ across the boundary $\partial\mathcal{V}$ per unit time is equal to the surface integral of II. kind

$$\int_{\partial\mathcal{V}}\varrho\boldsymbol{V}\cdot\boldsymbol{n}\mathrm{d}S=\int_{\partial\mathcal{V}}\varrho\boldsymbol{V}\cdot\mathrm{d}\boldsymbol{S}. \tag{2.16}$$

The mathematical expression of the law of conservation of matter therefore equates relations (2.15) and (2.16) and leads to the *continuity equation in integral conservative form*

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}}\varrho\mathrm{d}\boldsymbol{x}+\int_{\partial\mathcal{V}}\varrho\boldsymbol{V}\cdot\boldsymbol{n}\mathrm{d}S=0. \tag{2.17}$$

This equation can be further modified by first applying the Gauss theorem (Theorem 7, Chapter 1) and theorem about differentiation of an integral with respect to a parameter (Theorem 4), gradually obtaining

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}}\varrho\mathrm{d}\boldsymbol{x}+\int_{\mathcal{V}}\nabla\cdot\left(\varrho\boldsymbol{V}\right)\mathrm{d}\boldsymbol{x}&=0,\\ \int_{\mathcal{V}}\left[\frac{\partial\varrho}{\partial t}+\nabla\cdot\left(\varrho\boldsymbol{V}\right)\right]\mathrm{d}\boldsymbol{x}&=0.\end{aligned} \tag{2.18}$$

Now we consider that the volume $\mathcal{V}$ is chosen completely arbitrarily. Therefore, the integral (2.18) can only be equal to zero provided that the integrand is also equal to zero in the entire region where the material body is located, i.e.,

$$\frac{\partial\varrho}{\partial t}+\nabla\cdot\left(\varrho\boldsymbol{V}\right)=\frac{\partial\varrho}{\partial t}+\partial_j\left(\varrho V_j\right)=0. \tag{2.19}$$

Equation (2.19) is a partial differential equation and is called the *continuity equation in conservative* (differential) *form*.

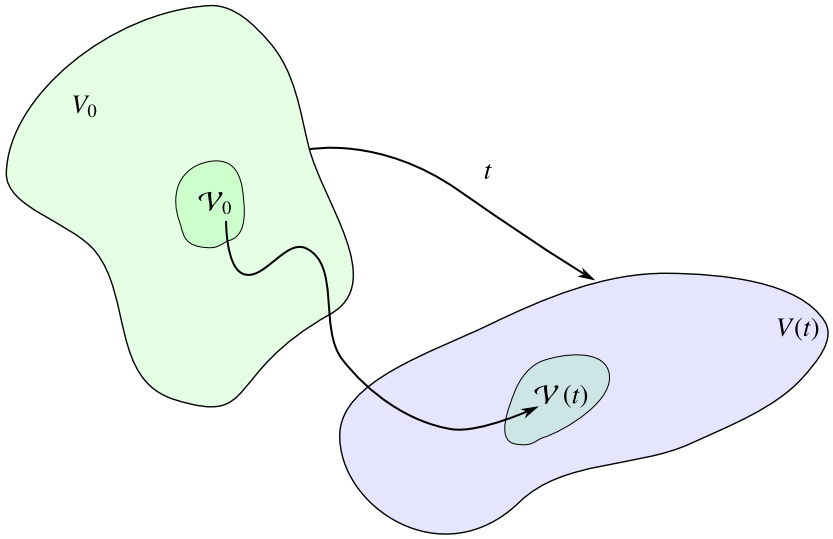

Figure 2.4: Lagrangian approach: Material body $V(t)$ and its evolution over time. Within $V(t)$, the control volume $\mathcal{V}(t)$ is chosen, which moves together with the material body.

2.9.2 Lagrangian approach using a finite volume

For the sake of interest, we will proceed to the derivation of the continuity equation using the *Lagrangian approach*, which follows the motion of a fixed material point, or a set of material points $\mathcal{V}_0 \subset V_0$ (giant. 2.4). The total mass in this volume is

$$M = \int_{\mathcal{V}_0} \rho(0, \boldsymbol{X}) \, \mathrm{d}\boldsymbol{X} = \int_{\mathcal{V}_0} \varrho(0, \boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}.$$

Over time, a set of material points with this (still the same) mass M changes its shape and size, so it holds at the same time that

$$M = \int_{\mathcal{V}(t)} \varrho(t, \boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \tag{2.20}$$

for each $t \in \mathcal{J}$. The region of integration in (2.20) changes over time, and generally $\mathcal{V}(t) \subset V(t)$ (see Section 2.2). By moving from spatial coordinates $\boldsymbol{x}$ to material coordinates $\boldsymbol{X}$, however, we get the integral over the time-invariant volume $\mathcal{V}_0$:

$$M = \int_{\mathcal{V}(t)} \varrho(t, \boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \int_{\mathcal{V}_0} \varrho(t, \boldsymbol{x}(t, \boldsymbol{X})) \left| \det \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}} \right| \mathrm{d}\boldsymbol{X} = \int_{\mathcal{V}_0} \rho(t, \boldsymbol{X}) \, |\det \mathbf{F}| \, \mathrm{d}\boldsymbol{X}, \tag{2.21}$$

considering that the Jacobian of the transformation $\det \mathbf{F} = \det\left(\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}}\right)$ is nonzero by the assumption (2.3) and has the same sign for all $\boldsymbol{X} \in V_0$. Hence, the absolute value can be removed and

$$\pm M = \int_{\mathcal{V}_0} \rho(t, \boldsymbol{X}) \det \mathbf{F} \mathrm{d}\boldsymbol{X}$$

holds. By differentiating this equality with respect to time, we obtain the *continuity equation in non-conservative integral form*

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{V}_0} \rho(t, \boldsymbol{X}) \det \mathbf{F} \mathrm{d}\boldsymbol{X} = 0. \tag{2.22}$$

Similarly to part 2.9.1, we can derive the appropriate differential form of this equation. By swapping the integral and the time derivative according to Theorem 4 and considering that the volume $\mathcal{V}_0$ was selected completely arbitrarily, we get the equality

$$\frac{\partial\left(\rho \det \mathbf{F}\right)}{\partial t} = 0, \tag{2.23}$$

which is the *continuity equation in the non-conservative* (differential) *form* expressed in *material coordinates*.

Let us show that equation (2.23) is equivalent to equation (2.19) derived in Section 2.9.1. We perform the time derivative of the product and obtain

$$\frac{\partial \rho}{\partial t} \det \mathbf{F} + \rho \frac{\partial \det \mathbf{F}}{\partial t} = 0. \tag{2.24}$$

Now we will use the relation ((2.26) proved as Lemma 74 in the following section 2.10)

$$\frac{\partial \det \mathbf{F}}{\partial t} = \det \mathbf{F} \nabla \cdot \boldsymbol{V}.$$

After dividing by the nonzero $\det \mathbf{F}$, we obtain the equality

$$\frac{\partial \rho}{\partial t} + \rho \nabla \cdot \boldsymbol{V} = 0$$

and finally we apply the definition of the material derivative (2.8) to get

$$\frac{\mathrm{D}\varrho}{\mathrm{D}t} + \varrho \nabla \cdot \boldsymbol{V} = 0, \tag{2.25}$$

which is the *continuity equation in the non-conservative* (differential) *form* expressed in *spatial coordinates*. Now it is easy to get the relationship (2.19), when we only break down the material derivative

$$\frac{\mathrm{D}\varrho}{\mathrm{D}t} + \nabla \cdot \boldsymbol{V} = \frac{\partial \varrho}{\partial t} + \boldsymbol{V} \cdot \nabla \varrho + \varrho \nabla \cdot \boldsymbol{V} = \frac{\partial \varrho}{\partial t} + \nabla \cdot \left(\varrho \boldsymbol{V}\right) = 0.$$

3.38

2.10 Reynolds transport theorem

First, we show an important auxiliary statement:

Lemma 74. *It holds that*

$$\frac{\partial \det \mathbf{F}}{\partial t} = \det \mathbf{F} \nabla \cdot \boldsymbol{V}. \tag{2.26}$$

Proof. Assuming sufficient differentiability of the function $\boldsymbol{x}(t, \boldsymbol{X})$, the assertion (2.26) can be derived from the expression of the determinant (1.18) and from the definition $\mathbf{F}$ (2.5), i.e.

$$\det \mathbf{F} = \frac{1}{3!} \varepsilon_{IJK} \varepsilon_{ijk} \frac{\partial x_I}{\partial X_i} \frac{\partial x_J}{\partial X_j} \frac{\partial x_K}{\partial X_k}.$$

using substitution of partial derivatives $\partial/\partial t$ and $\partial/\partial X_*$ we gradually manipulate the expression as follows:

$$\begin{aligned}\frac{\partial \det \mathbf{F}}{\partial t} &= \frac{1}{3!}\varepsilon_{IJK}\varepsilon_{ijk}\frac{\partial}{\partial t}\left(\frac{\partial x_I}{\partial X_i}\frac{\partial x_J}{\partial X_j}\frac{\partial x_K}{\partial X_k}\right)\\ &= \frac{1}{3!}\varepsilon_{IJK}\varepsilon_{ijk}\underbrace{\left(\frac{\partial v_I}{\partial X_i}\frac{\partial x_J}{\partial X_j}\frac{\partial x_K}{\partial X_k} + \underbrace{\frac{\partial x_I}{\partial X_i}\frac{\partial v_J}{\partial X_j}\frac{\partial x_K}{\partial X_k}}_{\text{index renaming } I\leftrightarrow J, i\leftrightarrow j} + \underbrace{\frac{\partial x_I}{\partial X_i}\frac{\partial x_J}{\partial X_j}\frac{\partial v_K}{\partial X_k}}_{\text{index renaming } I\leftrightarrow K, i\leftrightarrow k}\right)}_{\Longrightarrow\ 3\times\text{the same expression}} \qquad (2.27)\\ &= \frac{1}{2}\varepsilon_{IJK}\varepsilon_{ijk}\frac{\partial v_I}{\partial X_i}\frac{\partial x_J}{\partial X_j}\frac{\partial x_K}{\partial X_k} = \frac{1}{2}\varepsilon_{IJK}\varepsilon_{ijk}\frac{\partial V_I}{\partial x_\ell}\frac{\partial x_\ell}{\partial X_i}\frac{\partial x_J}{\partial X_j}\frac{\partial x_K}{\partial X_k}. \qquad (2.28)\end{aligned}$$

By the definition of the matrix $\mathbf{F}^{-1}$ and expressing its elements using the cofactors (1.19), we obtain

$$\frac{\partial X_i}{\partial x_I} = \frac{1}{\det \mathbf{F}}\Delta_{Ii} = \frac{1}{\det \mathbf{F}}\frac{1}{2}\varepsilon_{IJK}\varepsilon_{ijk}\frac{\partial x_J}{\partial X_j}\frac{\partial x_K}{\partial X_k}.$$

After substituting into (2.28), we get

$$\frac{\partial \det \mathbf{F}}{\partial t} = \det \mathbf{F}\frac{\partial X_i}{\partial x_I}\frac{\partial V_I}{\partial x_\ell}\frac{\partial x_\ell}{\partial X_i} = \det \mathbf{F}\underbrace{\frac{\partial X_i}{\partial x_I}\frac{\partial x_\ell}{\partial X_i}}_{\delta_{I\ell}}\frac{\partial V_I}{\partial x_\ell} = \det \mathbf{F}\delta_{I\ell}\frac{\partial V_I}{\partial x_\ell} = \det \mathbf{F}\frac{\partial V_I}{\partial x_I} = \det \mathbf{F}\nabla\cdot\boldsymbol{V}.$$

□

Now let $\mathcal{V}_0 \subset V_0$ be a fixed control volume of the material body and denote $\mathcal{V}(t) = \boldsymbol{x}(t,\mathcal{V}_0)$. Let $\phi : (0,T)\times V_0 \to \mathbb{R}$ be an arbitrary function and we define $\Phi(t,\boldsymbol{x}) = \phi(t,\boldsymbol{X})$ where $\boldsymbol{x} = \boldsymbol{x}(t,\boldsymbol{X})$. Then it holds that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)}\Phi(t,\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}_0}\Phi(t,\boldsymbol{x}(t,\boldsymbol{X}))\,|\det \mathbf{F}(t,\boldsymbol{X})|\,\mathrm{d}\boldsymbol{X} = \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}_0}\phi\,|\det \mathbf{F}|\,\mathrm{d}\boldsymbol{X}\\ &= \int_{\mathcal{V}_0}\frac{\partial}{\partial t}\left(\phi(t,\boldsymbol{X})\,|\det \mathbf{F}|\right)\mathrm{d}\boldsymbol{X} = \int_{\mathcal{V}_0}\frac{\partial \phi}{\partial t}\,|\det \mathbf{F}| + \phi(t,\boldsymbol{X})\frac{\partial\,|\det \mathbf{F}|}{\partial t}\mathrm{d}\boldsymbol{X}\\ &= \int_{\mathcal{V}_0}\left(\frac{\mathrm{D}\Phi}{\mathrm{D}t} + \Phi\nabla\cdot\boldsymbol{V}\right)\Big|_{(t,\boldsymbol{x}(t,\boldsymbol{X}))}\,|\det \mathbf{F}|\,\mathrm{d}\boldsymbol{X}\\ &= \int_{\mathcal{V}(t)}\frac{\mathrm{D}\Phi}{\mathrm{D}t} + \Phi\nabla\cdot\boldsymbol{V}\Big|_{(t,\boldsymbol{x})}\,\mathrm{d}\boldsymbol{x}. \qquad (2.29)\end{aligned}$$

After breaking down the material derivative operator, we get another useful form of the equality (2.29)

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)}\Phi(t,\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int_{\mathcal{V}(t)}\frac{\partial \Phi}{\partial t} + \boldsymbol{V}\cdot\nabla\Phi + \Phi\nabla\cdot\boldsymbol{V}\,\mathrm{d}\boldsymbol{x} = \int_{\mathcal{V}(t)}\frac{\partial \Phi}{\partial t} + \nabla\cdot(\Phi\boldsymbol{V})\,\mathrm{d}\boldsymbol{x}. \qquad (2.30)$$

Both (2.29) and (2.30) are referred to as the Reynolds transport theorem.

2.10.1 Continuity equation as a consequence of the Reynolds transport theorem

The law of conservation of mass in any volume $\mathcal{V}_0 \subset V_0$, which in time $t > 0$ transforms into volume $\mathcal{V}(t)$, can be formulated as

$$M(\mathcal{V}_0) = M(\mathcal{V}(t)) = \int_{\mathcal{V}(t)} \varrho(t, \boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \text{konst.},$$

from which

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{V}(t)} \varrho(t, \boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = 0$$

Substituting into (2.29) or (2.30), respectively, with the choice $\Phi = \varrho$, we immediately receive

$$\int_{\mathcal{V}(t)} \frac{\mathrm{D}\varrho}{\mathrm{D}t} + \varrho \nabla \cdot \boldsymbol{V} \mathrm{d}\boldsymbol{x} = \int_{\mathcal{V}(t)} \frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \boldsymbol{V}) \, \mathrm{d}\boldsymbol{x} = 0$$

regardless of the choice $\mathcal{V}_0$ (and hence regardless of the choice of $\mathcal{V}(t)$ as well), which means that

$$\frac{\mathrm{D}\varrho}{\mathrm{D}t} + \varrho \nabla \cdot \boldsymbol{V} = \frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \boldsymbol{V}) = 0.$$

This is a continuity equation in the forms (2.25) and (2.19), respectively.

2.10.2 Reynolds transport theorem for specific quantities

Let $F : (0, T) \times \mathbb{R}^3 \to \mathbb{R}$ be an arbitrary function (a physical quantity defined per unit mass, i.e. a specific quantity). Then substituting $\Phi = \varrho F$ int (2.29), we get

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{V}(t)} \varrho F \mathrm{d}\boldsymbol{x} = \int_{\mathcal{V}(t)} \frac{\mathrm{D}(\varrho F)}{\mathrm{D}t} + \varrho F \nabla \cdot \boldsymbol{V} \mathrm{d}\boldsymbol{x}. = \int_{\mathcal{V}(t)} \varrho \frac{\mathrm{D}F}{\mathrm{D}t} + \underbrace{F\left(\frac{\mathrm{D}\varrho}{\mathrm{D}t} + \varrho \nabla \cdot \boldsymbol{V}\right)}_{=0 \text{ by the continuity eq. (2.25)}} \mathrm{d}\boldsymbol{x} = \int_{\mathcal{V}(t)} \varrho \frac{\mathrm{D}F}{\mathrm{D}t} \mathrm{d}\boldsymbol{x}. \quad (2.31)$$

2.11 Description of deformation

In this section, we derive the form of some mathematical objects that describe deformation of the fluid during the flow. The study of these objects falls into the field of linear and general elasticity, from which, however, we only select the knowledge necessary for the interpretation of fluid dynamics in Chapter 3. In some more complex derivations, we will highlight some terms in the equations in color for clarity, while always adjusting the expression marked in red in order to obtain the expression in blue.

The *relative displacement vector* $\boldsymbol{u}$ (in the spatial description) is defined as

$$\boldsymbol{u}(t, \boldsymbol{X}) = \boldsymbol{x}(t, \boldsymbol{X}) - \boldsymbol{x}(0, \boldsymbol{X}) = \boldsymbol{x}(t, \boldsymbol{X}) - \boldsymbol{X} = (x_k(t, \boldsymbol{X}) - X_k)\boldsymbol{e}_k.$$

Consider two points $\boldsymbol{X}, \boldsymbol{Y} \in V_0$, whose mutual displacement will be denoted as

$$\mathrm{d}\boldsymbol{X} = \boldsymbol{Y} - \boldsymbol{X}.$$

At time t, these points get to a position

$$\begin{aligned} \boldsymbol{x} &= \boldsymbol{x}(t, \boldsymbol{X}) = \boldsymbol{X} + \boldsymbol{u}(t, \boldsymbol{X}), \\ \boldsymbol{y} &= \boldsymbol{x}(t, \boldsymbol{Y}) = \boldsymbol{Y} + \boldsymbol{u}(t, \boldsymbol{Y}). \end{aligned} \quad (2.32)$$

Their relative positions at time 0 and at time t (with dependence on t now being omitted for clarity) are bound by

$$\begin{aligned}
\mathrm{d}\boldsymbol{X} &= \boldsymbol{Y} - \boldsymbol{X},\\
\mathrm{d}\boldsymbol{x} &= \boldsymbol{y} - \boldsymbol{x} = \boldsymbol{x}(t, \boldsymbol{X} + \mathrm{d}\boldsymbol{X}) - \boldsymbol{x}(t, \boldsymbol{X})\\
&= \boldsymbol{x}(t, \boldsymbol{X}) + \nabla \boldsymbol{x}(t, \boldsymbol{X}) \cdot \mathrm{d}\boldsymbol{X} + \boldsymbol{o}(\mathrm{d}\boldsymbol{X}) - \boldsymbol{x}(t, \boldsymbol{X})\\
&= \nabla \boldsymbol{x}(t, \boldsymbol{X}) \cdot \mathrm{d}\boldsymbol{X} + \boldsymbol{o}(\mathrm{d}\boldsymbol{X}) = \mathbf{F}(t, \boldsymbol{X}) \cdot \mathrm{d}\boldsymbol{X} + \boldsymbol{o}(\mathrm{d}\boldsymbol{X}),
\end{aligned} \tag{2.33}$$

where we used the Taylor expansion $\boldsymbol{x}(t, \cdot)$ up to the 1st order, i.e.

$$\lim_{\mathrm{d}\boldsymbol{X} \to \mathbf{0}} \frac{\boldsymbol{o}(\mathrm{d}\boldsymbol{X})}{\|\mathrm{d}\boldsymbol{X}\|} = \mathbf{0}$$

holds. By writing down (2.33) component-wise, we get

$$\mathrm{d}x_i = \frac{\partial x_i}{\partial X_j} \mathrm{d}X_j + o(\mathrm{d}\boldsymbol{X}). \tag{2.34}$$

Next, we define (at the point $(t, \boldsymbol{X})$)

$$\mathbf{H} = \nabla \boldsymbol{u} = \left(\frac{\partial u_i}{\partial X_j} \right) = \left(\frac{\partial (x_i - X_i)}{\partial X_j} \right) = \left(\frac{\partial x_i}{\partial X_j} - \delta_{ij} \right) = \mathbf{F} - \mathbf{I} \tag{2.35}$$

and substituting (2.35) to (2.33), we get the expression using the displacement vector

$$\mathrm{d}\boldsymbol{x} = (\mathbf{H} + \mathbf{I}) \cdot \mathrm{d}\boldsymbol{X} + \boldsymbol{o}(\mathrm{d}\boldsymbol{X}) = \mathrm{d}\boldsymbol{X} + \nabla \boldsymbol{u} \cdot \mathrm{d}\boldsymbol{X} + \boldsymbol{o}(\mathrm{d}\boldsymbol{X}) \tag{2.36}$$

2.11.1 Lagrangian finite strain tensor

For the magnitude of the mutual position vector, i.e. the distance of the points $\boldsymbol{x}, \boldsymbol{y}$, we have

$$\begin{aligned}
\|\mathrm{d}\boldsymbol{x}\|^2 &= \|\mathrm{d}\boldsymbol{X} + \nabla \boldsymbol{u} \cdot \mathrm{d}\boldsymbol{X} + \boldsymbol{o}(\mathrm{d}\boldsymbol{X})\|^2 = \left(\mathrm{d}X_i + \frac{\partial u_i}{\partial X_j} \mathrm{d}X_j + o(\mathrm{d}\boldsymbol{X}) \right) \left(\mathrm{d}X_i + \frac{\partial u_i}{\partial X_k} \mathrm{d}X_k + o(\mathrm{d}\boldsymbol{X}) \right)\\
&= \mathrm{d}X_i \mathrm{d}X_i + \frac{\partial u_i}{\partial X_j} \mathrm{d}X_j \mathrm{d}X_i + \underbrace{\frac{\partial u_i}{\partial X_k} \mathrm{d}X_i \mathrm{d}X_k}_{\text{index naming: } i \to j, k \to i} + \underbrace{\frac{\partial u_i}{\partial X_j} \frac{\partial u_i}{\partial X_k} \mathrm{d}X_j \mathrm{d}X_k}_{\text{index naming: } i \leftrightarrow k} + o(\mathrm{d}\boldsymbol{X})\\
&= \|\mathrm{d}\boldsymbol{X}\|^2 + \frac{\partial u_i}{\partial X_j} \mathrm{d}X_j \mathrm{d}X_i + \frac{\partial u_j}{\partial X_i} \mathrm{d}X_j \mathrm{d}X_i + \frac{\partial u_k}{\partial X_j} \frac{\partial u_k}{\partial X_i} \mathrm{d}X_j \mathrm{d}X_i + o(\mathrm{d}\boldsymbol{X})\\
&= \|\mathrm{d}\boldsymbol{X}\|^2 + 2\epsilon_{ij} \mathrm{d}X_i \mathrm{d}X_j + o(\mathrm{d}\boldsymbol{X}),
\end{aligned} \tag{2.37}$$

where $\mathbf{e}$ is called the *Lagrangian finite strain tensor* (or the *Green-Lagrange strain tensor*)

$$\mathbf{e} = (\epsilon_{ij}), \ \epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i} + \frac{\partial u_k}{\partial X_j} \frac{\partial u_k}{\partial X_i} \right). \tag{2.38}$$

Neglecting the quadratic terms in (2.38), we obtain a symmetric *small strain tensor*

$$\tilde{\mathbf{e}} = (\tilde{\epsilon}_{ij}), \ \tilde{\epsilon}_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i} \right). \tag{2.39}$$

However, according to (1.15), it is nothing but the symmetric part of the tensor $\nabla \boldsymbol{u}$.

After substituting into (2.36) and utilizing (1.15) and (1.16), we get

$$\mathrm{d}\boldsymbol{x} + o(\mathrm{d}\boldsymbol{X}) = \mathrm{d}\boldsymbol{X} + \nabla \boldsymbol{u} \cdot \mathrm{d}\boldsymbol{X} = \mathrm{d}\boldsymbol{X} + (\nabla \boldsymbol{u})_{\mathrm{sym}} \cdot \mathrm{d}\boldsymbol{X} + (\nabla \boldsymbol{u})_{\mathrm{skew}} \cdot \mathrm{d}\boldsymbol{X} = \mathrm{d}\boldsymbol{X} + \tilde{\mathbf{e}} \cdot \mathrm{d}\boldsymbol{X} + \boldsymbol{w} \times \mathrm{d}\boldsymbol{X},$$

where according to (1.15) and (1.17), one can write

$$(\nabla \boldsymbol{u})_{\text{skew}} = \frac{1}{2}\left(\nabla \boldsymbol{u} - \nabla \boldsymbol{u}^{\mathrm{T}}\right) = \left(\frac{1}{2}\left(\frac{\partial u_i}{\partial X_j} - \frac{\partial u_j}{\partial X_i}\right)\right) = \begin{pmatrix} 0 & -w_3 & w_2 \\ w_3 & 0 & -w_1 \\ -w_2 & w_1 & 0 \end{pmatrix},$$

where

$$\boldsymbol{w} = \operatorname{rot} \boldsymbol{u}.$$

Going back to (2.32) and subtracting both equations, we obtain

$$\begin{aligned} \boldsymbol{u}(t,\boldsymbol{Y}) &= \boldsymbol{u}(t,\boldsymbol{X}) + \left(\boldsymbol{y}-\boldsymbol{x}\right) - (\boldsymbol{Y}-\boldsymbol{X}) \\ &= \boldsymbol{u}(t,\boldsymbol{X}) + \mathrm{d}\boldsymbol{x} - \mathrm{d}\boldsymbol{X} \\ &= \boldsymbol{u}(t,\boldsymbol{X}) + \tilde{\mathbf{e}}\cdot\mathrm{d}\boldsymbol{X} + \boldsymbol{w}\times\mathrm{d}\boldsymbol{X} + o(\mathrm{d}\boldsymbol{X}). \end{aligned}$$

This means that the movement of $\boldsymbol{Y}$ can be decomposed into

- $\boldsymbol{u}(t,\boldsymbol{X})\ldots$ displacement of any reference point $\boldsymbol{X}$,
- $\tilde{\mathbf{e}}\cdot\mathrm{d}\boldsymbol{X}\ \ldots$ dilation/contraction of the position of $\boldsymbol{Y}$ relative to the position of $\boldsymbol{X}$ (Symmetric tensor $\tilde{\mathbf{e}}$ is diagonalizable, has real eigenvalues and their corresponding three eigenvectors represent the three main dilation/contraction directions)
- $\boldsymbol{w}\times\mathrm{d}\boldsymbol{X}\ldots$ rotation of $\boldsymbol{Y}$ around the point $\boldsymbol{X}$
- $o(\mathrm{d}\boldsymbol{X})\ldots$ deformation of an order higher than the distance of the points $\boldsymbol{X}$, $\boldsymbol{Y}$

2.11.2 Strain rate tensor

By differentiating the equality (2.33) with respect to time, we get the rate of change of $\mathrm{d}\boldsymbol{x}$ per unit time (for fixed $\boldsymbol{X},\boldsymbol{Y}$)

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathrm{d}\boldsymbol{x}) = \frac{\mathrm{d}}{\mathrm{d}t}\nabla\boldsymbol{u}(t,\boldsymbol{X})\cdot\mathrm{d}\boldsymbol{X} = \nabla\boldsymbol{v}(t,\boldsymbol{X})\cdot\mathrm{d}\boldsymbol{X} = \left(\frac{\partial v_i}{\partial X_j}\mathrm{d}X_j\right),$$

where the tensor $\nabla\boldsymbol{v}(t,\boldsymbol{X}) = \left(\frac{\partial v_i}{\partial X_j}\right)$ is the *velocity gradient* [Rud19] in material coordinates. With the use of (2.34), one can proceed further as

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathrm{d}\boldsymbol{x}) = \left(\frac{\partial v_i}{\partial X_j}\mathrm{d}X_j\right) = \left(\frac{\partial V_i}{\partial x_k}\frac{\partial x_k}{\partial X_j}\mathrm{d}X_j\right) = \left(\frac{\partial V_i}{\partial x_k}\mathrm{d}x_k\right) + \boldsymbol{o}(\mathrm{d}\boldsymbol{X}) = \left(\frac{\partial V_i}{\partial x_j}\mathrm{d}x_j\right) + \boldsymbol{o}(\mathrm{d}\boldsymbol{X}) = \nabla\boldsymbol{V}(t,\boldsymbol{x})\cdot\mathrm{d}\boldsymbol{x} + \boldsymbol{o}(\mathrm{d}\boldsymbol{X}),$$

where the tensor $\nabla\boldsymbol{V}(t,\boldsymbol{x}) = \left(\frac{\partial V_i}{\partial x_j}\right)$ is the velocity gradient in the current coordinates.

The relative rate of dilation of the line segment between material points $\boldsymbol{X},\boldsymbol{Y}$, located at positions $\boldsymbol{x},\boldsymbol{y}$ in the mutual distance $\|\mathrm{d}\boldsymbol{x}\|$ at time t, can be expressed as

$$\frac{\frac{\mathrm{d}}{\mathrm{d}t}\|\mathrm{d}\boldsymbol{x}\|}{\|\mathrm{d}\boldsymbol{x}\|} = \frac{1}{2}\frac{\frac{\mathrm{d}}{\mathrm{d}t}\left(\|\mathrm{d}\boldsymbol{x}\|^2\right)}{\|\mathrm{d}\boldsymbol{x}\|^2} = \frac{1}{2}\frac{\frac{\mathrm{d}}{\mathrm{d}t}\left(2\epsilon_{ij}\mathrm{d}X_i\mathrm{d}X_j\right)}{\|\mathrm{d}\boldsymbol{x}\|^2} = \frac{1}{2}\frac{2\dot{\epsilon}_{ij}\mathrm{d}X_i\mathrm{d}X_j}{\|\mathrm{d}\boldsymbol{x}\|^2}. \tag{2.40}$$

We further modify the expression

$$\begin{aligned} 2\dot{\epsilon}_{ij}\mathrm{d}X_i\mathrm{d}X_j &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i} + \frac{\partial u_k}{\partial X_j}\frac{\partial u_k}{\partial X_i}\right)\mathrm{d}X_i\mathrm{d}X_j \\ &= \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} + \frac{\partial v_k}{\partial X_j}\frac{\partial u_k}{\partial X_i} + \frac{\partial u_k}{\partial X_j}\frac{\partial v_k}{\partial X_i}\right)\mathrm{d}X_i\mathrm{d}X_j \\ &= 2\left(\frac{\partial v_j}{\partial X_i} + \frac{\partial v_k}{\partial X_j}\frac{\partial u_k}{\partial X_i}\right)\mathrm{d}X_i\mathrm{d}X_j. \end{aligned}$$

Using (2.35), we continue as

$$2\dot{\epsilon}_{ij}\mathrm{d}X_i\mathrm{d}X_j = 2\left(\frac{\partial v_j}{\partial X_i} + \frac{\partial v_k}{\partial X_j}\left(\frac{\partial x_k}{\partial X_i} - \delta_{ik}\right)\right)\mathrm{d}X_i\mathrm{d}X_j = 2\left(\frac{\partial v_j}{\partial X_i} - \frac{\partial v_i}{\partial X_j} + \frac{\partial v_k}{\partial X_j}\frac{\partial x_k}{\partial X_i}\right)\mathrm{d}X_i\mathrm{d}X_j$$
$$= 2\left(\underbrace{\frac{\partial v_j}{\partial X_i}\mathrm{d}X_i\mathrm{d}X_j - \frac{\partial v_i}{\partial X_j}\mathrm{d}X_i\mathrm{d}X_j}_{=0 \text{ (just renaming of } i,j)} + \frac{\partial v_k}{\partial X_j}\frac{\partial x_k}{\partial X_i}\mathrm{d}X_i\mathrm{d}X_j\right)$$
$$= 2\frac{\partial v_k}{\partial X_j}\frac{\partial x_k}{\partial X_i}\mathrm{d}X_i\mathrm{d}X_j = 2\frac{\partial V_k}{\partial x_\ell}\frac{\partial x_\ell}{\partial X_j}\frac{\partial x_k}{\partial X_i}\mathrm{d}X_i\mathrm{d}X_j = 2\frac{\partial V_k}{\partial x_\ell}\frac{\partial x_k}{\partial X_i}\mathrm{d}X_i\frac{\partial x_\ell}{\partial X_j}\mathrm{d}X_j$$

and using (2.34), we finally get

$$2\dot{\epsilon}_{ij}\mathrm{d}X_i\mathrm{d}X_j = 2\frac{\partial V_k}{\partial x_\ell}\mathrm{d}x_k\mathrm{d}x_l + o\left(\|\mathrm{d}\boldsymbol{x}\|^2\right) \underset{(k,l)\curvearrowright(i,j) \text{ a } (j,i)}{=} \frac{\partial V_i}{\partial x_j}\mathrm{d}x_i\mathrm{d}x_j + \frac{\partial V_i}{\partial x_j}\mathrm{d}x_i\mathrm{d}x_j + o\left(\|\mathrm{d}\boldsymbol{x}\|^2\right)$$
$$= \left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i}\right)\mathrm{d}x_i\mathrm{d}x_j + o\left(\|\mathrm{d}\boldsymbol{x}\|^2\right).$$

After substituting back into (2.40), we have

$$\frac{\frac{\mathrm{d}}{\mathrm{d}t}\|\mathrm{d}\boldsymbol{x}\|}{\|\mathrm{d}\boldsymbol{x}\|} = \frac{1}{2}\left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i}\right)\frac{\mathrm{d}x_i\mathrm{d}x_j}{\mathrm{d}x_k\mathrm{d}x_k} + O(\mathrm{d}\boldsymbol{x}) = \mathbf{D}\boldsymbol{\alpha} + O(\mathrm{d}\boldsymbol{x}),$$

where

$$\mathbf{D} = \left(d_{ij}\right) = \left(\frac{1}{2}\left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i}\right)\right) = \frac{1}{2}\left[\nabla\boldsymbol{V} + (\nabla\boldsymbol{V})^{\mathrm{T}}\right] \tag{2.41}$$

is the *strain rate tensor* in the current coordinates and $\boldsymbol{\alpha}$ is a unit vector in the direction $\mathrm{d}\boldsymbol{x}$. $\mathbf{D}$ is the symmetric part of the velocity gradient tensor $\nabla\boldsymbol{V}$.

CHAPTER

3 Fluid dynamics equations

Mathematical description of continuum dynamics, i.e. description of the movement and deformation of a given material body depending on the action of external and internal forces, can be derived from the laws of conservation in classical mechanics, i.e.

1. the law of conservation of mass (Lomonosov 1758, Lavoisier 1774) - see the continuity equation (3),
2. of the law of conservation of linear momentum (a direct consequence of Newton's three laws of motion)
3. the law of conservation of energy (the first law of thermodynamics),

and, in addition, from the physical properties of the material.

3.1 Forces and II. Newton's law in a fluid

- postulate: in the continuum, there are only surface and body (volume) forces (it should be possible to prove - see [Tru92])
- the specific body force $\boldsymbol{F}$ or the body force intensity $\boldsymbol{F}_V$ defined as the limit

$$\boldsymbol{F}(\boldsymbol{x}) = \lim_{R\to 0+} \frac{\boldsymbol{F}_V(B_R(\boldsymbol{x}))}{M(B_R(\boldsymbol{x}))} = \lim_{R\to 0+} \frac{\boldsymbol{F}_V(B_R(\boldsymbol{x}))}{\frac{4}{3}\pi R^3} \frac{\frac{4}{3}\pi R^3}{M(B_R(\boldsymbol{x}))} = \frac{1}{\varrho(\boldsymbol{x})} \lim_{R\to 0+} \frac{\boldsymbol{F}_V(B_R(\boldsymbol{x}))}{\frac{4}{3}\pi R^3}.$$

- the surface force per unit area acting at the surface around the a point $\boldsymbol{x}$ with the normal vector $\boldsymbol{n}(\boldsymbol{x})$ is

$$\boldsymbol{T}(t, \boldsymbol{x}, \boldsymbol{n}(\boldsymbol{x})).$$

  The fact that $\boldsymbol{T}$ does not depend on other properties of the surface, e.g., on the mean curvature $\kappa = \nabla \cdot \boldsymbol{n}$ or higher derivatives of the normal vector, is stated by the so-called Cauchy's hypothesis. In 1957, Walter Noll proved this hypothesis using Cauchy's fundamental lemma (which we discuss below) [Tru92], [Gur81, p. 97].

- internal and external forces
  - internal force acts within the studied system

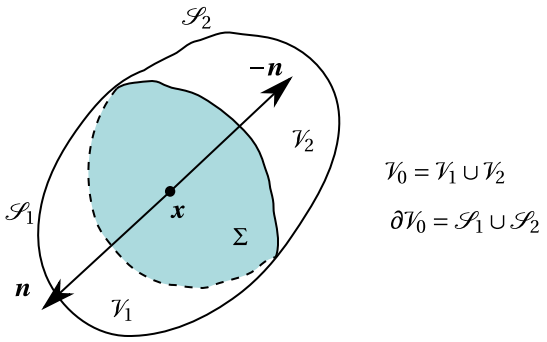

Figure 3.1: On derivation of Cauchy's lemma, i.e. the principle of action and reaction of surface forces

– external force acts through objects outside the studied system

We formulate the laws of conservation of linear momentum and angular momentum (i.e., the laws of force) in a general form. Let again $\mathcal{V}_0 \subset V_0$ be a fixed but arbitrarily chosen control volume of the material body. The momentum of the mass contained within this volume and located in the region $\mathcal{V}(t)$ at time t, is subject to the law of force

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{V}(t)} \varrho \boldsymbol{V}\,\mathrm{d}\boldsymbol{x} = \int\limits_{\partial\mathcal{V}(t)} \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n})\,\mathrm{d}S + \int\limits_{\mathcal{V}(t)} \varrho \boldsymbol{F}\,\mathrm{d}\boldsymbol{x} \tag{3.1}$$

and the angular momentum of this mass (with respect to the origin of the coordinate system[1]) satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{V}(t)} \varrho \boldsymbol{x}\times\boldsymbol{V}\,\mathrm{d}\boldsymbol{x} = \int\limits_{\partial\mathcal{V}(t)} \boldsymbol{x}\times\boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n})\,\mathrm{d}S + \int\limits_{\mathcal{V}(t)} \varrho \boldsymbol{x}\times\boldsymbol{F}\,\mathrm{d}\boldsymbol{x}. \tag{3.2}$$

From the fact that relation (3.1) is valid regardless of the selection of $\mathcal{V}_0$, we arrive at the differential equations describing the balance (law of conservation) of linear momentum. Relationship (3.2) does not lead to another independent equation describing the flow, because the angular momentum of each finite volume $\mathcal{V}_0$ can be described using the linear momenta of elementary subvolumes $\mathrm{d}\mathcal{V}_0 \subset \mathcal{V}_0$, satisfying (3.1). However, relationship (3.2) taken for $|\mathcal{V}_0| \to 0$ has consequences for the form of the force $\boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n})$, which we will show shortly.

3.2 Stress tensor

Consider the division of volume $\mathcal{V}_0$ into two parts $\mathcal{V}_0 = \mathcal{V}_1 \cup \mathcal{V}_2$ and let us denote the common boundary in between by Σ. At time $t > 0$, the respective sets have the shape $\boldsymbol{x}(t,\mathcal{V}_1)$, $\boldsymbol{x}(t,\mathcal{V}_2)$, $\boldsymbol{x}(t,\Sigma)$. If $\boldsymbol{n}$ is the outer normal to $\boldsymbol{x}(t,\mathcal{V}_1)$ at point $\boldsymbol{\xi} \in \boldsymbol{x}(t,\Sigma)$, then $-\boldsymbol{n}$ is the outer normal to $\boldsymbol{x}(t,\mathcal{V}_2)$ at the same point. If we formulate (3.1) separately for $\mathcal{V}_1, \mathcal{V}_2$, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\boldsymbol{x}(t,\mathcal{V}_1)} \varrho \boldsymbol{V}\,\mathrm{d}\boldsymbol{x} = \int\limits_{\boldsymbol{x}(t,\Sigma)} \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n})\,\mathrm{d}S + \int\limits_{\boldsymbol{x}(t,\mathscr{S}_1)} \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n})\,\mathrm{d}S + \int\limits_{\boldsymbol{x}(t,\mathcal{V}_1)} \varrho \boldsymbol{F}\,\mathrm{d}\boldsymbol{x}, \tag{3.3}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\boldsymbol{x}(t,\mathcal{V}_2)} \varrho \boldsymbol{V}\,\mathrm{d}\boldsymbol{x} = \int\limits_{\boldsymbol{x}(t,\Sigma)} \boldsymbol{T}(t,\boldsymbol{x},-\boldsymbol{n})\,\mathrm{d}S + \int\limits_{\boldsymbol{x}(t,\mathscr{S}_2)} \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n})\,\mathrm{d}S + \int\limits_{\boldsymbol{x}(t,\mathcal{V}_2)} \varrho \boldsymbol{F}\,\mathrm{d}\boldsymbol{x}. \tag{3.4}$$

[1] Momentum balance relative to any point $\boldsymbol{x}_0$ we would gain by replacing $\boldsymbol{x}$ expression $(\boldsymbol{x}-\boldsymbol{x}_0)$ in (3.2).

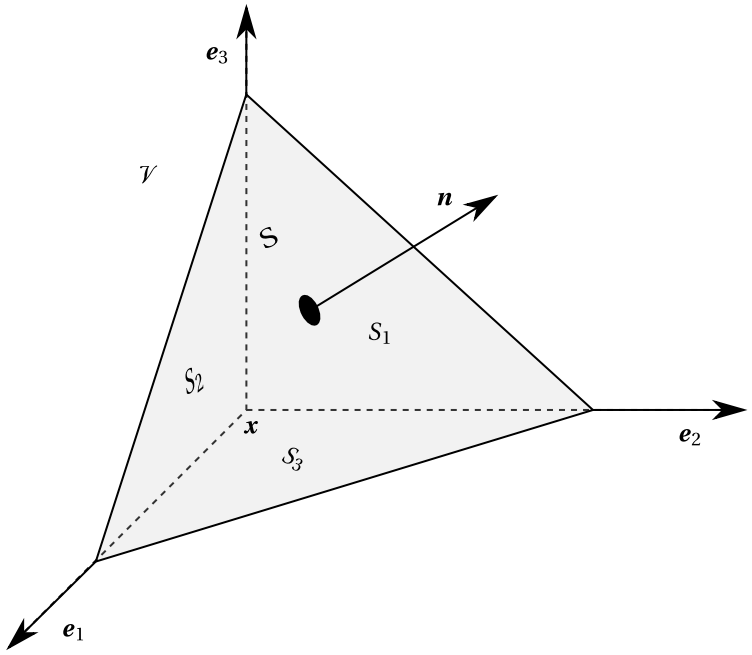

Figure 3.2: A tetrahedron argument to derive the existence of the stress tensor. Without loss of generality, one of the vertices of the tetrahedron is placed at the origin of the coordinate system, i.e. $\boldsymbol{x} \equiv \boldsymbol{0}$.

By summing (3.3)-(3.4) we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{V}(t)} \varrho \boldsymbol{V}\mathrm{d}\boldsymbol{x} = \int\limits_{\boldsymbol{x}(t,\Sigma)} [\boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n}) + \boldsymbol{T}(t,\boldsymbol{x},-\boldsymbol{n})]\,\mathrm{d}S + \int\limits_{\partial\mathcal{V}(t)} \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n})\,\mathrm{d}S + \int\limits_{\mathcal{V}(t)} \varrho \boldsymbol{F}\mathrm{d}\boldsymbol{x} \tag{3.5}$$

and subtracting (3.1) finally yields

$$\int\limits_{\boldsymbol{x}(t,\Sigma)} [\boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n}) + \boldsymbol{T}(t,\boldsymbol{x},-\boldsymbol{n})]\,\mathrm{d}S = 0.$$

Since the respective volume $\mathcal{V}_0$ and its cut Σ were chosen arbitrarily,

$$\boldsymbol{T}(t,\boldsymbol{x},-\boldsymbol{n}) = -\boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n}) \;\; \forall \boldsymbol{x}, \forall \boldsymbol{n}$$

must hold, which is called *Cauchy's fundamental lemma* and is de facto the III. Newton's law (law of action and reaction).

Let us now imagine such a control volume $\mathcal{V}_0$ that its shape at time t is a tetrahedron $\mathcal{V} := \mathcal{V}(t) = \boldsymbol{x}(t,\mathcal{V}_0)$, with three faces S_1, S_2, S_3 perpendicular to the axes of the coordinate system (Fig. 3.2). The outward-pointing normal to the face S_i is $\boldsymbol{n}_i = -\boldsymbol{e}_i$. The fourth face S has a unit outward-pointing normal vector $\boldsymbol{n}$. According to the mean value theorem, the action of surface forces on the tetrahedron can be expressed as

$$\int\limits_{\partial\mathcal{V}} \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n}(\boldsymbol{x}))\,\mathrm{d}S = \boldsymbol{T}(t,\boldsymbol{\xi},\boldsymbol{n})\,|S| + \boldsymbol{T}\left(t,\boldsymbol{\xi}_1,\boldsymbol{n}_1\right)|S_1| + \boldsymbol{T}\left(t,\boldsymbol{\xi}_2,\boldsymbol{n}_2\right)|S_2| + \boldsymbol{T}\left(t,\boldsymbol{\xi}_3,\boldsymbol{n}_3\right)|S_3|, \tag{3.6}$$

where $\boldsymbol{\xi}_j \in S_j$, $\boldsymbol{\xi} \in S$. Further:

- From Cauchy's lemma, it holds that $\boldsymbol{T}\left(t,\boldsymbol{\xi}_j,\boldsymbol{n}_j\right) = \boldsymbol{T}\left(t,\boldsymbol{\xi}_j,-\boldsymbol{e}_j\right) = -\boldsymbol{T}\left(t,\boldsymbol{\xi}_j,\boldsymbol{e}_j\right)$.

- The surface S_j is the projection of the surface S to the plane with the normal $\boldsymbol{e}_j$, and therefore its area satisfies
$$\frac{|S_j|}{|S|} = n_j,$$
where $\boldsymbol{n} = (n_j)$. n_j is the projection of the normal vector $\boldsymbol{n}$ to the direction $\boldsymbol{e}_j$.

Substituting these facts into (3.6), we get according to (3.1) the momentum balance for the tetrahedron $\mathcal{V}$ as

$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho v)\big|_{(t,\boldsymbol{\xi}_\mathcal{V})}|\mathcal{V}| = \big(\boldsymbol{T}(t,\boldsymbol{\xi},\boldsymbol{n}) - \boldsymbol{T}(t,\boldsymbol{\xi}_1,\boldsymbol{e}_1)n_1 - \boldsymbol{T}(t,\boldsymbol{\xi}_2,\boldsymbol{e}_2)n_2 - \boldsymbol{T}(t,\boldsymbol{\xi}_3,\boldsymbol{e}_3)n_3\big)|S| + \varrho F\big|_{(t,\tilde{\boldsymbol{\xi}}_\mathcal{V})}|\mathcal{V}|, \tag{3.7}$$

where the mean value theorem for volume integrals was again used, i.e. $\in \mathcal{V}_0$, $\boldsymbol{\xi}_\mathcal{V}, \tilde{\boldsymbol{\xi}}_\mathcal{V} \in \mathcal{V}$. Now let us scale all sides of the tetrahedron $\mathcal{V}$ by the factor ϵ. Since $|S| = O(\epsilon^2)$ and $|\mathcal{V}| = O(\epsilon^3) = o(\epsilon)$, by dividing (3.7) by the number ϵ^2 and taking the limits $\epsilon \to 0$, we get

$$0 = \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n}) - \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{e}_1)n_1 - \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{e}_2)n_2 - \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{e}_3)n_3,$$

or

$$\boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n}) = \mathbf{T}(t,\boldsymbol{x})\cdot\boldsymbol{n}, \tag{3.8}$$

where

$$\mathbf{T}(t,\boldsymbol{x}) = \begin{pmatrix} \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{e}_1) & \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{e}_2) & \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{e}_3) \end{pmatrix} = \big(\boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{e}_j)_i\big) = (\tau_{ij})$$

is the *stress tensor* whose j-th column expresses the surface force vector acting on the unit surface with normal $\boldsymbol{e}_j$.

3.2.1 Symmetry of the stress tensor

With the use of (3.8), the surface integral in (3.2) can be rewritten into the form

$$\int_{\partial\mathcal{V}(t)} \boldsymbol{x}\times\boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n})\,\mathrm{d}S = \int_{\partial\mathcal{V}(t)} \boldsymbol{x}\times(\mathbf{T}\cdot\boldsymbol{n})\,\mathrm{d}S = \int_{\partial\mathcal{V}(t)} \varepsilon_{ijk}x_j(\mathbf{T}\cdot\boldsymbol{n})_k\boldsymbol{e}_i\,\mathrm{d}S = \varepsilon_{ijk}\boldsymbol{e}_i\int_{\partial\mathcal{V}(t)} x_j\tau_{kl}n_l\,\mathrm{d}S.$$

$$\ldots\text{by Green's formula (Theorem 5)}\ldots$$

$$= \varepsilon_{ijk}\boldsymbol{e}_i\int_{\mathcal{V}(t)} \frac{\partial}{\partial x_l}(x_j\tau_{kl})\,\mathrm{d}\boldsymbol{x} = \varepsilon_{ijk}\boldsymbol{e}_i\int_{\mathcal{V}(t)} \left(\delta_{jl}\tau_{kl} + x_j\frac{\partial\tau_{kl}}{\partial x_l}\right)\mathrm{d}\boldsymbol{x}$$

$$= \varepsilon_{ijk}\boldsymbol{e}_i\int_{\mathcal{V}(t)} \left(\tau_{kj} + x_j\frac{\partial\tau_{kl}}{\partial x_l}\right)\mathrm{d}\boldsymbol{x}. \tag{3.9}$$

At the left hand side of (3.2), we use the Reynolds transport theorem for specific quantities (2.31) and we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} \varrho\boldsymbol{x}\times\boldsymbol{V}\,\mathrm{d}\boldsymbol{x} = \int_{\mathcal{V}(t)} \varrho\frac{\mathrm{D}}{\mathrm{D}t}(\boldsymbol{x}\times\boldsymbol{V})\,\mathrm{d}\boldsymbol{x} = \int_{\mathcal{V}(t)} \varrho\left(\underbrace{\frac{\mathrm{D}\boldsymbol{x}}{\mathrm{D}t}\times\boldsymbol{V}}_{=\boldsymbol{V}\times\boldsymbol{V}=0} + \boldsymbol{x}\times\frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t}\right)\mathrm{d}\boldsymbol{x} = \int_{\mathcal{V}(t)} \varrho\left(\boldsymbol{x}\times\frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t}\right)\mathrm{d}\boldsymbol{x}. \tag{3.10}$$

After the replacement of both terms (3.9) and (3.10) rewritten in this way back to (3.2), we already have all terms under the volume integral

$$\int_{\mathcal{V}(t)} \varrho\left(\boldsymbol{x}\times\frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t}\right)\mathrm{d}\boldsymbol{x} = \int_{\mathcal{V}(t)} \varepsilon_{ijk}\boldsymbol{e}_i\left(\tau_{kj} + x_j\frac{\partial\tau_{kl}}{\partial x_l}\right)\mathrm{d}\boldsymbol{x} + \int_{\mathcal{V}(t)} \varrho\boldsymbol{x}\times\boldsymbol{F}\,\mathrm{d}\boldsymbol{x}. \tag{3.11}$$

Now let us denote $\epsilon = \operatorname{diam} \mathcal{V}(t)$ and without loss of generality, let us choose $\mathcal{V}_0$ such that $\mathbf{0} \in \mathcal{V}(t)$. This only means that we represent the angular momentum about a point that is inside $\mathcal{V}(t)$, which corresponds to the appropriate choice of $\boldsymbol{x}_0$ in (3.2) - see Remark 1 on page 54. Then of course $\|\boldsymbol{x}\| = O(\epsilon)$. If we divide (3.11) by ϵ^3, we scale the volume $\mathcal{V}(t)$ around the point $\mathbf{0}$ ($=\boldsymbol{x}_0$) and take a limit transition for $\epsilon \to 0$, all terms in (3.11) multiplied by $\boldsymbol{x}$ will have a limit equal to zero, leaving only one term for which, therefore,

$$\varepsilon_{ijk} \boldsymbol{e}_i \tau_{kj}\big|_{(t,\boldsymbol{x}_0)} = \mathbf{0}$$

must hold. So component-wise, we have

$$\begin{aligned}
\varepsilon_{1jk}\tau_{kj} = 0 &\iff \tau_{23} = \tau_{32}, \\
\varepsilon_{2jk}\tau_{kj} = 0 &\iff \tau_{13} = \tau_{31}, \\
\varepsilon_{3jk}\tau_{kj} = 0 &\iff \tau_{12} = \tau_{21},
\end{aligned}$$

which means that the stress tensor $\mathbf{T}$ is symmetric. Hence, it has real eigenvalues and three mutually perpendicular eigenvectors which are called *principal stresses* and *principal stress directions*, respectively.

3.3 Equation of the momentum conservation law in general form

Let us take the equation

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{V}(t)} \varrho \boldsymbol{V} \mathrm{d}\boldsymbol{x} = \int_{\partial\mathcal{V}(t)} \boldsymbol{T}(t,\boldsymbol{x},\boldsymbol{n}) \,\mathrm{d}S + \int_{\mathcal{V}(t)} \varrho \boldsymbol{F} \mathrm{d}\boldsymbol{x}. \tag{3.1}$$

The i-th component of this vector equation indicates the balance of the i-th momentum component, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{V}(t)} \varrho V_i \mathrm{d}\boldsymbol{x} = \int_{\partial\mathcal{V}(t)} T_i(t,\boldsymbol{x},\boldsymbol{n}) \,\mathrm{d}S + \int_{\mathcal{V}(t)} \varrho F_i \mathrm{d}\boldsymbol{x}. \tag{3.12}$$

Now we use the Reynolds transport theorem with the choice $\Phi = \varrho V_i$ and relationship 3.8. Ny substituting into (3.12), we get

$$\int_{\mathcal{V}(t)} \frac{\partial}{\partial t}\left(\varrho V_i\right) + \nabla \cdot \left(\varrho V_i \boldsymbol{V}\right) \mathrm{d}\boldsymbol{x} = \int_{\partial\mathcal{V}(t)} \left(\mathbf{T}(t,\boldsymbol{x}) \cdot \boldsymbol{n}\right)_i \mathrm{d}S + \int_{\mathcal{V}(t)} \varrho F_i \mathrm{d}\boldsymbol{x},$$

which can also be written using Einstein summation as

$$\int_{\mathcal{V}(t)} \frac{\partial}{\partial t}\left(\varrho V_i\right) + \partial_j\left(\varrho V_i V_j\right) \mathrm{d}\boldsymbol{x} = \int_{\partial\mathcal{V}(t)} \tau_{ij} n_j \mathrm{d}S + \int_{\mathcal{V}(t)} \varrho F_i \mathrm{d}\boldsymbol{x}, \tag{3.13}$$

Next, we apply Green's formula to the surface integral in (3.13), which gives

$$\int_{\mathcal{V}(t)} \frac{\partial}{\partial t}\left(\varrho V_i\right) + \partial_j\left(\varrho V_i V_j\right) \mathrm{d}\boldsymbol{x} = \int_{\mathcal{V}(t)} \partial_j \tau_{ij} \mathrm{d}\boldsymbol{x} + \int_{\mathcal{V}(t)} \varrho F_i \mathrm{d}\boldsymbol{x}.$$

Given an arbitrary choice of the volume $\mathcal{V}$, equality of integrands must also hold, i.e.,

$$\frac{\partial\left(\varrho V_i\right)}{\partial t} + \partial_j\left(\varrho V_i V_j\right) = \partial_j \tau_{ij} + \varrho F_i, \; i \in \{1,2,3\}, \tag{3.14}$$

which is the *law of conservation of linear momentum in conservative* (differential) *form* for a general fluid. Using $V_i V_j = (\boldsymbol{V} \otimes \boldsymbol{V})_{ij}$, the system of equations (3.14) can also be rewritten in vector form

$$\frac{\partial(\rho \boldsymbol{V})}{\partial t} + \nabla \cdot (\rho \boldsymbol{V} \otimes \boldsymbol{V}) = \nabla \cdot \mathbf{T} + \rho \boldsymbol{F}. \tag{3.15}$$

Alternatively, instead of (2.30), it is possible to use the Reynolds transport theorem for specific quantities (2.31) to manipulate the left hand side of (3.12), and thereby obtain the law of conservation of linear momentum in a non-conservative form

$$\rho \frac{\mathrm{D}V_i}{\mathrm{D}t} = \partial_j \tau_{ij} + \rho F_i, \ i \in \{1,2,3\}. \tag{3.16}$$

or, respectively, in vector form

$$\rho \frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t} = \nabla \cdot \mathbf{T} + \rho \boldsymbol{F}. \tag{3.17}$$

3.4 Simple fluids

The fluid is called *simple,* if the stress tensor (3.8) has the form

$$\mathbf{T} = -P\mathbf{I} + \mathbf{T}_D \tag{3.18}$$

where

$$\mathbf{T}_D = (\tilde{\tau}_{ij}) \tag{3.19}$$

is called the *tensor of viscous stresses*, or the *dynamic/viscous stress tensor*. In addition, it must depend on $t, \boldsymbol{x}$ only through the velocity of the fluid and its derivatives and $\mathbf{T}_D = \mathbf{0}$ must hold whenever $\boldsymbol{V}$ and its derivatives are equal to zero. A scalar quantity P is called the *thermodynamic* or *hydrostatic pressure* [Haz13], which corresponds to the force per unit area acting perpendicularly to the given surface in a material body that is at rest. It satisfies the general relation $P = P(\rho, T)$, where T is the *absolute* (thermodynamic) *temperature*, as given by the fluid's *equation of state* (see section 6.2.1). The law of conservation of linear momentum for a simple fluid has the form (conservative, respectively non-conservative)

$$\frac{\partial(\rho V_i)}{\partial t} + \partial_j(\rho V_i V_j) = \rho \frac{\mathrm{D}V_i}{\mathrm{D}t} = -\partial_i P + \partial_j \tilde{\tau}_{ij} + \rho F_i, \ i \in \{1,2,3\}, \tag{3.20}$$

or, respectively, in vector form

$$\frac{\partial(\rho \boldsymbol{V})}{\partial t} + \nabla \cdot (\rho \boldsymbol{V} \otimes \boldsymbol{V}) = \rho \frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t} = -\nabla P + \nabla \cdot \mathbf{T}_D + \rho \boldsymbol{F}. \tag{3.21}$$

Our further study will be limited to simple fluids.

3.5 Newtonian fluids and Navier-Stokes equations

In this section, we derive the constitutive relations for the viscous stress tensor $\mathbf{T}_D$ for the so-called Newtonian fluids, which is a model applicable to a number of fluids often encountered in practice (air, water, oil, ...). However, the theory of constitutive relations can be built in a much more rigorous way, which is beyond the scope of this subject [Mar11, Haz13].

3.5.1 Objective quantities

The form of the stress tensor (and in general other thermodynamic quantities such as Helmholtz free energy, which we do not consider here), depends on the particular material on intensive physical quantities, which are *objective* [Haz13, Chapter 5], i.e. independent of the transformation of the coordinate system in the form

$$\boldsymbol{x}'(t) = \mathbf{Q}(t)\,\boldsymbol{x} + \boldsymbol{C}(t), \tag{3.22}$$

where $\boldsymbol{C}$ is the translation vector a $\mathbf{Q}$ is a time-dependent orthogonal transformation. A vector quantity $\boldsymbol{A}$ is called objective if its magnitude does not change by the transformation of coordinates. Specifically, for the mutual position vector

$$\boldsymbol{A} = \boldsymbol{x} - \boldsymbol{y}$$

it holds by the use of (3.22) that

$$\boldsymbol{A}' = \mathbf{Q}(t)\,\boldsymbol{A},$$

from which (using $\mathbf{Q}^{\mathrm{T}}\mathbf{Q} = \mathbf{I}$) it follows that

$$\left\|\boldsymbol{A}'\right\|^2 = \|\boldsymbol{A}\|^2.$$

Similarly, the tensor $\mathbf{M}$ (as a matrix - see section 1.2.8) is objective if and only if it transforms objective vectors into objective ones, i.e.

$$\mathbf{M}'\boldsymbol{A}' = \mathbf{Q}(t)\,\mathbf{M}\boldsymbol{A},$$

from which

$$\mathbf{M}' = \mathbf{Q}^{\mathrm{T}}\mathbf{M}\mathbf{Q}. \tag{3.23}$$

On the other hand, e.g., velocity and acceleration vectors are not objective. Using (3.23), it can be shown that the velocity gradient $\nabla\boldsymbol{V}$ is not an objective quantity, whereas its symmetric part, i.e. the strain rate tensor $\mathbf{D}$ given by the relation (2.41), is objective. Therefore, we will consider the dependence of $\mathbf{T}_D$ on the rate of mechanical deformation only through $\mathbf{D}$.

3.5.2 Newtonian fluids

Let us assume that $\mathbf{T}_D$ is dependent only on the strain rate tensor $\mathbf{D}$ (i.e. independent of, e.g., the temperature gradient). In addition, let us assume that the fluid has no internal structure and is so-called isotropic (its properties are independent of direction). This means that $\mathbf{T}_D$ is an isotropic tensor function of $\mathbf{D}$. For any $n \in \mathbb{N}$, the function $\mathbf{F}(\mathbf{D}) = \mathbf{D}^n = \underbrace{\mathbf{D}\mathbf{D}\mathbf{D}\cdots\mathbf{D}}_{n\times}$ is obviously isotropic, as by Definition (1.20), it is true for any orthogonal $\mathbf{Q}$ that

$$\mathbf{Q}^{\mathrm{T}}\mathbf{F}(\mathbf{D})\,\mathbf{Q} = \mathbf{Q}^{\mathrm{T}}\mathbf{D}^n\mathbf{Q} = \left(\mathbf{Q}^{\mathrm{T}}\mathbf{D}\mathbf{Q}\right)^n = \mathbf{F}\left(\mathbf{Q}^{\mathrm{T}}\mathbf{D}\mathbf{Q}\right).$$

In addition, the tensor $\mathbf{D}$ is symmetric, so every power of it also satisfies $(\mathbf{D}^n)^{\mathrm{T}} = \mathbf{D}^n$. Let us consider the dependence in the form of a finite sum [Haz13, Chapter 7]

$$\mathbf{T}_D(\mathbf{D}) = \sum_n \tilde{\alpha}_n \mathbf{D}^n,$$

where $\tilde{\alpha}_n$ are numbers that can no longer depend on the tensor elements $\mathbf{D} = \left(d_{ij}\right)$ in a specific basis, but they may still depend on its invariants. Without loss of generality, dependence on the principal invariants

$$\tilde{\alpha} = \tilde{\alpha}\left({}_{\mathbf{D}}I_1, {}_{\mathbf{D}}I_2, {}_{\mathbf{D}}I_3\right)$$

can be assumed (see Section 1.2.10), as any other invariant can be calculated from them by a formula independent of $\mathbf{D}$. Then $\mathbf{T}_D$ is a symmetric tensor and also is an isotropic function of $\mathbf{D}$. According to the Cayley-Hamilton theorem,

$$l\left(\mathbf{D}\right) = -\mathbf{D}^3 + {}_{\mathbf{D}}I_1\mathbf{D}^2 - {}_{\mathbf{D}}I_2\mathbf{D} + {}_{\mathbf{D}}I_3\mathbf{I} = \mathbf{0},$$

which means that all powers $\mathbf{D}^n$ for $n \geq 3$ can be expressed using $\mathbf{I}, \mathbf{D}, \mathbf{D}^2$ and the invariants. It can therefore be written

$$\mathbf{T}_D\left(\mathbf{D}\right) = \alpha_0\mathbf{I} + \alpha_1\mathbf{D} + \alpha_2\mathbf{D}^2 \tag{3.24}$$

for certain $\alpha_0, \alpha_1, \alpha_2$, which are functions of ${}_{\mathbf{D}}I_1, {}_{\mathbf{D}}I_2, {}_{\mathbf{D}}I_3$. This is the general constitutive relation for the so-called *Reiner-Rivlin* fluids [Haz13, Chapter 7].

If, however, we consider a strictly linear dependence on $\mathbf{D}$, we get a constitutive relation for *Newtonian* liquids. In that case, apparently $\alpha_2 = 0$, $\alpha_1 = \text{const.}$ and α_0 can only be in the form

$$\alpha_0 = \mu'{}_{\mathbf{D}}I_1 = \mu'\mathrm{Tr}\,\mathbf{D} = \mu' d_{ii} = \mu'\nabla\cdot\boldsymbol{V},$$

because the invariants ${}_{\mathbf{D}}I_2, {}_{\mathbf{D}}I_3$ have quadratic and cubic dependence on $\mathbf{D}$, respectively - see Section 1.2.10. We substitute into (3.24) and using the convention $\alpha_1 = 2\mu$,we get

$$\begin{aligned}\mathbf{T}_D\left(\mathbf{D}\right) &= \mu'\left(\nabla\cdot\boldsymbol{V}\right)\mathbf{I} + 2\mu\mathbf{D},\\ \mathbf{T}\left(\mathbf{D}\right) &= \left(-P + \mu'\nabla\cdot\boldsymbol{V}\right)\mathbf{I} + 2\mu\mathbf{D}.\end{aligned} \tag{3.25}$$

The coefficient μ, which generally depends on temperature T and density ϱ, is called the *dynamic viscosity coefficient* and μ' is called *the second (dilation) viscosity coefficient* .

Remark. Relationship for $\mathbf{T}_D$ can also be derived from the assumption of its isotropic linear dependence on the velocity tensor deformation $\mathbf{D}$ in the form

$$\tau_{ij} = \alpha_{ijk\ell}d_{k\ell} + \beta_{ij},$$

where $\mathbf{A} = \left(\alpha_{ijk\ell}\right)$, $\mathbf{B} = \left(\beta_{ij}\right)$ are isotropic tensors (see section 1.2.11).

By writing it down $\mathbf{T}_D = \left(\tilde{\tau}_{ij}\right)$, we get component-wise

$$\tilde{\tau}_{ij} = \mu'\delta_{ij}\nabla\cdot\boldsymbol{V} + \mu\left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i}\right) = \mu'\delta_{ij}\partial_k V_k + \mu\left(\partial_j V_i + \partial_i V_j\right), \tag{3.26}$$

, or, respectively, in the expanded form

$$\tilde{\tau}_{ii} = \mu'\partial_k V_k + 2\mu\partial_i V_i, \tag{3.27}$$

$$\tilde{\tau}_{ij} = \tilde{\tau}_{ji} = \mu\left(\partial_j V_i + \partial_i V_j\right),\ i \neq j. \tag{3.28}$$

The given relations can be interpreted as an effect of the viscosity of the fluid, where fluid layers moving at different velocities "rub" against each other and exert a force on each other, which is proportional to their mutual velocity.

If we substitute the relations (3.27)–(3.28) into the equations (3.20), we get the so-called *Navier-Stokes equations*[2] *in non-conservative* (differential) *form*, which describe the compressible flow of a viscous Newtonian fluid

[2] In a broader sense, we mean the entire system of equations by the Navier-Stokes equations describing the flow, i.e. equation (3.30)–(3.32) together with the continuity equation and the energy equation (see Sect 3.9).

$$\varrho\frac{\mathrm{D}V_i}{\mathrm{D}t} = -\partial_i P + \partial_j\left(\mu'\delta_{ij}\partial_k V_k + \mu\left(\partial_j V_i + \partial_i V_j\right)\right) + \varrho F_i,\ i \in \{1,2,3\}, \tag{3.29}$$

or, respectively, in the expanded form

$$\varrho\frac{\mathrm{D}V_1}{\mathrm{D}t} = -\frac{\partial P}{\partial x_1} + \frac{\partial}{\partial x_1}\left(\mu'\nabla\cdot\boldsymbol{V} + 2\mu\frac{\partial V_1}{\partial x_1}\right) + \frac{\partial}{\partial x_2}\left[\mu\left(\frac{\partial V_1}{\partial x_2} + \frac{\partial V_2}{\partial x_1}\right)\right] + \frac{\partial}{\partial x_3}\left[\mu\left(\frac{\partial V_1}{\partial x_3} + \frac{\partial V_3}{\partial x_1}\right)\right] + \varrho F_1 \tag{3.30}$$

$$\varrho\frac{\mathrm{D}V_2}{\mathrm{D}t} = -\frac{\partial P}{\partial x_2} + \frac{\partial}{\partial x_1}\left[\mu\left(\frac{\partial V_2}{\partial x_1} + \frac{\partial V_1}{\partial x_2}\right)\right] + \frac{\partial}{\partial x_2}\left(\mu'\nabla\cdot\boldsymbol{V} + 2\mu\frac{\partial V_2}{\partial x_2}\right) + \frac{\partial}{\partial x_3}\left[\mu\left(\frac{\partial V_2}{\partial x_3} + \frac{\partial V_3}{\partial x_2}\right)\right] + \varrho F_2, \tag{3.31}$$

$$\varrho\frac{\mathrm{D}V_3}{\mathrm{D}t} = -\frac{\partial P}{\partial x_3} + \frac{\partial}{\partial x_1}\left[\mu\left(\frac{\partial V_3}{\partial x_1} + \frac{\partial V_1}{\partial x_3}\right)\right] + \frac{\partial}{\partial x_2}\left[\mu\left(\frac{\partial V_3}{\partial x_2} + \frac{\partial V_2}{\partial x_3}\right)\right] + \frac{\partial}{\partial x_3}\left(\mu'\nabla\cdot\boldsymbol{V} + 2\mu\frac{\partial V_3}{\partial x_3}\right) + \varrho F_3. \tag{3.32}$$

3.5.3 Stokes hypothesis

The so-called *mechanical pressure* is often [Bur15] defined as

$$P_{\mathrm{mech}} = -\frac{1}{3}\mathrm{Tr}\,\mathbf{T} = -\frac{1}{3}\tau_{ii}, \tag{3.33}$$

i.e. as the average of the forces acting on three unit surfaces oriented perpendicularly to the axes of the coordinate system. The choice of the coordinate system does not matter because (3.33) is an invariant of $\mathbf{T}$ (see Section 1.2.10). For simple fluids defined by the relation (3.18), and therefore also for Newtonian fluids, it holds at rest that $P_{\mathrm{mech}} = P$. But how about when the fluid is moving?

The strain rate tensor $\mathbf{D}$ can be written as the sum of its isotropic (volumetric) part

$$\mathbf{D}_{\mathrm{iso}} = \frac{1}{3}\left(\mathrm{Tr}\,\mathbf{D}\right)\mathbf{I} = \frac{1}{3}\left(\nabla\cdot\boldsymbol{V}\right)\mathbf{I}$$

and the remaining, so-called *deviatoric* parts with zero trace

$$\mathbf{D}_{\mathrm{dev}} = \mathbf{D} - \mathbf{D}_{\mathrm{iso}} = \left(\frac{1}{2}\left(\left(\partial_i V_j + \partial_j V_i\right) - \frac{2}{3}\delta_{ij}\partial_k V_k\right)\right).$$

Substituting into the stress tensor in the form (3.25), we have

$$\mathbf{T} = \left(-P + \mu'\nabla\cdot\boldsymbol{V}\right)\mathbf{I} + 2\mu\left(\mathbf{D}_{\mathrm{iso}} + \mathbf{D}_{\mathrm{dev}}\right) = \left(-P + \left(\underbrace{\mu' + \frac{2}{3}\mu}_{:=\kappa}\right)\nabla\cdot\boldsymbol{V}\right)\mathbf{I} + 2\mu\mathbf{D}_{\mathrm{dev}}$$

$$= \left(-P + \kappa\nabla\cdot\boldsymbol{V}\right)\mathbf{I} + 2\mu\mathbf{D}_{\mathrm{dev}},$$

where $\kappa = \mu' + \frac{2}{3}\mu$ is called the *bulk viscosity coefficient* (or *volumetric viscosity*) and the dynamic viscosity μ is also called *shear viscosity* in this context. According to (3.33),

$$P_{\mathrm{mech}} = P - \kappa\nabla\cdot\boldsymbol{V}$$

then holds. The usual assumption is that the hydrostatic and mechanical pressures are equal even during movement, which expresses the so-called Stokes hypothesis by relation

$$\kappa = 0 \text{ or } \mu' = -\frac{2}{3}\mu. \tag{3.34}$$

In [Gad95] and more recently in [Bur15], it is discussed that for certain fluids (monatomic sufficiently dilute gases), this relationship can also be justified by the kinetic theory of gases, but it does not apply in general. There are experimental methods [Gad95] by which one can measure κ, and in very common materials (gases such as oxygen, nitrogen), κ is apparently of the same order as μ. In CO_2, κ is even (roughly) a thousand times greater than μ. The reason why Stokes hypothesis can still be used and achieve realistic results of flow simulations is rather that (not only) for these materials, it normally holds that

$$|\kappa \nabla \cdot \boldsymbol{V}| \ll P.$$

Exceptions are extreme situations such as supersonic flow during entry of a cosmic module into a planetary atmosphere with high CO_2 concentration. In many cases, on the other hand, the Stokes hypothesis is not needed at all, as we will learn further in Section 3.7.

3.6 Inviscid flow - Euler's equations

In some cases, the viscosity of the fluid can be neglected. Then we speak of the so-called *inviscid (ideal)* liquid. By putting $\mu = \mu' = 0$ in (3.30)–(3.32) or, respectively, $\tilde{\tau}_{ij} = 0$ in (3.20), we get the so-called *Euler's equations in non-conservative* (differential) *form*

$$\varrho \frac{\mathrm{D}V_i}{\mathrm{D}t} = -\partial_i P + \varrho F_i. \tag{3.35}$$

Their vector form

$$\rho \frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t} = -\nabla P + \varrho \boldsymbol{F},$$

can be obtained by substituting $\mathbf{T}_D = 0$ into (3.17).

3.7 Incompressible flow

In *incompressible flow*, the volumetric measure in any control volume of fluid $\mathcal{V}_0 \subset V_0$ does not change over time, i.e., (as in v 2.21) we have

$$m_3(\mathcal{V}_0) = \int_{\mathcal{V}_0} \mathrm{d}\boldsymbol{X} \overset{!}{=} \int_{\mathcal{V}(t)} \mathrm{d}\boldsymbol{x} = \int_{\mathcal{V}_0} \left| \det \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}} \right| \mathrm{d}\boldsymbol{X} = \int_{\mathcal{V}_0} |\det \mathbf{F}| \, \mathrm{d}\boldsymbol{X}, \tag{3.36}$$

from which

$$\int_{\mathcal{V}_0} (1 - |\det \mathbf{F}|) \, \mathrm{d}\boldsymbol{X} = 0$$

and given an arbitrary choice of $\mathcal{V}_0$, it follows that

$$|\det \mathbf{F}| = 1. \tag{3.37}$$

Now by differentiating (3.37) w.r.t. time and using (2.26), we get

$$\nabla \cdot \boldsymbol{V} = \partial_j V_j = 0, \tag{3.38}$$

Under this assumption, the continuity equation (2.19) emerges in the form of the so-called *transport equation*

$$0 = \frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \boldsymbol{V}) = \frac{\partial \varrho}{\partial t} + \boldsymbol{V} \cdot \nabla \varrho + \varrho \underbrace{\nabla \cdot \boldsymbol{V}}_{=0} = \frac{\partial \varrho}{\partial t} + \boldsymbol{V} \cdot \nabla \varrho = \frac{\mathrm{D}\varrho}{\mathrm{D}t} = \frac{\partial \rho}{\partial t}. \tag{3.39}$$

The density ρ expressed in material coordinates is therefore independent of time. From this it can be seen that the condition of incompressibility is satisfied by the flow if any initial density distribution just drifts along with the flow. If the fluid is initially homogeneous, i.e. $\rho = \text{const.}$, then $\varrho = \text{const.}$ must apply at any time t and for each $\boldsymbol{x} \in V(t)$.

3.8 Equations of incompressible fluid flow

For simplicity, let us now assume

$$\varrho = \text{const.}$$

Then directly from the continuity equation (2.19), we get the incompressibility condition (3.38). Let us also assume that the kinematic viscosity (and therefore the dynamic viscosity μ) is also constant. By direct substitution of (3.38) into (3.30), we obtain

$$\begin{aligned} \varrho \frac{\mathrm{D}V_i}{\mathrm{D}t} &= -\partial_i P + \mu \partial_j \left(\left(\partial_j V_i + \partial_i V_j \right) \right) + \varrho F_i \\ &= -\partial_i P + \mu \left(\partial_{jj} V_i + \underbrace{\partial_{ij} V_j}_{=0} \right) + \varrho F_i \; i \in \{1,2,3\}, \\ &= -\partial_i P + \mu \partial_{jj} V_i. \end{aligned} \tag{3.40}$$

The marked term is equal to zero because it is a derivative of the continuity equation $\partial_k V_k = 0$ w.r.t. x_i (assuming interchangeability of derivatives). In vector form, we have

$$\varrho \frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t} = -\nabla P + \mu \Delta \boldsymbol{V} + \varrho \boldsymbol{F}. \tag{3.41}$$

After dividing by the density ϱ, we get the frequently used form

$$\frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t} = -\nabla \tilde{P} + \nu \Delta \boldsymbol{V} + \boldsymbol{F}, \tag{3.42}$$

where

$$\nu = \frac{\mu}{\varrho} \tag{3.43}$$

is called *kinematic viscosity* and

$$\tilde{P} = \frac{P}{\varrho} \tag{3.44}$$

is the *kinematic* (standardized) *pressure*.

Under the given assumptions, the system of equations (3.38), (3.42) supplemented by the state equation of the fluid (see section 3.10) is closed and solvable without using the law of conservation of energy, which we derive in the following section. The same is true for inviscid flow at constant temperature.

3.9 Conservation of energy

3.9.1 Conservation of total energy

We will now consider the law of conservation of total energy for simple liquids. As in part 3.1, let $\mathcal{V}_0$ be a fixed control volume of the material body V_0 whose shape transforms over time to $\mathcal{V}(t)$. Let us denote by $E(t,\boldsymbol{x})$ the *specific internal energy* (per unit mass). Total (kinetic and internal) energy of the substance contained in the volume $\mathcal{V}(t)$ is then

$$\mathscr{E}(t) = \int_{\mathcal{V}(t)} \varrho\left(E + \frac{1}{2}\boldsymbol{V}^2\right)\mathrm{d}\boldsymbol{x}, \tag{3.45}$$

where we denoted $\boldsymbol{V}^2 := \boldsymbol{V}\cdot\boldsymbol{V} = V_i V_i = \|\boldsymbol{V}\|^2$. The change of this value per unit time is the sum of:

1. Power of surface forces (pressure and viscous forces) at the boundary of the volume $\partial\mathcal{V}$, i.e.
$$\int_{\partial\mathcal{V}(t)} \boldsymbol{V}\cdot(\mathbf{T}\boldsymbol{n})\,\mathrm{d}S = \int_{\partial\mathcal{V}} V_i\,(\mathbf{T}\boldsymbol{n})_i\,\mathrm{d}S = \int_{\partial\mathcal{V}} V_i\tau_{ij}n_j\mathrm{d}S = \int_{\mathcal{V}(t)} \partial_j\left(V_i\tau_{ij}\right)\mathrm{d}\boldsymbol{x}. \tag{3.46}$$
2. Power of volume forces on the substance in the entire volume $\mathcal{V}$
$$\int_{\mathcal{V}(t)} \boldsymbol{F}\cdot\left(\varrho\boldsymbol{V}\mathrm{d}\boldsymbol{x}\right) = \int_{\mathcal{V}(t)} \varrho F_i V_i\mathrm{d}\boldsymbol{x}. \tag{3.47}$$
3. Flux of internal energy across the boundary $\partial\mathcal{V}$ due to the diffusion (conduction) of heat through the material. Heat flux *into* the volume $\mathcal{V}$ across the surface $\mathrm{d}S$ with *outer* normal $\boldsymbol{n}$ due to heat conduction is given by Fourier's law
$$\lambda\frac{\partial T}{\partial\boldsymbol{n}}\mathrm{d}S = \lambda\nabla T\cdot\boldsymbol{n}\mathrm{d}S \tag{3.48}$$
where $\lambda\ \left[\mathrm{W}\cdot\mathrm{m}^{-1}\cdot\mathrm{K}^{-1}\right]$ is the thermal conductivity coefficient. Therefore, the total heat flux across the boundary $\partial\mathcal{V}$ caused by heat conduction is
$$\int_{\partial\mathcal{V}(t)} \lambda\nabla T\cdot\boldsymbol{n}\mathrm{d}S = \int_{\partial\mathcal{V}(t)} \lambda\partial_i T n_i\mathrm{d}S = \int_{\mathcal{V}(t)} \partial_i\left(\lambda\partial_i T\right)\mathrm{d}S = \int_{\mathcal{V}(t)} \nabla\cdot(\lambda\nabla T)\,\mathrm{d}x. \tag{3.49}$$
4. Power of volumetric heat sources in the volume $\mathcal{V}$. If the heating power of volumetric heat sources per unit mass is equal to $\dot{Q}$, the total heating power in the volume $\mathcal{V}(t)$ is
$$\int_{\mathcal{V}(t)} \varrho\dot{Q}\mathrm{d}\boldsymbol{x}. \tag{3.50}$$

By summing up all the contributions (3.46)–(3.50), we get the total energy balance

$$\frac{\mathrm{d}\mathscr{E}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} \varrho\left(E + \frac{1}{2}\boldsymbol{V}^2\right)\mathrm{d}\boldsymbol{x} = \int_{\mathcal{V}(t)} \partial_j\left(V_i\tau_{ij}\right) + \varrho F_i V_i + \partial_i\left(\lambda\partial_i T\right) + \varrho\dot{Q}\mathrm{d}\boldsymbol{x}.$$

Using the Reynolds transport theorem for specific quantities (2.31) with the choice $\Phi = E + \frac{1}{2}\boldsymbol{V}^2$ and considering that the choice $\mathcal{V}_0$ was arbitrary, we get the equality of integrands in the form

$$\varrho\frac{\mathrm{D}}{\mathrm{D}t}\left(E + \frac{1}{2}\boldsymbol{V}^2\right) = \partial_j\left(V_i\tau_{ij}\right) + \varrho F_i V_i + \partial_i\left(\lambda\partial_i T\right) + \varrho\dot{Q}, \tag{3.51}$$

or the *law of conservation of total energy* in the (non-conservative) differential form. The conservative form (obtained using (2.30)) is not mention, as it is not so compact.

3.9.2 Conservation of internal energy

It is clear that kinetic energy, like momentum, is not an objective quantity (see section 3.5.1). Equation (3.51) can be simplified, however. We start from the general momentum balance equations

$$\varrho \frac{\mathrm{D}V_i}{\mathrm{D}t} = \partial_j \tau_{ij} + \varrho F_i,\ i \in \{1,2,3\}, \tag{3.16}$$

which we multiply by V_i and we sum over i, which gives

$$\varrho \underbrace{\frac{\mathrm{D}V_i}{\mathrm{D}t} V_i}_{\frac{\mathrm{D}}{\mathrm{D}t}\frac{1}{2}V^2} = V_i \partial_j \tau_{ij} + \varrho F_i V_i. \tag{3.52}$$

By subtracting (3.52) from (3.51), we obtain

$$\varrho \frac{\mathrm{D}E}{\mathrm{D}t} = \tau_{ij}\partial_j V_i + \partial_i (\lambda \partial_i T) + \varrho \dot{Q}, \tag{3.53}$$

or, respectively, in vector form

$$\varrho \frac{\mathrm{D}E}{\mathrm{D}t} = \mathbf{T} \cdot \nabla \boldsymbol{V} + \nabla \cdot (\lambda \nabla T) + \varrho \dot{Q}, \tag{3.54}$$

which is *the law of conservation of internal energy in non-conservative* (differential) *form.*

3.9.3 Conservation of internal energy for simple fluids

By substituting the relation (3.18) into (3.53), we get the internal energy balance equation for simple fluids

$$\begin{aligned} \varrho \frac{\mathrm{D}E}{\mathrm{D}t} &= \left(-P\delta_{ij} + \tilde{\tau}_{ij}\right)\partial_j V_i + \partial_i (\lambda \partial_i T) + \varrho \dot{Q}, \\ &= -P\partial_i V_i + \tilde{\tau}_{ij}\partial_j V_i + \partial_i (\lambda \partial_i T) + \varrho \dot{Q}, \end{aligned}$$

or, in vector form,

$$\varrho \frac{\mathrm{D}E}{\mathrm{D}t} = -P\nabla \cdot \boldsymbol{V} + \mathbf{T}_D \cdot \nabla \boldsymbol{V} + \nabla \cdot (\lambda \nabla T) + \varrho \dot{Q}.$$

3.9.4 Conservation of internal energy for inviscid flow

In the case of inviscid flow described by Euler's equations (see part 3.6), heat conduction is also usually neglected, i.e. we put $\mu = 0$ and $\lambda = 0$. The law of conservation of internal energy then has the form

$$\varrho \frac{\mathrm{D}E}{\mathrm{D}t} = -P\nabla \cdot \boldsymbol{V} + \varrho \dot{Q}. \tag{3.55}$$

3.10 Closure of the system of equations for fluid flow

So far, we have derived several equations that express the processes during fluid flow following from the conservation laws of fundamental physical quantities. It is 1 equation for the mass conservation law (Section 2.9), 3 equations for the conservation of linear momentum components (part 3.3)

and 1 equation for the conservation of energy (Sect 3.9). Hence, we have a total of 5 equations for the density ϱ, 3 momentum components ϱV_i, internal energy E, absolute temperature T and pressure P [3]. There are 7 unknown quantities and it is obvious that 2 more equations will be needed for the system to be well-posed. These equations are

1. the relationship between internal energy and absolute temperature,
2. equation of state of the fluid.

These relationships will be explored in more detail in Sections 6.1 and 6.2.

3.11 Potential flow equation

We assume a stationary non-eddy inviscid and isentropic flow. *Stationary* means that the partial derivatives of all quantities with respect to time are equal to zero. *Non-eddy* in 3D means

$$\operatorname{curl} \boldsymbol{V} = 0, \tag{3.56}$$

which is equivalent to the existence of a flow potential, i.e. a function Φ such that

$$\boldsymbol{V} = \nabla\Phi.$$

Condition (3.56) corresponds to the exactness (and therefore integrability) of the differential form $V_i \mathrm{d}x_i$. In the two-dimensional domain, the corresponding condition is the exactness of the differential form

$$V_1 \mathrm{d}x_1 + V_2 \mathrm{d}x_2,$$

i.e.,

$$\partial_2 V_1 - \partial_1 V_2 = 0$$

must hold.

The system of Euler's equations in conservative form for stationary flow can be written as

$$\begin{aligned} \partial_1(\varrho V_1) + \partial_2(\varrho V_2) &= 0, \\ \partial_1(\varrho V_1^2 + P) + \partial_2(\varrho V_1 V_2) &= 0, \\ \partial_1(\varrho V_1 V_2) + \partial_2(\varrho V_2^2 + P) &= 0. \end{aligned}$$

From Euler's equations in non-conservative form, it can be derived that

$$-\frac{1}{2}\rho \mathrm{d}\left(V_1^2 + V_2^2\right) = \mathrm{d}p$$

and because for the local speed of sound, we have

$$a^2 = \frac{\mathrm{d}p}{\mathrm{d}\rho},$$

we obtain

$$\mathrm{d}\rho = -\frac{\mathrm{d}p}{a^2} = -\frac{\rho}{2a^2}\mathrm{d}\left(V_1^2 + V_2^2\right)$$

from which $\partial_1\rho, \partial_2\rho$ can be calculated. After substituting into the continuity equation and expressing $V_1 = \partial_1\Phi$, $V_2 = \partial_2\Phi$, we get *the full potential equation* (without explicit occurrence of ρ) in the form

$$\partial_{11}\Phi\left(1 - \frac{1}{a^2}(\partial_1\Phi)^2\right) + \partial_{22}\Phi\left(1 - \frac{1}{a^2}(\partial_2\Phi)^2\right) - \frac{2}{a^2}\partial_1\Phi\partial_2\Phi\partial_{12}\Phi = 0.$$

[3] The symbolism corresponds to the Eulerian approach and the corresponding conservative form equations. We will follow this marking throughout the section (3.10).

CHAPTER

4 Mathematical analysis of flow equations

In this chapter, we will briefly get acquainted with some principles and mathematical tools that are used in the mathematical analysis of flow problems. The aim of this analysis is to show whether, under what conditions and in what form there is a solution to flow problems, and if so, if it is unique.

4.1 Formulation of the incompressible flow problem

Let $\Omega \subset \mathbb{R}^3$ be a domain with a Lipschitz boundary (see Definition 29) a $\mathcal{J} = (0, t_{\max})$ be the time interval. The problem we will investigate is that of incompressible flow, in the form

$$\nabla \cdot \boldsymbol{V} = 0, \tag{3.38}$$

$$\frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t} = -\nabla \tilde{P} + \nu \Delta \boldsymbol{V} + \boldsymbol{F}, \tag{3.42}$$

for the unknowns $\boldsymbol{V}$ and $\tilde{P}$, where $\nu = \frac{\mu}{\varrho}$ is called *kinematic viscosity* and $\tilde{P} = \frac{p}{\varrho}$ is the *kinematic pressure* (see sections 3.7 and 3.8), with a boundary condition

$$\boldsymbol{V}(t, \boldsymbol{x})|_{\partial\Omega} = \boldsymbol{W}(t, \boldsymbol{x}). \tag{4.1}$$

By integrating (3.38) over Ω and using the Gauss theorem (Corollary 7), we find that the function $\boldsymbol{W}$ has to satisfy

$$\int_{\partial\Omega} \boldsymbol{W} \cdot \boldsymbol{n} \mathrm{d}S = 0.$$

The initial condition is given by

$$\boldsymbol{V}(0, \boldsymbol{x}) = \boldsymbol{V}_0(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega, \tag{4.2}$$

satisfying the *divergence-free* condition

$$\nabla \cdot \boldsymbol{V}_0(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \Omega. \tag{4.3}$$

4.2 Pressure Poisson Equation

If we apply the divergence operator to (3.42), we get

$$\nabla \cdot \frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t} = -\nabla \cdot \nabla \tilde{P} + \nu \nabla \cdot \Delta \boldsymbol{V} + \nabla \cdot \boldsymbol{F}. \tag{4.4}$$

Let's denote $\Phi = \nabla \cdot \boldsymbol{V}$. On the left hand side of (4.4), we get from the definition of the material derivative (2.8)

$$\nabla \cdot \frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t} = \nabla \cdot \left(\frac{\partial \boldsymbol{V}}{\partial t} + \boldsymbol{V} \cdot \nabla \boldsymbol{V} \right) = \frac{\partial \Phi}{\partial t} + \nabla \cdot (\boldsymbol{V} \cdot \nabla \boldsymbol{V}).$$

On the right hand side of (4.4), one can rewrite

$$\nu \nabla \cdot \Delta \boldsymbol{V} = \nu \partial_i \partial_{kk} V_i = \nu \partial_{kki} V_i = \nu \partial_{ikk} V_i = \nu \partial_{kk} \partial_i V_i = \nu \Delta \Phi.$$

(4.4) can therefore be written as

$$\Delta \tilde{P} + \nabla \cdot (\boldsymbol{V} \cdot \nabla \boldsymbol{V}) - \nabla \cdot \boldsymbol{F} = \nu \Delta \Phi - \frac{\partial \Phi}{\partial t}. \tag{4.5}$$

From the incompressibility condition (3.38), i.e $\Phi = 0$, we obtain the so-called (simplified) *Pressure Poisson Equation* or *PPE*

$$\Delta \tilde{P} = -\nabla \boldsymbol{V} \cdot \nabla \boldsymbol{V} + \nabla \cdot \boldsymbol{F}. \tag{4.6}$$

The incompressibility condition therefore induces a pressure field that is up to a constant uniquely determined by the current value of the velocity field $\boldsymbol{V}$ and its changes propagate at infinite speed throughout the domain based on the changes of $\boldsymbol{V}$. If, on the other hand, we assume the validity of (4.6), we get, according to (4.5), a heat equation for the quantity Φ in the form

$$\frac{\partial \Phi}{\partial t} = \nu \Delta \Phi. \tag{4.7}$$

If we consider the boundary condition

$$\Phi|_{\partial\Omega} = 0 \tag{4.8}$$

or

$$\left. \frac{\partial \Phi}{\partial \boldsymbol{n}} \right|_{\partial\Omega} = 0, \tag{4.9}$$

then together with the initial condition (4.3) equation (4.7) implies $\Phi \equiv 0$ independently of t and $\boldsymbol{x}$. $\tilde{P}$ therefore appears in the equation (3.42) as the Lagrange multiplier ensuring the condition (3.38). Equation (4.7) together with the boundary condition (4.8) ensures that the initial value of $\nabla \cdot \boldsymbol{V}$ diffuses over time to zero, although the initial condition (4.2) does not meet (4.3), i.e. $\nabla \cdot \boldsymbol{V}_0$ does not generally hold in Ω . In numerical algorithms (see also section **??**) based on this form of PPE, the divergence of velocity relaxes to zero, which in practice makes it possible to get rid of a hard-to-fulfill condition (4.3).

Alternatively to (4.6), it is possible to only use $\frac{\partial \Phi}{\partial t} = 0$ as a consequence of incompressibility, plug this into (4.5) and obtain a seemingly equivalent, so-called *consistent* pressure Poisson equation in the form

$$\Delta \tilde{P} = -\nabla \boldsymbol{V} \cdot \nabla \boldsymbol{V} + \nu \nabla \cdot \Delta \boldsymbol{V} + \nabla \cdot \boldsymbol{F}. \tag{4.10}$$

Solution (4.10) implies in turn

$$\frac{\partial \Phi}{\partial t} = 0,$$

which means that the divergence value $\boldsymbol{V}$ does not change over time. With the initial condition (4.3) the equivalence with the incompressibility condition (3.38) is guaranteed.

Equations (4.6) and (4.10) also require boundary conditions for their solution, which the original problem does not include. A suitable boundary condition can be obtained by extending the validity

of (3.42) to the boundary $\partial\Omega$. Since this is a vector equation, there seems to be a choice. If we project (3.42) to the direction of the external normal $\boldsymbol{n}$ to $\partial\Omega$, we get the Neumann boundary condition

$$\frac{\partial \tilde{P}}{\partial \boldsymbol{n}} = \boldsymbol{n}\cdot\nabla\tilde{P} = -\frac{\mathrm{D}V_n}{\mathrm{D}t} + \nu\Delta V_n + F_n, \tag{4.11}$$

where V_n, F_n are the normal components of the vectors $\boldsymbol{V}, \boldsymbol{F}$. In the article [GS87], the authors show that, assuming sufficient regularity of both the solution and the boundary, taking the projection into the tangential direction yields an equivalent boundary condition. Furthermore, when using (4.11), the equations (4.6) and (4.10) are equivalent.

4.3 Weak solution of the incompressible flow problem

Now consider the problem (3.42), (3.38), (4.2) with a boundary condition

$$\boldsymbol{V}|_{\partial\Omega} = \boldsymbol{0} \tag{4.12}$$

for simplicity. Condition (4.12) is commonly referred to as the *no-slip* condition for viscous liquids on the walls - see section 7.1. For the more general case (e.g. domain with inflow and outflow), the problem can be reformulated using a vector field $\tilde{\boldsymbol{V}}_W$ fulfilling $\nabla\cdot\tilde{\boldsymbol{V}}_W = 0$, $\tilde{\boldsymbol{V}}_W\big|_{\partial\Omega} = \boldsymbol{W}$. Then just look for a solution to the problem in the form $\tilde{\boldsymbol{V}} = \boldsymbol{V} - \tilde{\boldsymbol{V}}_W$, which satisfies (3.42) and (4.12).

The following interpretation is inspired by the original course [Neu06a]. For a more detailed study, one can also use well-prepared materials for the course on the Navier-Stokes theory at the Charles University [Pok20a].

4.3.1 Weak equality

Consider again the Navier–Stokes equations (3.42) and let's expand the material derivative, i.e.

$$\frac{\partial \boldsymbol{V}}{\partial t} + \boldsymbol{V}\cdot\nabla\boldsymbol{V} = -\nabla\tilde{P} + \nu\Delta\boldsymbol{V} + \boldsymbol{F}.$$

From Helmholtz's theorem 2.4 it follows that for a (sufficiently smooth) vector field $\boldsymbol{F}$, there is potential Φ such that

$$\boldsymbol{F} = \nabla\Phi + \boldsymbol{F}_\sigma, \tag{4.13}$$

where $\nabla\cdot\boldsymbol{F}_\sigma = 0$. If we substitute this into (4.14), we will get

$$\frac{\partial \boldsymbol{V}}{\partial t} + \underbrace{\boldsymbol{V}\cdot\nabla\boldsymbol{V}}_{(1)} = \underbrace{-\nabla\left(\tilde{P}-\Phi\right)}_{(2)} + \underbrace{\nu\Delta\boldsymbol{V}}_{(3)} + \boldsymbol{F}_{\boldsymbol{\sigma}}. \tag{4.14}$$

We multiply the equation (4.14) by a sufficiently smooth scalar function $\boldsymbol{\varphi} : \Omega \to \mathbb{R}^3$, which has a compact support in Ω and satisfies $\nabla\cdot\boldsymbol{\varphi} = 0$ in Ω. We integrate over Ω and for the individual terms from left to right. we obtain

$$\begin{aligned}
(1)\qquad \int_\Omega (\boldsymbol{V}\cdot\nabla\boldsymbol{V})\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x} &= \int_\Omega V_j\left(\partial_j V_i\right)\varphi_i\,\mathrm{d}\boldsymbol{x} = \int_{\partial\Omega} V_j V_i \underbrace{\varphi_i}_{=0}\,\mathrm{d}\boldsymbol{x} - \int_\Omega \partial_j\left(V_j\varphi_i\right)V_i\,\mathrm{d}\boldsymbol{x} \\
&\quad - \int_\Omega \underbrace{\left(\partial_j V_j\right)}_{=0}\varphi_i V_j\,\mathrm{d}\boldsymbol{x} - \int_\Omega V_i\partial_j\varphi_i V_j\,\mathrm{d}\boldsymbol{x} = -\int_\Omega \boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}\,\mathrm{d}x, \qquad (4.15)\\
(2)\qquad -\int_\Omega \nabla\left(\tilde{P}-\Phi\right)\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x} &= -\int_\Omega \left(\partial_i\left(\tilde{P}-\Phi\right)\right)\varphi_i\,\mathrm{d}\boldsymbol{x} = -\int_{\partial\Omega}\left(\tilde{P}-\Phi\right)\underbrace{\varphi_i}_{=0}\,\mathrm{d}\boldsymbol{x} - \int_\Omega\left(\tilde{P}-\Phi\right)\underbrace{\left(\partial_i\varphi_i\right)}_{=0}\mathrm{d}\boldsymbol{x} = 0,\\
(3)\qquad \int_\Omega \Delta\boldsymbol{V}\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x} &= \int_\Omega\left(\partial_{jj}V_i\right)\varphi_i\,\mathrm{d}\boldsymbol{x} = \int_{\partial\Omega}\left(\partial_j V_i\right)\underbrace{\varphi_i}_{=0}n_j\,\mathrm{d}\boldsymbol{x} - \int_\Omega\left(\partial_j V_i\right)\left(\partial_j\varphi_i\right)\mathrm{d}\boldsymbol{x} = -\int_\Omega \nabla\boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\mathrm{d}\boldsymbol{x}.
\end{aligned}$$

After performing these operations, we arrive at

$$\int_\Omega \frac{\partial \boldsymbol{V}}{\partial t}\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x} - \int_\Omega \boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}\,\mathrm{d}\boldsymbol{x} + \int_\Omega \nu\nabla\boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x} = \int_\Omega \boldsymbol{F}_\sigma\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x}. \tag{4.16}$$

Next, we multiply (4.16) by a smooth function $\vartheta : \mathscr{J} \to \mathbb{R}$ satisfying $\vartheta(t_{\max}) = 0$ and we integrate over $\mathscr{J}$. In the first term, we get

$$\begin{aligned}\int_{\mathscr{J}}\int_\Omega \frac{\partial \boldsymbol{V}}{\partial t}\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x}\vartheta\,\mathrm{d}t &= \int_{\mathscr{J}}\left(\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \boldsymbol{V}\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x}\right)\vartheta\,\mathrm{d}t = \text{[per partes]}\\ &= \left[\int_\Omega \boldsymbol{V}\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x}\vartheta\right]_0^{t_{\max}} - \int_{\mathscr{J}}\int_\Omega \boldsymbol{V}\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x}\dot{\vartheta}\,\mathrm{d}t\\ &= -\vartheta(0)\int_\Omega \boldsymbol{V_0}\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x} - \int_{\mathscr{J}}\int_\Omega \boldsymbol{V}\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x}\dot{\vartheta}\,\mathrm{d}t.\end{aligned}$$

After these steps, we obtain from (4.16) the so-called *weak equality*

$$\int_{\mathscr{J}}\int_\Omega -\boldsymbol{V}\cdot\boldsymbol{\varphi}\dot{\vartheta} - \boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}\vartheta + \nu\nabla\boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\vartheta - \boldsymbol{F}\cdot\boldsymbol{\varphi}\vartheta\,\mathrm{d}\boldsymbol{x}\mathrm{d}t = \vartheta(0)\int_\Omega \boldsymbol{V}_0\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x}. \tag{4.17}$$

Note that:

1. In (4.17), the conditions for the regularity of the function $\boldsymbol{V}$ are significantly weaker than in the original equation (4.14). It does not have to be differentiable w.r.t. time and must be (together with its first derivatives) defined almost everywhere.

2. In (4.17), neither the pressure $\tilde{P}$ nor the potential Φ of (4.13) appear. Without loss of generality, we can therefore assume $\Phi = 0$, i.e. $\boldsymbol{F} = \boldsymbol{F}_\sigma$, and so $\nabla\cdot\boldsymbol{F} = 0$.

3. Each sufficiently smooth, so-called *classic* solution of the problem of incompressible flow (3.42), (3.38), (4.12), (4.2) satisfies a weak equality for any choice of functions $\boldsymbol{\varphi}, \vartheta$ with the above properties.

The question is whether, on the contrary, it is possible to use the weak equality (4.17) to define a function that is, in a sense, a solution to the original problem. For example, it follows from the above procedure that to derive (4.17), the condition of incompressibility (3.38) played an important role, but it no longer exists in the weak equality itself. What else needs to be assumed about the function $\boldsymbol{V}$, so that satisfying the weak equality identifies the function that is related to the original problem? Can it be guaranteed that such a function even exists? We will try to answer some of these questions in the following.

4.3.2 Special function spaces

At this moment, it is appropriate to recall the definitions of function spaces from Section 1.7.4. In addition, let's introduce the following spaces:

$\mathrm{L}_2(\Omega)^3$ Hilbert space of vector functions $\boldsymbol{u}:\Omega\to\mathbb{R}^3$, whose components[1] are in $\mathrm{L}_2(\Omega)$, with an inner product

$$(\boldsymbol{u},\boldsymbol{v})_{\mathrm{L}_2(\Omega)^3}=\int_\Omega \boldsymbol{u}\cdot\boldsymbol{v}\mathrm{d}\boldsymbol{x}=\sum_{i=1}^{3}\int_\Omega u_i(\boldsymbol{x})\,v_i(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}=\sum_{i=1}^{3}(u_i,v_i)_{\mathrm{L}_2(\Omega)}$$

and the induced norm

$$\begin{aligned}\|\boldsymbol{u}\|_{\mathrm{L}_2(\Omega)^3}&=\sqrt{\int_\Omega\|\boldsymbol{u}(\boldsymbol{x})\|^2\,\mathrm{d}\boldsymbol{x}}=\sqrt{\int_\Omega\sum_{i=1}^{3}u_i^2(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}}=\sqrt{\sum_{i=1}^{3}\int_\Omega u_i^2(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}}\\&=\left\|\left(\|u_i\|_{\mathrm{L}_2(\Omega)}\right)\right\|=\sqrt{\sum_{i=1}^{3}\|u_i\|^2_{\mathrm{L}_2(\Omega)}}.\end{aligned}\tag{4.18}$$

$\mathrm{H}_0^1(\Omega)^3$ Hilbert space of vector functions $\boldsymbol{u}:\Omega\to\mathbb{R}^3$, whose components are in $\mathrm{H}_0^1(\Omega)$, with an inner product

$$(\boldsymbol{u},\boldsymbol{v})_{\mathrm{H}_0^1(\Omega)^3}\equiv((\boldsymbol{u},\boldsymbol{v}))=\int_\Omega\nabla\boldsymbol{u}\cdot\nabla\boldsymbol{v}\mathrm{d}\boldsymbol{x}=\int_\Omega\partial_j u_i\partial_j v_i\mathrm{d}\boldsymbol{x}\tag{4.19}$$

and the induced norm

$$\begin{aligned}\|\boldsymbol{u}\|_{\mathrm{H}_0^1(\Omega)^3}&=\sqrt{((\boldsymbol{u},\boldsymbol{u}))}=\sqrt{\int_\Omega\nabla\boldsymbol{u}\cdot\nabla\boldsymbol{u}\mathrm{d}\boldsymbol{x}}=\sqrt{\sum_{i=1}^{3}\int_\Omega\sum_{j=1}^{3}\left(\partial_j u_i\right)^2\mathrm{d}\boldsymbol{x}}\\&=\left\|\left(\|u_i\|'_{\mathrm{H}_0^1(\Omega)}\right)\right\|=\sqrt{\sum_{i=1}^{3}\|u_i\|'^2_{\mathrm{H}_0^1(\Omega)}}.\end{aligned}\tag{4.20}$$

Remark 75. The expression (4.19) is evidently a symmetric bilinear form. Thanks to the modifications (4.20), we see that

$$((\boldsymbol{u},\boldsymbol{u}))=\sum_{i=1}^{3}\|u_i\|'^2_{\mathrm{H}_0^1(\Omega)},$$

where on the right hand side, there is a norm denoted by a prime introduced as a result of Corollary 1.7.9. That's why $((\cdot,\cdot))$ is also positive definite and is therefore indeed an inner product. According to Remark 57, there further exists $k>0$ such that

$$\|\boldsymbol{u}\|_{\mathrm{L}_2(\Omega)^3}\le k\|\boldsymbol{u}\|_{\mathrm{H}_0^1(\Omega)^3}.\tag{4.21}$$

$\mathrm{L}_{2,\mathrm{div}}(\Omega)^3$ space of vector-valued functions $\boldsymbol{u}$ with components in $\mathrm{L}_2(\Omega)$, for which in addition $\nabla\cdot\boldsymbol{u}\in\mathrm{L}_2(\Omega)$. The norm in this space is

$$\|\boldsymbol{u}\|_{\mathrm{L}_{2,\mathrm{div}}(\Omega)^3}=\|\boldsymbol{u}\|_{\mathrm{L}_2(\Omega)^3}+\|\nabla\cdot\boldsymbol{u}\|_{\mathrm{L}_2(\Omega)}.$$

[1] This definition assigns properties to the components of vector functions - i.e. elements of space $\mathrm{L}_2(\Omega)^3$ are triples of functions z $\mathrm{L}_2(\Omega)$, which, if they are calculated at a point (which is generally only possible almost everywhere), together creates a column vector of function values that lies in $\mathbb{R}^3$. Alternatively, one can define $\mathrm{L}_2(\Omega)^3$ as the tensor product of vector spaces

$$\mathrm{L}_2(\Omega)^3=\mathrm{L}_2(\Omega)\otimes\mathrm{L}_2(\Omega)\otimes\mathrm{L}_2(\Omega),$$

whose elements are formal vectors of elements of $\mathrm{L}_2(\Omega)$, i.e. evaluation at a point is not discussed at all. This view will be used in the proof of the statement 78, although a direct definition of the tensor product of vector spaces is avoided

Theorem 76. (on traces II) *There is continuous map* $T : \mathrm{L}_{2,div}(\Omega)^3 \to \mathrm{L}_2(\partial\Omega)$ *such that for each* $\boldsymbol{f} \in \mathrm{C}^1(\bar{\Omega})^3$,

$$T\boldsymbol{f} = \boldsymbol{f} \cdot \boldsymbol{n}\big|_{\partial\Omega}$$

holds.

Remark. Functions from $\mathrm{L}_2(\Omega)^3$ cannot generally be (continuously) extended onto the boundary of Ω , but functions from $\mathrm{L}_{2,\mathrm{div}}(\Omega)^3$ can be continuously extended to $\partial\Omega$ by taking their normal component.

$\mathrm{C}^\infty_{0,\sigma}(\Omega)^3$ space of vector-valued functions $\boldsymbol{u}$ with components from $\mathrm{C}^\infty_0(\Omega)$, satisfying in addition $\nabla \cdot \boldsymbol{u} = 0$ (σ ... *solenoidal* function).

$\mathrm{H} = \mathrm{L}_{2,\sigma}(\Omega)^3$ closure of the space $\mathrm{C}^\infty_{0,\sigma}(\Omega)^3$ in $\mathrm{L}_2(\Omega)^3$, with the inner product $(\boldsymbol{u},\boldsymbol{v})_\mathrm{H} = (\boldsymbol{u},\boldsymbol{v})_{\mathrm{L}_2(\Omega)^3}$ and norm $\|\cdot\|_\mathrm{H} = \|\cdot\|_{\mathrm{L}_2(\Omega)^3}\big|_\mathrm{H}$.

Remark. The closure of $\mathrm{C}^\infty_0(\Omega)^3$ (without „σ“) in $\mathrm{L}_2(\Omega)^3$ is the whole $\mathrm{L}_2(\Omega)^3$, i.e. $\mathrm{C}^\infty_0(\Omega)^3$ is dense in $\mathrm{L}_2(\Omega)^3$. Space H can also be thought of as a space of functions from $\mathrm{L}_2(\Omega)^3$, whose divergence *in terms of distributions* (see section 1.7.5) is zero and their normal component at the boundary $\partial\Omega$ is (according to Theorem 76) zero.

V closure of the space $\mathrm{C}^\infty_{0,\sigma}(\Omega)^3$ in $\mathrm{H}^1_0(\Omega)^3$, i.e. Hilbert space with inner product $(\cdot,\cdot)_\mathrm{V} = ((\cdot,\cdot))|_{\mathrm{V}\times\mathrm{V}}$ and with the norm $\|\cdot\|_\mathrm{V} = \|\cdot\|_{\mathrm{H}^1_0(\Omega)^3}\Big|_\mathrm{V}$.

Remark. The space V can also be thought of as a space of functions from $\mathrm{H}^1_0(\Omega)^3$, whose divergence is equal to zero almost everywhere in Ω. (In particular, unlike H, the functions from V have derivatives almost everywhere.)

Lemma 77. $\mathrm{V} \subset \mathrm{H}$ *holds.*

Proof. According to Remark 75, boundedness of a function u in the norm of the space $\mathrm{H}^1_0(\Omega)^3$ also implies boundedness in the norm of $\mathrm{L}_2(\Omega)^3$, from which it follows that

$$\mathrm{H}^1_0(\Omega)^3 \subset \mathrm{L}_2(\Omega)^3 . \tag{4.22}$$

Alternatively, to prove the inclusion (4.22) the first part of the proof of the next statement 78 (where even something more is proven) can be used. Now consider an arbitrary element $\boldsymbol{u} \in \mathrm{V}$. By definition of V as the closure of $\mathrm{C}^\infty_{0,\sigma}(\Omega)^3$ in $\mathrm{H}^1_0(\Omega)^3$, it can be expressed as a limit element of a sequence of functions $(\boldsymbol{u}_n) \subset \mathrm{C}^\infty_{0,\sigma}(\Omega)^3$ in the norm of the space $\mathrm{H}^1_0(\Omega)^3$, i.e.

$$\lim_{n\to\infty} \|\boldsymbol{u}_n - \boldsymbol{u}\|_{\mathrm{H}^1_0(\Omega)^3} = 0$$

holds. Thanks again to Remark 75, however,

$$\lim_{n\to\infty} \|\boldsymbol{u}_n - \boldsymbol{u}\|_{\mathrm{L}_2(\Omega)^3} = 0$$

also holds, which means that $\boldsymbol{u}$ is the limit element of the same sequence of functions $(\boldsymbol{u}_n) \subset \mathrm{C}^\infty_{0,\sigma}(\Omega)^3$, even in the norm of the space $\mathrm{L}_2(\Omega)^3$. In other words, it lies in the closure of $\mathrm{C}^\infty_{0,\sigma}(\Omega)^3$ in $\mathrm{L}_2(\Omega)^3$, which is H. Thereby, the proof is concluded. □

Proposition 78. $\mathrm{V} \hookrightarrow\hookrightarrow \mathrm{H}$ *holds.*

Proof. According to the consequence of the Rellich-Kondrachov theorem 1.7.10, it holds that

$$\mathrm{H}^1(\Omega) \hookrightarrow\hookrightarrow \mathrm{L}_2(\Omega).$$

If $\mathscr{B}_1 \hookrightarrow\hookrightarrow \mathscr{B}_2$ and $\mathscr{X} \Subset \mathscr{B}_1$ is a subspace of $\mathscr{B}_1$ (with the same norm!), then apparently also $\mathscr{X} \hookrightarrow\hookrightarrow \mathscr{B}_2$, which follows immediately from the definitions of compact embedding (Def. 68) and compact operator. Thanks to that, we specifically have

$$\mathrm{H}_0^1(\Omega) \hookrightarrow\hookrightarrow \mathrm{L}_2(\Omega). \tag{4.23}$$

We first show that

$$\mathrm{H}_0^1(\Omega)^3 \hookrightarrow\hookrightarrow \mathrm{L}_2(\Omega)^3. \tag{4.24}$$

Space $\mathrm{H}_0^1(\Omega)^3$ is a Hilbert space, and thus is (note 20) reflexive. The identical operator

$$\iota : \mathrm{H}_0^1(\Omega)^3 \to \mathrm{L}_2(\Omega)^3 \tag{4.25}$$

is therefore compact (Definition 65) if and only if (Remark 66) it is completely continuous (Definition 60). Therefore, it suffices to show from the definition that ι is completely continuous. So let $(\boldsymbol{u}^n)$ be a weakly convergent sequence of elements of $\mathrm{H}_0^1(\Omega)^3$, i.e.

$$\lim_{n\to\infty} \underline{\boldsymbol{w}}\left(\boldsymbol{u}^n\right) = \underline{\boldsymbol{w}}(\boldsymbol{u}) \ , \ \forall \underline{\boldsymbol{w}} \in \mathrm{H}_0^1(\Omega)^{3\prime}. \tag{4.26}$$

From the definition of the addition operation by components and linearity of $\underline{\boldsymbol{w}}$, one can write [2]

$$\underline{\boldsymbol{w}}\left(\boldsymbol{u}^n\right) = \underline{\boldsymbol{w}}\left(\begin{pmatrix} u_1^n \\ 0 \\ 0 \end{pmatrix}\right) + \underline{\boldsymbol{w}}\left(\begin{pmatrix} 0 \\ u_2^n \\ 0 \end{pmatrix}\right) + \underline{\boldsymbol{w}}\left(\begin{pmatrix} 0 \\ 0 \\ u_3^n \end{pmatrix}\right) = \sum_{i=1}^{3} \underline{\boldsymbol{w}}_i\left(u_i^n\right)$$

where $\underline{\boldsymbol{w}}_i \in \mathrm{H}_0^1(\Omega)'$ are three generally different functionals on $\mathrm{H}_0^1(\Omega)'$. If we choose $\underline{\boldsymbol{w}}_i$ arbitrarily and $\underline{\boldsymbol{w}}_j = \underline{0}$ for $j \neq i$, we get thanks to (4.26)

$$\lim_{n\to\infty} \underline{\boldsymbol{w}}_i\left(u_i^n\right) = \lim_{n\to\infty} \underline{\boldsymbol{w}}\left(u^n\right) \overset{(4.26)}{=} \underline{\boldsymbol{w}}\left(u^n\right) = \underline{\boldsymbol{w}}_i(u_i) \ , \ \forall \underline{\boldsymbol{w}}_i \in \mathrm{H}_0^1(\Omega)' \ \forall i \in \{1,2,3\}.$$

This means that even individual components u_i^n weakly converge to u_i in $\mathrm{H}_0^1(\Omega)$, and therefore thanks to (4.23), they converge strongly in $\mathrm{L}_2(\Omega)$. But then, from the definition of the norm on $\mathrm{L}_2(\Omega)^3$ by components using (4.18), it follows that the sequence of entire vectors $\boldsymbol{u}^n$ also converges in $\mathrm{L}^2(\Omega)^3$. This proves the complete continuity (and thus compactness) of the operator (4.25), that is, the compact embedding (4.24). Ultimately, because $\mathrm{V} \Subset \mathrm{H}_0^1(\Omega)^3$, we have $\mathrm{V} \hookrightarrow\hookrightarrow \mathrm{L}_2(\Omega)^3$, but because $\mathrm{V} \subset \mathrm{H}$ by Lemma 77, $\mathrm{V} \hookrightarrow\hookrightarrow \mathrm{H}$ holds. □

4.3.3 Energy inequality and the definition of a weak solution

We will perform the so-called a priori estimate of the solution to the problem (3.42), (3.38), (4.12), (4.2). We assume that it exists and by modifying (4.14), we arrive at an inequality that this solution must satisfy. This inequality will represent its boundedness in terms norms of certain function spaces. Thanks to this, we will find out to which function spaces the solution must belong.

We start from the relationship (4.16) and we substitute $\boldsymbol{\varphi} = \boldsymbol{V}$, which gives

$$\underbrace{\int_\Omega \frac{\partial \boldsymbol{V}}{\partial t} \cdot \boldsymbol{V} \mathrm{d}\boldsymbol{x}}_{(1)} \underbrace{- \int_\Omega \boldsymbol{V} \cdot \nabla \boldsymbol{V} \cdot \boldsymbol{V} \mathrm{d}\boldsymbol{x}}_{(2)} + \int_\Omega \nu \nabla \boldsymbol{V} \cdot \nabla \boldsymbol{V} \mathrm{d}\boldsymbol{x} = \int_\Omega \boldsymbol{F} \cdot \boldsymbol{V} \mathrm{d}\boldsymbol{x}. \tag{4.27}$$

[2] Formally, it can be simplified to $\boldsymbol{u}^n = u_i^n \boldsymbol{e}_i$, but the components of the vector are functions and the multiplication operation only meanins $\boldsymbol{u}^n(\boldsymbol{x}) = u_i^n(\boldsymbol{x})\,\boldsymbol{e}_i$ almost everywhere on Ω.

It holds at the same time

$$(1) = \int_\Omega \frac{\partial \boldsymbol{V}}{\partial t} \cdot \boldsymbol{V} \mathrm{d}\boldsymbol{x} = \int_\Omega \frac{1}{2} \frac{\partial \boldsymbol{V}^2}{\partial t} \mathrm{d}\boldsymbol{x} = \frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \frac{1}{2} \boldsymbol{V}^2 \mathrm{d}\boldsymbol{x}$$

If we recall the derived relation (4.15), i.e.

$$\int_\Omega \boldsymbol{V} \cdot \nabla \boldsymbol{V} \cdot \boldsymbol{\varphi} \mathrm{d}\boldsymbol{x} = -\int_\Omega \boldsymbol{V} \cdot \nabla \boldsymbol{\varphi} \cdot \boldsymbol{V} \mathrm{d}\boldsymbol{x},$$

then by substitution $\boldsymbol{\varphi} = \boldsymbol{V}$ (at this point we need from $\boldsymbol{V}$ the same properties as from $\boldsymbol{\varphi}$, i.e. especially (4.12)!), we receive immediately

$$(2) = \int_\Omega \boldsymbol{V} \cdot \nabla \boldsymbol{V} \cdot \boldsymbol{V} \mathrm{d}\boldsymbol{x} = 0.$$

By substituting back using the definitions of the spaces in Section 4.3.2 (and especially (4.20)), we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \frac{1}{2} \boldsymbol{V}^2 \mathrm{d}\boldsymbol{x} + \nu \|\boldsymbol{V}\|_{\mathrm{V}}^2 = \int_\Omega \boldsymbol{F} \cdot \boldsymbol{V} \mathrm{d}\boldsymbol{x}.$$

Using Schwarz, Poincaré (Remark 57 considered with a proportionality constant k) and (generalized) Young's inequalities, the right-hand side can be estimated as

$$\begin{aligned} \int_\Omega \boldsymbol{F} \cdot \boldsymbol{V} \mathrm{d}\boldsymbol{x} = (\boldsymbol{F}, \boldsymbol{V})_{\mathrm{L}_2(\Omega)^3} &\leq \|\boldsymbol{F}\|_{\mathrm{L}_2(\Omega)^3} \|\boldsymbol{V}\|_{\mathrm{L}_2(\Omega)^3} \\ &\leq k \|\boldsymbol{F}\|_{\mathrm{H}} \|\boldsymbol{V}\|_{\mathrm{V}} \\ &\leq \nu \frac{1}{2} \|\boldsymbol{V}\|_{\mathrm{V}}^2 + \frac{k}{2\nu} \|\boldsymbol{F}\|_{\mathrm{H}}^2. \end{aligned}$$

This further yields

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \frac{1}{2} \boldsymbol{V}^2 \mathrm{d}\boldsymbol{x} + \nu \frac{1}{2} \|\boldsymbol{V}\|_{\mathrm{V}}^2 \leq \frac{k^2}{2\nu} \|\boldsymbol{F}\|_{\mathrm{H}}^2.$$

By integrating over the time interval $(0, t)$, we get the so-called *energy inequality*

$$\underbrace{\int_\Omega \frac{1}{2} \boldsymbol{V}^2 \mathrm{d}\boldsymbol{x}\Big|_t}_{\text{current kinetic energy}} + \underbrace{\int_0^t \nu \frac{1}{2} \|\boldsymbol{V}(\tau,\cdot)\|_{\mathrm{V}}^2 \mathrm{d}\tau}_{\substack{\text{dissipation of kin. en.} \\ \text{from } t=0 \text{ to } t}} \leq \underbrace{\int_\Omega \frac{1}{2} \boldsymbol{V}^2 \mathrm{d}\boldsymbol{x}\Big|_{t=0}}_{\text{initial kin. energy}} + \underbrace{\frac{k^2}{2\nu} \int_0^t \|\boldsymbol{F}(\tau,\cdot)\|_{\mathrm{H}}^2 \mathrm{d}\tau}_{\substack{\approx \text{work of volumetric foces}^3 \\ \text{from time 0 to } t}}. \tag{4.28}$$

If we neglect the second term on the left-hand side of (4.28) and multiply the inequality by 2, we can proceed to the estimate

$$\int_\Omega \frac{1}{2} \boldsymbol{V}^2 \mathrm{d}\boldsymbol{x}\Big|_t \leq \int_\Omega \frac{1}{2} \boldsymbol{V_0}^2 \mathrm{d}\boldsymbol{x} + \frac{k^2}{2\nu} \int_{\mathscr{J}} \|\boldsymbol{F}\|_{\mathrm{H}}^2 \mathrm{d}t,$$

[3] More precisely, the work of volume forces in the entire domain Ω for time t would be equal

$$\int_0^t \int_\Omega |\boldsymbol{F}(\tau,\boldsymbol{x}) \cdot \boldsymbol{V}(\tau,\boldsymbol{x})| \, \mathrm{d}\boldsymbol{x} \mathrm{d}t.$$

which can be further rewritten using the definitions of norms on the appropriate spaces as

$$\|\boldsymbol{V}(t,\cdot)\|_{\mathrm{H}}^2 \leq \|\boldsymbol{V}_0\|_{\mathrm{H}}^2 + \frac{k^2}{\nu}\|\boldsymbol{F}\|_{\mathrm{L}_2(\mathscr{J};\mathrm{H})}^2 . \tag{4.29}$$

This is true for (*almost*) every $t \in \mathscr{J}$. In other words, even the (essential) supremum of the left hand side, which is the norm in the Bochner space $\mathrm{L}_\infty(\mathscr{J};\mathrm{H})$ satisfies the same inequality, i.e.

$$\|\boldsymbol{V}\|_{\mathrm{L}_\infty(\mathscr{J};\mathrm{H})}^2 \leq \|\boldsymbol{V}_0\|_{\mathrm{H}}^2 + \frac{k^2}{\nu}\|\boldsymbol{F}\|_{\mathrm{L}_2(\mathscr{J};\mathrm{H})}^2 . \tag{4.30}$$

On the other hand, if we neglect the first term in the energy inequality (4.28), we get for $t = t_{\max}$ (and after multiplying by $\frac{2}{\nu}$)

$$\|\boldsymbol{V}\|_{\mathrm{L}_2(\mathscr{J};\mathrm{V})}^2 = \int_{\mathscr{J}} \|\boldsymbol{V}\|_{\mathrm{V}}^2 \,\mathrm{d}t \leq \frac{1}{\nu}\|\boldsymbol{V}_0\|_{\mathrm{H}}^2 + \frac{k^2}{\nu^2}\|\boldsymbol{F}\|_{\mathrm{L}_2(\mathscr{J};\mathrm{H})}^2 . \tag{4.31}$$

A priori estimates (4.30) and (4.31) thus suggest that a possible solution to the incompressible flow problem should lie in the spaces $\mathrm{L}_\infty(\mathscr{J};\mathrm{H})$ and $\mathrm{L}_2(\mathscr{J};\mathrm{V})$, and in addition satisfy the mentioned inequalities. Thanks to this, we can proceed to the definition of a weak solution to the incompressible flow problem:

Definition 79. Let $\boldsymbol{V}_0 \in \mathrm{H}$, $\boldsymbol{F} \in \mathrm{L}_2(\mathscr{J};\mathrm{H})$. A function $\boldsymbol{V} \in \mathrm{L}_\infty(\mathscr{J};\mathrm{H}) \cap \mathrm{L}_2(\mathscr{J};\mathrm{V})$ satisfying the weak equality

$$\int_{\mathscr{J}}\int_{\Omega} -\boldsymbol{V}\cdot\boldsymbol{\varphi}\dot{\vartheta} - \boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}\vartheta + \nu\nabla\boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\vartheta - \boldsymbol{F}\cdot\boldsymbol{\varphi}\vartheta \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t = \vartheta(0)\int_{\Omega}\boldsymbol{V}_0\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x} \tag{4.17}$$

for all $\boldsymbol{\varphi} \in \mathrm{C}_{0,\sigma}^\infty(\Omega)^3$ and all $\vartheta \in \mathrm{C}_0^\infty([0,\mathrm{T}_{\max}))$ is called the *weak solution* of the incompressible flow problem (3.42), (3.38), (4.12), (4.2).

Remark. The choice $\vartheta \in \mathrm{C}_0^\infty([0,\mathrm{T}_{\max}))$ ensures $\vartheta(t_{\max}) = 0$, but does not force $\vartheta(0) = 0$ (ϑ must have compact support in a semi-closed interval).

Remark. The freedom of choice of the test functions is analogous to the freedom in selecting the volume $\mathcal{V}_0$ in the integral form of the conservation laws. In both these cases, lower regularity of the solutions is required compared to classical solutions ofthe equations in differential form.

Remark. When describing real flow situations, discontinuities may actually exist in physical quantities. In transonic flow (which is always compressible, however!), the interface between subsonic and supersonic flow is formed by a surface (so-called shock wave), where pressure, density and temperature are discontinuous. From a physical point of view, the weak solution is therefore more appropriate for describing real situations compared to the classical solution of the original problem (3.42), (3.38), (4.12), (4.2). On the other hand, in our particular setting of incompressible flow, the manner in which functions from Sobolev spaces can be discontinuous is strictly controlled by Theorems 45 and 46.

4.4 Existence (and uniqueness) of a weak solution

We find the weak solution as the limit of the sequence of its approximations using the Galerkin method. This method relies on the existence of a countable orthonormal basis of the underlying space, i.e. a complete orthonormal system of functions. We can find these functions as the eigenfunctions of the so-called Stokes operator.

4.4.1 Functional-analytic intermezzo: the Stokes operator

We define the *Stokes operator* $A : \mathrm{V} \to \mathrm{V}'$ using a relationship

$$(A\boldsymbol{u})(\boldsymbol{v}) = ((\boldsymbol{u}, \boldsymbol{v})), \tag{4.32}$$

where $((\cdot,\cdot))$ is the inner product on V defined by the relation (4.19). Then

1. A is (apparently) linear:

$$(A(\alpha\boldsymbol{u}_1 + \boldsymbol{u}_2))(\boldsymbol{v}) = ((\alpha\boldsymbol{u}_1 + \boldsymbol{u}_2, \boldsymbol{v})) = \alpha((\boldsymbol{u}_1, \boldsymbol{v})) + ((\boldsymbol{u}_2, \boldsymbol{v})) = \alpha(A\boldsymbol{u}_1)(\boldsymbol{v}) + (A\boldsymbol{u}_2)(\boldsymbol{v}).$$

2. A is continuous (bounded) on V:

$$\|A\boldsymbol{u}\|_{\mathrm{V}'} = \sup_{\substack{\boldsymbol{v}\in\mathrm{V} \\ \|\boldsymbol{v}\|_{\mathrm{V}}=1}} |(A\boldsymbol{u})(\boldsymbol{v})| = \sup_{\substack{\boldsymbol{v}\in\mathrm{V} \\ \|\boldsymbol{v}\|_{\mathrm{V}}=1}} |((\boldsymbol{u}, \boldsymbol{v}))|$$
$$\underbrace{=}_{\text{Schwarz}} ((\boldsymbol{u}, \frac{\boldsymbol{u}}{\|\boldsymbol{u}\|_{\mathrm{V}}})) = \frac{1}{\|\boldsymbol{u}\|_{\mathrm{V}}}\|\boldsymbol{u}\|_{\mathrm{V}}^2 = \|\boldsymbol{u}\|_{\mathrm{V}}.$$

3. A is a bijection $A : \mathrm{V} \to \mathrm{V}'$, i.e. A is invertible.

   According to Riesz's theorem 1.7.2, for each $\underline{\boldsymbol{w}} \in \mathrm{V}'$, there exists one and only one element $\boldsymbol{u} \in \mathrm{V}$ such that

$$\underline{\boldsymbol{w}}(\boldsymbol{v}) = ((\boldsymbol{u}, \boldsymbol{v})) = (A\boldsymbol{u})(\boldsymbol{v}),$$

   i.e. exactly one solution to the equation

$$A\boldsymbol{u} = \underline{\boldsymbol{w}}.$$

Remark. If we had introduced the inner product on V using

$$(\boldsymbol{u}, \boldsymbol{v})_{\mathrm{V}} = \int_\Omega \boldsymbol{u}\cdot\boldsymbol{v} + \nabla\boldsymbol{u}\cdot\nabla\boldsymbol{v}\,\mathrm{d}\boldsymbol{x},$$

which corresponds to the norm (1.36) on $\mathrm{H}_0^1(\Omega)$ (the one "without prime"), we would use The Lax-Milgram Lemma 19 here instead of Riesz's theorem 1.7.2. From Poincaré's inequality 1.7.9, however, the norm induced by this scalar product and the norm induced by $((\boldsymbol{u}, \boldsymbol{v}))$ are equivalent and therefore dual spaces are the same when using both norms (a functional is continuous in one norm just as it is in the other). That's why we can take $((\boldsymbol{u}, \boldsymbol{v}))$ as the „primary" inner product on V and all procedures will be simplified.

Remark. As $\mathrm{V} \subset \mathrm{H}$, then obviously $\mathrm{H}' \subset \mathrm{V}'$ (continuity of functionals is assumed in the norm H, i.e. $\mathrm{L}_2(\Omega)^3$).

Theorem 80. *Let $\underline{\boldsymbol{w}} \in \mathrm{H}'$. Then the solution of the equation*

$$A\boldsymbol{u} = \underline{\boldsymbol{w}},$$

satisfies

$$\boldsymbol{u} \in \mathrm{H}^2(\Omega)^3 \cap \mathrm{H}_0^1(\Omega)^3 \cap \mathrm{L}_{2,\sigma}(\Omega)^3 = \mathrm{H}^2(\Omega)^3 \cap \mathrm{H}_0^1(\Omega)^3 \cap \mathrm{V}.$$

Let us denote

$$D_{\tilde{A}} = \mathrm{H}^2(\Omega)^3 \cap \mathrm{H}_0^1(\Omega)^3 \cap \mathrm{V} \tag{4.33}$$

and further denote as $\tilde{A}$ the operator A restricted to $D_{\tilde{A}}$.

In Hilbert space H, the isomorphism $\mathrm{H}' \equiv \mathrm{H}$ holds and by Riesz's theorem (1.7.2), every element $\tilde{A}\boldsymbol{u} \in \mathrm{H}'$ for $\boldsymbol{u} \in D_{\tilde{A}}$ is represented uniquely by an element $\boldsymbol{z} \in \mathrm{H}$ such that (according to the definition of the Stokes operator (4.32)

$$(\boldsymbol{z}, \boldsymbol{v})_{\mathrm{H}} = \left(\tilde{A}\boldsymbol{u}\right)(\boldsymbol{v}) = ((\boldsymbol{u}, \boldsymbol{v})) = \int_\Omega \nabla \boldsymbol{u} \cdot \nabla \boldsymbol{v} \mathrm{d}\boldsymbol{x}.$$

According to Green's formula (Theorem 5), this representative is

$$\boldsymbol{z} = -\Delta \boldsymbol{u},$$

which is, thanks to the form of $D_{\tilde{A}}$ (4.33), a function defined almost everywhere in Ω (because $\boldsymbol{u}$ is in $\mathrm{H}^2(\Omega)$).

So let us consider in this sense $\tilde{A}$ as an operator

$$\tilde{A} : D_{\tilde{A}} \to \mathrm{H},$$

with values

$$\tilde{A}\boldsymbol{u} = \boldsymbol{z} = -\Delta \boldsymbol{u}.$$

The latter is (again according to Riesz's theorem and the derivation above) bounded on $D_{\tilde{A}}$ and in addition, it is symmetric:

$$\left(\tilde{A}\boldsymbol{u}, \boldsymbol{v}\right) = ((\boldsymbol{u}, \boldsymbol{v})) = ((\boldsymbol{v}, \boldsymbol{u})) = \left(\tilde{A}\boldsymbol{v}, \boldsymbol{u}\right) = \left(\boldsymbol{u}, \tilde{A}\boldsymbol{v}\right).$$

$\tilde{A}$ is therefore a self-adjoint and invertible operator. Operator $\tilde{A}^{-1} : \mathrm{H} \to D_{\tilde{A}}$ is thus also self-adjoint and due to compact embedding $D_{\tilde{A}} \subset \mathrm{V} \hookrightarrow\hookrightarrow \mathrm{H}$ (see Proposition 78) it is also compct according to Theorem 71. Further, by Theorem 67, there is a countable orthonormal basis of the space H.

4.4.2 Galerkin method

According to the previous section 4.4.1, there is an orthonormal basis $(\boldsymbol{W}_n)$ of the space H , which satisfies the condition of orthonormality in H, i.e.

$$(\boldsymbol{W}_k, \boldsymbol{W}_\ell)_{\mathrm{H}} = \delta_{k\ell}. \tag{4.34}$$

Because $\boldsymbol{W}_n$ are at the same time the eigenfunctions of the Stokes operator $\tilde{A}$[4], it also holds that $\boldsymbol{W}_n \in \mathrm{V}$ and in addition,

$$((\boldsymbol{W}_k, \boldsymbol{W}_\ell)) = \left(\tilde{A}\boldsymbol{W}_k, \boldsymbol{W}_\ell\right)_{\mathrm{H}} = \left(\mu_k \boldsymbol{W}_k, \boldsymbol{W}_\ell\right)_{\mathrm{H}} = \mu_k \delta_{k\ell}. \tag{4.35}$$

Let us now denote

$$\mathrm{V}_n = \mathrm{span}\,(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_n). \tag{4.36}$$

[4] $\boldsymbol{W}_n$ are eigenfunctions of the operator $\tilde{A}^{-1}$, i.e. $\tilde{A}^{-1}\boldsymbol{W}_n = \lambda_n \boldsymbol{W}_n \in \mathrm{V}$ holds with $\lambda_n \neq 0$, because $\tilde{A}^{-1}$ is (as well as $\tilde{A}$) injective. Then of course

$$\tilde{A}\boldsymbol{W}_n = \tilde{A}\left(\frac{1}{\lambda_n}\tilde{A}^{-1}\boldsymbol{W}_n\right) = \frac{1}{\lambda_n}\boldsymbol{W}_n,$$

i.e, $\boldsymbol{W}_n$ is also an eigenfunction of the operator $\tilde{A}$ corresponding to its eigenvalue $\mu_n = \lambda_n^{-1}$.

The Galerkin method consists in the construction of a sequence of approximations of the weak solution, i.e. function $\boldsymbol{V}$ satisfying the weak equality by definition 79. Let's look for the n-th approximation as a function $\boldsymbol{V}_n : \mathscr{J} \to \mathrm{V}_n$ in the form

$$\boldsymbol{V}_n(t, \boldsymbol{X}) = \sum_{k=1}^{n} a_k(t)\, \boldsymbol{W}_k(\boldsymbol{x}),$$

which satisfies (4.16), i.e.

$$\int_\Omega \frac{\partial \boldsymbol{V_n}}{\partial t} \cdot \boldsymbol{\varphi} \mathrm{d}\boldsymbol{x} - \int_\Omega \boldsymbol{V}_n \cdot \nabla \boldsymbol{\varphi} \cdot \boldsymbol{V}_n \mathrm{d}\boldsymbol{x} + \int_\Omega \nu \nabla \boldsymbol{V}_n \cdot \nabla \boldsymbol{\varphi} \mathrm{d}\boldsymbol{x} = \int_\Omega \boldsymbol{F} \cdot \boldsymbol{\varphi} \mathrm{d}\boldsymbol{x}, \tag{4.37}$$

for each $\boldsymbol{\varphi} \in \mathrm{V}_n$. From the construction of V_n, this is equivalent with (4.37) being satisfied for each $\boldsymbol{\varphi} \in \{\boldsymbol{W}_1, \ldots, \boldsymbol{W}_n\}$. After plugging $\boldsymbol{\varphi} = \boldsymbol{W}_\ell$, we get

$$\sum_{k=1}^{n} \dot{a}_k(t) (\boldsymbol{W}_k, \boldsymbol{W}_\ell)_{\mathrm{H}} - \sum_{k=1}^{n}\sum_{j=1}^{n} a_k(t)\, a_j(t) \int_\Omega \boldsymbol{W}_k \cdot \nabla \boldsymbol{W}_\ell \cdot \boldsymbol{W}_j \mathrm{d}\boldsymbol{x} + \nu \sum_{k=1}^{n} a_k(t) ((\boldsymbol{W}_k, \boldsymbol{W}_\ell)) = (\boldsymbol{F}, \boldsymbol{W}_\ell)_{\mathrm{H}}.$$

Using orthogonality relations (4.34) and (4.35), we can further write

$$\dot{a}_\ell(t) - \sum_{k=1}^{n}\sum_{j=1}^{n} a_k(t)\, a_j(t) \int_\Omega \boldsymbol{W}_k \cdot \nabla \boldsymbol{W}_\ell \cdot \boldsymbol{W}_j \mathrm{d}\boldsymbol{x} + \nu \mu_\ell a_\ell(t) = (\boldsymbol{F}, \boldsymbol{W}_\ell)_{\mathrm{H}}. \tag{4.38}$$

Equation (4.38) for $\ell \in \{0, 1, \ldots, n\}$ forms a system of ordinary differential equations for the unknown functions $a_1(t), \ldots, a_n(t)$. The initial conditions for this system are obtained as

$$a_\ell(0) = \beta_\ell, \text{ kde } \boldsymbol{V}_0 = \sum_{k=1}^{+\infty} \beta_k \boldsymbol{W}_k, \tag{4.39}$$

which means that the n- th approximation satisfies the n-th initial condition

$$\boldsymbol{V}_n(0, \cdot) = \boldsymbol{V}_{0,n} := \sum_{k=1}^{n} \beta_k \boldsymbol{W}_k.$$

We show that the problem (4.38), (4.39) has a solution on the entire interval $\mathscr{J}$. Because it is a so-called *autonomous* system in the form $\dot{\boldsymbol{a}} = \boldsymbol{f}(\boldsymbol{a})$ where $\boldsymbol{a} = (a_\ell)$, i.e. without an explicit dependence of the right-hand side on time, only two distinct cases can occur:

1. the solution exists on the entire interval $\mathscr{J}$, or
2. at time $T_{\mathrm{b}} < T_{\mathrm{end}}$ there is a so-called „blow-up", i.e.

$$\lim_{t \to T_{\mathrm{b}}} \|\boldsymbol{a}(t)\|_{\mathbb{R}^n} = +\infty. \tag{4.40}$$

We will now rule out this second possibility.

It holds that

$$\|\boldsymbol{V}_n\|_{\mathrm{H}}^2 = \int_\Omega \boldsymbol{V}_n \cdot \boldsymbol{V}_n \mathrm{d}\boldsymbol{x} = \sum_{k=1}^{n}\sum_{j=1}^{n} a_k a_j \left(\boldsymbol{W}_k, \boldsymbol{W}_j\right)_{\mathrm{H}} = \sum_{k=1}^{n}\sum_{j=1}^{n} a_k a_j \delta_{kj} = \sum_{k=1}^{n} a_k^2 = \|\boldsymbol{a}\|_{\mathbb{R}^n}^2.$$

Therefore, by estimating the value of $\|\boldsymbol{V}_n\|_{\mathrm{H}}$, it is also possible to estimate the norm of the solution of the ODE system, i.e. $\|\boldsymbol{a}\|$. We make this estimate again in terms of the energy inequality (4.28). By

choosing $\boldsymbol{\varphi} = \boldsymbol{V}_n$ in (4.37), we get a relation analogous to (4.27), only with $\boldsymbol{V}_n$ in place of $\boldsymbol{V}$. By making all adjustments up to (4.29), we obtain

$$\|\boldsymbol{a}\|^2_{\mathbb{R}^n} = \|\boldsymbol{V}_n(t,\cdot)\|^2_{\mathrm{H}} \leq \left\|\boldsymbol{V}_{0,n}\right\|^2_{\mathrm{H}} + \frac{k^2}{\nu}\|\boldsymbol{F}\|^2_{\mathrm{L}_2(\mathscr{J};\mathrm{H})}, \tag{4.41}$$

that is, uniform boundedness of $\boldsymbol{a}$ independent of t, which rules out (4.40). Analogously to (4.30) and (4.31), we also have a priori estimates available:

$$\|\boldsymbol{V}_n\|^2_{\mathrm{L}_\infty(\mathscr{J};\mathrm{H})} \leq \left\|\boldsymbol{V}_{0,n}\right\|^2_{\mathrm{H}} + \frac{k^2}{\nu}\|\boldsymbol{F}\|^2_{\mathrm{L}_2(\mathscr{J};\mathrm{H})}, \tag{4.42}$$

$$\|\boldsymbol{V}_n\|^2_{\mathrm{L}_2(\mathscr{J};\mathrm{V})} \leq \frac{1}{\nu}\left\|\boldsymbol{V}_{0,n}\right\|^2_{\mathrm{H}} + \frac{k^2}{\nu^2}\|\boldsymbol{F}\|^2_{\mathrm{L}_2(\mathscr{J};\mathrm{H})}. \tag{4.43}$$

4.4.3 Passage to the limit

Because the space V is Hilbert, the Bochner space $\mathrm{L}_2(\mathscr{J};\mathrm{V})$ is also Hilber according to Remark 48, and therefore it is (according to Remark 20) reflexive. Theorem 23 therefore ensures that from a bounded (thanks to (4.43)) sequence $\boldsymbol{V}_n$ in $\mathrm{L}_2(\mathscr{J};\mathrm{V})$, it is possible to select a subsequence that converges weakly, i.e.

$$\boldsymbol{V}_{k_n} \rightharpoonup \boldsymbol{V} \in \mathrm{L}_2(\mathscr{J};\mathrm{V}).$$

From now on, to simplify the notation, we will denote this subsequence again as $\boldsymbol{V}_n := \boldsymbol{V}_{k_n}$. Our aim is to show that the weak limit $\boldsymbol{V}$ is at the same time a weak solution to the problem by Definition 79.

Again, we realize that the solution of the ODE system (4.38), (4.39) is a function $\boldsymbol{V}_n$, which actually satisfies (4.37) for each $t \in \mathscr{J}$ and each $\boldsymbol{\varphi} \in \mathrm{V}_n$ (in contrast to the formal construction of the weak equality, where we only *assume* that the function $\boldsymbol{V}$ in the equality (4.16) exists!).

By multiplying (4.37) by a test function $\vartheta \in \mathrm{C}_0^\infty([0,\mathrm{T}_{\max}))$ and by integrating over $\mathscr{J}$, we obtain an equivalent of the weak equality (4.17) in the the form

$$\int_{\mathscr{J}}\int_{\Omega} \underbrace{-\boldsymbol{V}_n\cdot\boldsymbol{\varphi}\dot{\vartheta}}_{(1)} \underbrace{-\boldsymbol{V}_n\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}_n\vartheta}_{(2)} + \underbrace{\nu\nabla\boldsymbol{V}_n\cdot\nabla\boldsymbol{\varphi}\vartheta}_{(3)} - \boldsymbol{F}\cdot\boldsymbol{\varphi}\vartheta\,\mathrm{d}\boldsymbol{x}\mathrm{d}t = \vartheta(0)\int_{\Omega}\underbrace{\boldsymbol{V}_{0,n}\cdot\boldsymbol{\varphi}}_{(4)}\mathrm{d}\boldsymbol{x}, \tag{4.44}$$

which is satisfied for every $\vartheta \in \mathrm{C}_0^\infty([0,\mathrm{T}_{\max}))$ and every $\boldsymbol{\varphi} \in \mathrm{V}_n$.

Integrals of (1) and (3) represent linear functionals on $\mathrm{L}_2(\mathscr{J};\mathrm{V})$ applied to $\boldsymbol{V}_n$, and therefore thanks to $\boldsymbol{V}_{k_n} \rightharpoonup \boldsymbol{V}$, it holds for them that (see definition of weak convergence 21)

$$\int_{\mathscr{J}}\int_{\Omega}(1)\mathrm{d}\boldsymbol{x}\mathrm{d}t = \int_{\mathscr{J}}\int_{\Omega}\boldsymbol{V}_n\cdot\boldsymbol{\varphi}\dot{\vartheta}\mathrm{d}\boldsymbol{x}\mathrm{d}t \xrightarrow{n\to+\infty} \int_{\mathscr{J}}\int_{\Omega}\boldsymbol{V}\cdot\boldsymbol{\varphi}\dot{\vartheta}\mathrm{d}\boldsymbol{x}\mathrm{d}t,$$

$$\int_{\mathscr{J}}\int_{\Omega}(3)\mathrm{d}\boldsymbol{x}\mathrm{d}t = \int_{\mathscr{J}}\int_{\Omega}\nu\nabla\boldsymbol{V}_n\cdot\nabla\boldsymbol{\varphi}\vartheta\mathrm{d}\boldsymbol{x}\mathrm{d}t \xrightarrow{n\to+\infty} \int_{\mathscr{J}}\int_{\Omega}\nu\nabla\boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\vartheta\mathrm{d}\boldsymbol{x}\mathrm{d}t,$$

that is, they converge to the respective expressions in the weak equality (4.17). The same applies to the member (4), because by choice of the n-th initial condition (4.39), we have

$$\boldsymbol{V}_{0,n} \to \boldsymbol{V}_0$$

in V, so

$$\int_{\Omega}(4)\mathrm{d}\boldsymbol{x} = \int_{\Omega}\boldsymbol{V}_{0,n}\cdot\boldsymbol{\varphi}\mathrm{d}\boldsymbol{x} \xrightarrow{n\to+\infty} \int_{\Omega}\boldsymbol{V}_0\cdot\boldsymbol{\varphi}\mathrm{d}\boldsymbol{x}.$$

However, passage to the limit in the integral of (2) remains a problem, as weak convergence $\boldsymbol{V}_n \rightharpoonup \boldsymbol{V}$ in $\mathrm{L}_2(\mathscr{J};\mathrm{V})$ is not sufficient for this.

The solution is as follows:

1. First, consider the time derivative $\frac{\partial \boldsymbol{V}_n}{\partial t}$ as a function mapping to the dual space

$$\frac{\partial \boldsymbol{V}_n}{\partial t} : \mathscr{J} \to \mathrm{V}'$$

pursuant

$$\underbrace{\left(\frac{\partial \boldsymbol{V}_n}{\partial t}(t)\right)}_{\in \mathrm{V}'}(\boldsymbol{\varphi}) = \left(\frac{\partial \boldsymbol{V}_n}{\partial t}(t,\cdot), \boldsymbol{\varphi}\right)_{\mathrm{H}} = \int_\Omega \frac{\partial \boldsymbol{V}_n}{\partial t}(t,\cdot)\cdot\boldsymbol{\varphi}\,\mathrm{d}\boldsymbol{x} \qquad \forall \boldsymbol{\varphi} \in \mathrm{V}.$$

Then it can be shown [Pok20a] the boundedness of $\frac{\partial \boldsymbol{V}_n}{\partial t}$ in the norm

$$\left\|\frac{\partial \boldsymbol{V}_n}{\partial t}\right\|_{\mathrm{L}_{p_1}(\mathscr{J};\mathrm{V}')} = \left\|\left\|\frac{\partial \boldsymbol{V}_n}{\partial t}\right\|_{\mathrm{V}'}\right\|_{\mathrm{L}_{p_1}(\mathscr{J})} = \left\|\sup_{\boldsymbol{\varphi}\in\mathrm{V},\|\boldsymbol{\varphi}\|_{\mathrm{V}}=1}\left|\underbrace{\left(\frac{\partial \boldsymbol{V}_n}{\partial t}(t)\right)}_{\in\mathrm{V}'}(\boldsymbol{\varphi})\right|\right\|_{\mathrm{L}_{p_1}(\mathscr{J})} \leq \cdots$$

For $\Omega \subset \mathbb{R}^2$, the choice $p_1 = 2$ can be used, but for $\Omega \subset \mathbb{R}^3$, we need $p_1 = \frac{4}{3}$.

2. Subsequently, we use the Lions-Aubin lemma 73, where we choose $\mathscr{B}_0 = \mathrm{V}$, $\mathscr{B} = \mathrm{H}$, $\mathscr{B}_1 = \mathrm{V}'$, $p_0 = 2$ and $p_1 \in \{2, \frac{4}{3}\}$ according to the dimension of the domain Ω (see the previous point). According to Remark 78, we have $\mathrm{V} \hookrightarrow\hookrightarrow \mathrm{H}$ and in addition, from Remark 69 (i.e. we know that $\mathrm{V} \hookrightarrow \mathrm{H}$) and Theorem 70 (i.e. $\mathrm{V} \hookrightarrow \mathrm{H} \implies \mathrm{H}' \hookrightarrow \mathrm{V}$), it follows that

$$\mathrm{H} \equiv \mathrm{H}' \hookrightarrow \mathrm{V}',$$

where we identified $\mathrm{H} \equiv \mathrm{H}'$ according to Remark 18. The statement of the Lions-Aubin lemma is in this case

$$\mathscr{Y} \hookrightarrow\hookrightarrow \mathrm{L}_2\left(\mathscr{J};\mathrm{H}\right) \tag{4.45}$$

where $\mathscr{Y}$ is the subspace of $\mathrm{L}_2\left(\mathscr{J};\mathrm{V}\right)$ containing functions with bounded derivatives, i.e. all approximations $\boldsymbol{V}_n$ thanks to the argument given above..

3. Thanks to the compact embedding (4.45) we know (see Definition 68 and 65) that

$$\boldsymbol{V}_n \xrightarrow[\text{(strongly)}]{} \boldsymbol{V} \text{ in } \mathrm{L}_2\left(\mathscr{J};\mathrm{H}\right).$$

Due to the strong convergence, we can complete the passage to the limit in the nonlinear term (2).

Let us now fix $m \in \mathbb{N}$ and choose $\boldsymbol{\varphi} \in \mathrm{V}_m$. Moreover, assume that

$$\boldsymbol{\varphi} \in \mathrm{C}^\infty_{0,\sigma}(\Omega)^3, \tag{4.46}$$

which we will use to conclude the proof. Let it $n \geq m$ and $\vartheta \in \mathrm{C}^\infty_0([0,\mathrm{T}_{\max}))$. We will show that

$$\left|\int_{\mathscr{J}}\int_\Omega \boldsymbol{V}_n\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}_n\vartheta\,\mathrm{d}\boldsymbol{x}\mathrm{d}t - \int_{\mathscr{J}}\int_\Omega \boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}\vartheta\,\mathrm{d}\boldsymbol{x}\mathrm{d}t\right| \xrightarrow{n\to+\infty} 0. \tag{4.47}$$

We manipulate the left hand side as

$$\begin{aligned}
&\left|\int_{\mathscr{J}}\int_\Omega \left(\boldsymbol{V}_n\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}_n - \boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}\right)\vartheta\,\mathrm{d}\boldsymbol{x}\mathrm{d}t\right| \\
&= \left|\int_{\mathscr{J}}\int_\Omega \left(\boldsymbol{V}_n\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}_n - \underbrace{\boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}_n + \boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}_n}_{\text{artificially added and subtracted}} - \boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}\right)\vartheta\,\mathrm{d}\boldsymbol{x}\mathrm{d}t\right| \\
&\leq \underbrace{\int_{\mathscr{J}}\int_\Omega \left|(\boldsymbol{V}_n-\boldsymbol{V})\cdot\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}_n\vartheta\right|\mathrm{d}\boldsymbol{x}\mathrm{d}t}_{(A)} + \underbrace{\int_{\mathscr{J}}\int_\Omega \left|\boldsymbol{V}\cdot\nabla\boldsymbol{\varphi}\cdot(\boldsymbol{V}_n-\boldsymbol{V})\,\vartheta\right|\mathrm{d}\boldsymbol{x}\mathrm{d}t}_{(B)}
\end{aligned}$$

Term (B) is a linear functional on the space $\mathrm{L}_2\left(\mathscr{J};\mathrm{H}\right)$, applied to the difference $(\boldsymbol{V}_n - \boldsymbol{V})$. Even from weak convergence

$$\boldsymbol{V}_n \rightharpoonup \boldsymbol{V}$$

in $\mathrm{L}_2\left(\mathscr{J};\mathrm{H}\right)$, it follows that

$$(B) \xrightarrow{n\to+\infty} 0.$$

We further esitmate the term (A) using Hölder's inequality 53 (for the integral over $\mathscr{J}$) and Hölder's inequality for vector functions 54 with $\frac{1}{p} = \frac{1}{q} = \frac{1}{2}$

$$(A) \leq \sqrt{\underbrace{\int_{\mathscr{J}}\int_{\Omega} \|\boldsymbol{V}_n - \boldsymbol{V}\|^2 \,\mathrm{d}\boldsymbol{x}\mathrm{d}t}_{(A1)}} \sqrt{\underbrace{\int_{\mathscr{J}}\int_{\Omega} \left\|\nabla\boldsymbol{\varphi}\cdot\boldsymbol{V}_n\right\|^2 \mathrm{d}\boldsymbol{x}}_{(A2)}\vartheta^2\mathrm{d}t},$$

where

$$(A1) = \|\boldsymbol{V}_n - \boldsymbol{V}\|^2_{\mathrm{H}} \xrightarrow{n\to+\infty} 0.$$

To prove (4.47), boundedness of $(A2)$ is sufficient. We will estimate it further

$$(A2) = \int_{\Omega}\sum_{j=1}^{3}\left(\underbrace{\sum_{i=1}^{3}\partial_j\varphi_i V_{n,i}}_{[\text{Hölder}p=q=\frac{1}{2}]}\right)^2 \mathrm{d}\boldsymbol{x} \leq \int_{\Omega}\sum_{j=1}^{3}\sum_{i=1}^{3}\left(\partial_j\varphi_i\right)^2\sum_{i=1}^{3}V_{n,i}^2\mathrm{d}\boldsymbol{x}$$
$$= \int_{\Omega}\left(\nabla\boldsymbol{\varphi}\cdot\nabla\boldsymbol{\varphi}\right)\|\boldsymbol{V}_n\|^2\,\mathrm{d}\boldsymbol{x}.$$

We use Hölder's inequality one more time (see Corollary 54) with the choice $\frac{1}{p} = \frac{1}{3}, \frac{1}{q} = \frac{2}{3}$ to get

$$(A2) \leq \underbrace{\left(\int_{\Omega}\|\boldsymbol{V}_n\|^6\,\mathrm{d}\boldsymbol{x}\right)^{\frac{1}{3}}}_{\|\boldsymbol{V}_n\|^2_{\mathrm{L}_6(\Omega)^3}}\left(\int_{\Omega}\left(\nabla\boldsymbol{\varphi}\cdot\nabla\boldsymbol{\varphi}\right)^{\frac{3}{2}}\mathrm{d}\boldsymbol{x}\right)^{\frac{2}{3}}\mathrm{d}t.$$

The second integral is finite from the additional assumption of regularity of the function $\boldsymbol{\varphi}$ (4.46), The norm $\|\boldsymbol{V}_n\|_{\mathrm{L}_6(\Omega)^3}$ is also bounded because at the same time, $\boldsymbol{V}_n(t,\cdot) \in \mathrm{V}$ and from the Rellich-Kondrachov lemma 72 for $\Omega\subset\mathbb{R}^2$ and $\Omega\subset\mathbb{R}^3$, because we have[5]

$$\mathrm{H}^1(\Omega) \hookrightarrow \mathrm{L}_6(\Omega).$$

Thus, we have shown that the limit $\boldsymbol{V}$ satisfies the weak equality (4.17) for $\boldsymbol{\varphi} \in \mathrm{V}_m \cap \mathrm{C}^{\infty}_{0,\sigma}(\Omega)^3$, where of course m is arbitrarily large. From the construction of V_m using (4.36), it follows that for each element

$$\boldsymbol{\psi} \in \mathrm{C}^{\infty}_{0,\sigma}(\Omega)^3 = \mathrm{H}\cap\mathrm{C}^{\infty}_{0,\sigma}(\Omega)^3,$$

[5] A lemma to be precise 72 implies

$$\mathrm{H}^1(\Omega) \hookrightarrow \mathrm{L}_{\mathscr{P}}(\Omega)$$

for $\mathscr{P} \in [1,6]$ when $\Omega\subset\mathbb{R}^3$ and for $\mathscr{P}\in[2,+\infty)$ for $\Omega\subset\mathbb{R}^2$. For member estimation $(A2)$ hence Hölder's inequality with choice can be used $2p = \mathscr{P} \in [2,6]$ but also $p > 1$ (that $\exists q > 1$ so that $\frac{1}{p}+\frac{1}{q} = 1$). In total, then. $p\in(1,3]$. By choosing the maximum possible $p = 3$ we put on $\nabla\boldsymbol{\varphi}$ minimum possible requirements for regularity. Assuming (4.46), which we use, but can be chosen p and otherwise.

„Sorcery" with estimates using Hölder's inequality can be found in the literature in various variants (see e.g. [Pok20a, p. 36]), while a specific procedure is required to prove some other statements.

there is a sequence $\boldsymbol{\varphi}_m \in V_m \cap C^\infty_{0,\sigma}(\Omega)^3$ such that $\lim_{m\to+\infty}\boldsymbol{\varphi}_m = \boldsymbol{\psi}$. Also, $\boldsymbol{V}$ satisfies (4.17) with the choice $\boldsymbol{\varphi} = \boldsymbol{\varphi}_m$ for each $m \in \mathbb{N}$. By the limit transition for $m \to +\infty$, we find that (4.17) is also satisfied for $\boldsymbol{\varphi} = \boldsymbol{\psi}$ (all terms are linear with respect to $\boldsymbol{\varphi}_m$, i.e. no problem will occur)[6]. We conclude that $\boldsymbol{V}$ satisfies the weak equality (4.17) for each

$$\boldsymbol{\varphi} \in C^\infty_{0,\sigma}(\Omega)^3,$$

and is therefore by definition 79 a weak solution to the incompressible flow problem.

4.4.4 Uniqueness of solutions, undiscussed and open problems

The investigation of solutions to the Navier-Stokes equations is far from being limited to the proof of existence of a weak solution:

- uniqueness of the solution in $\mathbb{R}^2$ has been proved
- uniqueness of solution v $\mathbb{R}^3$
  - only partial results are known
- the existence of a function P, which has the sense of pressure (exists for a sufficiently smooth region boundary)
  - if $\boldsymbol{V}$ is sufficiently smooth that there is also a classical solution, then P also exists [Neu06b]
- issues of locality vs. globality of solutions, questions of regularity, connection with initial regularity conditions
  - a smooth solution exists only locally in time (Ladyženská, Kyselev 1957)
- energy inequality
  - We have found a solution that satisfies the energy inequality.
  - The question whether every weak solution must satisfy the energy inequality is an open problem

A number of statements are proved in [Pok20a] and a summary of known and unknown results can be found in [Pok20b]. Advanced parts of the NS equation analysis for compressible flow can be found in [NS04, FN17].

[6] This is sometimes called a closure argument because

$$\overline{\bigcup_{m=1}^{+\infty}\left[V_m \cap C^\infty_{0,\sigma}(\Omega)^3\right]} = H \cap C^\infty_{0,\sigma}(\Omega)^3 = C^\infty_{0,\sigma}(\Omega)^3.$$

CHAPTER

5 Turbulent flow and turbulence modeling

5.1 Turbulent flow

- principle: kinetic energy is stored in vortices of different sizes (cascade eddies)
- the transfer of kinetic energy is from larger scales to smaller, but in theory also vice versa
- on the smallest scales, kinetic energy is dissipated into internal energy

5.2 Averaging quantities

5.2.1 Reynolds averaging

- decomposition of a quantity $f \in \{P, \varrho, V_i, T\}$ to mean values and fluctuations

$$f = \bar{f} + f' \tag{5.1}$$

  - time averaging (suitable for stationary flow)

$$\bar{f}_T(t, \boldsymbol{x}) = \lim_{T \to +\infty} \frac{1}{T} \int_t^{t+T} f(\tau, \boldsymbol{x}) \, \mathrm{d}\tau,$$

  - averaging in space (suitable for homogeneous flow)

$$\bar{f}_{\mathcal{V}}(t, \boldsymbol{x}) = \lim_{|\mathcal{V}(\boldsymbol{x})| \to +\infty} \frac{1}{|\mathcal{V}(\boldsymbol{x})|} \int_{\mathcal{V}(\boldsymbol{x})} f(t, \boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi},$$

    where $\boldsymbol{x} \in \mathcal{V}(\boldsymbol{x})$,

  - averaging over a statistical ensemble (*ensemble averaging*), i.e. N-times repeating the same process (experiment)

$$\bar{f}_E(t, \boldsymbol{x}) = \lim_{N \to +\infty} \frac{1}{N} \sum_k f(t, \boldsymbol{x})$$

- In practice $T \to +\infty$, $|\mathcal{V}| \to +\infty$ means that the interval (or the control volume) for averaging has an order of magnitude larger temporal (or spatial) scale than the turbulent phenomena.

5.2.2 Reynolds averaging rules

For averaged quantities f, g and $\alpha \in \mathbb{R}$, it holds under the assumption of stationary, or homogeneous flow

$$\begin{aligned}\overline{\alpha f} &= \alpha \bar{f},\\ \overline{f+g} &= \bar{f} + \bar{g},\\ \overline{fg} &= \bar{f}\bar{g} + \overline{f'g'},\\ \overline{\partial_i f} &= \partial_i \bar{f}\end{aligned}$$

and further

$$\bar{\bar{f}} = \bar{f},$$

from which it also flows

$$\overline{f'} = 0.$$

In the case of non-stationary inhomogeneous flow, the method of (e.g. time) averaging can be changed to

$$\bar{f}_T(t, \boldsymbol{x}) = \lim_{T\to+\infty} \frac{1}{\delta t} \int_t^{t+\delta t} f(\tau, \boldsymbol{x})\, \mathrm{d}\tau,$$

where $\delta t \ll t_0$ and t_0 is the time scale of slow (macroscopic) flow changes. For

$$\frac{\delta t}{t_0} \to 0,$$

one can show from the Taylor expansion

$$f(t+\delta t) = f(t) + \frac{\partial f}{\partial t}(t)\,\delta t + \cdots$$

that

$$\bar{\bar{f}} \to \bar{f}, \overline{\frac{\partial f}{\partial t}} \to \frac{\partial \bar{f}}{\partial t},$$

and likewise the asymptotic fulfillment of other averaging rules.

5.2.3 Reynolds-averaged Navier–Stokes (RANS) equations

- for *incompressible* flow, they can be derived from the equations (3.42) by applying Reynolds averaging to V_i, respectively P
- leads to formally the same form (NS equations) for the averaged quantities but in addition, the so-called Reynolds stress tensor

  $$\mathbf{T}^{\mathrm{R}} = \left(\tau^{\mathrm{R}}_{ij}\right),\ \tau^{\mathrm{R}}_{ij} = -\varrho v'_i v'_j = -\varrho\left(\overline{v_i v_j} - \bar{v}_i \bar{v}_j\right)$$

  appears

  - the form of the Reynolds stress tensor does not follow from this procedure, a *model* is required
    - k-ε model, k-ω model...

5.2.4 Favre averaging, compressible flow

- Reynolds averaging can be used when modeling compressible flow for all quantities (not only P and V_i, but alo ϱ and T), but the resulting equations must be supplemented with correlations modeling fluctuations density
- it is better to apply Reynolds averaging to ϱ and P and *Favre's* averaging on V_i, T, E, H
- Favre's averaging is given by the relation

$$\tilde{f} = \frac{1}{\bar{\varrho}} \lim_{T \to +\infty} \frac{1}{T} \int_t^{t+T} \varrho f \, \mathrm{d}t,$$

  where $\bar{\varrho}$ is the Reynolds averaged density.
- similarly to Reynolds averaging (5.1), so the relevant quantity can be decomposed into the averaged and fluctuating parts, respectively

5.2.5 Favre and Reynolds averaged Navier–Stokes equations

- **TODO:** see [Bla15], p. 220
- Favre averaged Reynolds stress tensor

5.3 Boundary conditions

- boundary conditions for k, ε, ω

5.4 Large Eddy Simulation

- LES .. large eddy simulation
- is based on spatial filtering

$$f = \bar{f} + f',$$

  where $\bar{f}$ is the macroscopic (resolved on a numerical grid) part of f and f' is the microscopic (*subgrid-size*) component
  - Smagorinsky
  - small eddies are filtered out, large ones are processed on a sufficiently fine mesh

5.5 Modern methods of turbulence modeling

- DNS simulation and machine learning approaches

CHAPTER

6 Fundamentals of fluid thermodynamics

6.1 Relationship between internal energy and absolute temperature

We start from the definitions of specific heat capacities (i.e. per unit mass) at constant volume and constant pressure

$$c_V = \left(\frac{\partial E}{\partial T}\right)_V, \; c_P = \left(\frac{\partial H}{\partial T}\right)_P, \tag{6.1}$$

where

$$H = E + \frac{P}{\varrho}$$

is the *specific enthalpy*. The notation

$$\left(\frac{\partial E}{\partial T}\right)_V$$

in (6.1) is usual in thermodynamics and should be understood in the following way. Internal energy is generally a function of the state variables P, V, T. The lower index V means that the process takes place at constant volume. It therefore follows from the equation of state that pressure is already a function of temperature only, i.e. $P = P(T)$ and the internal energy can therefore be expressed as a function

$$\mathscr{E}(T) = E(\Phi(T)),$$

where

$$\Phi(T) = (P(T), V, T).$$

Then the change in the internal energy of the system depending on the temperature is according to the chain rule of differentiation given by the relation

$$c_V = \left(\frac{\partial E}{\partial T}\right)_V := \frac{\mathrm{d}\mathscr{E}(T)}{\mathrm{d}T} = \frac{\partial E}{\partial P}\frac{\partial P}{\partial T} + \frac{\partial E}{\partial V}\underbrace{\frac{\partial V}{\partial T}}_{=0} + \frac{\partial E}{\partial T}\frac{\partial T}{\partial T} = \frac{\partial E}{\partial P}\frac{\partial P}{\partial T} + \frac{\partial E}{\partial T}.$$

Analogous reasoning applies to the calculation of c_P.

For liquids that can be considered incompressible (ϱ = konst.), it follows that

$$c_P = \left(\frac{\partial H}{\partial T}\right)_P = \left(\frac{\partial E}{\partial T}\right)_P + \underbrace{\left(\frac{\partial\left(\frac{P}{\varrho}\right)}{\partial T}\right)_P}_{=0} = \left(\frac{\partial E}{\partial T}\right)_P.$$

Some liquids can be considered so-called *perfect* gases for which the internal energy depends only on temperature. The internal energy can then be expressed for them as

$$E(T) = \int_{T_{\mathrm{ref},i}}^{T} c_V(\tau)\,\mathrm{d}\tau,\ H(T) = \int_{T_{\mathrm{ref},i}}^{T} c_P(\tau)\,\mathrm{d}\tau \tag{6.2}$$

where T_{ref} is an arbitrary reference temperature. As the internal energy only appears in the equations in the differential terms (but never directly), the value of T_{ref} can be chosen arbitrarily, e.g. $T_{\mathrm{ref}} = 0$. In many applications, the temperature varies over the range where the heat capacity can be considered constant. Then from (6.2), the relationships

$$E = c_V T,\ H = c_P T \tag{6.3}$$

follow. Values of c_V and c_P for different fluids have been measured and can be found in the respective charts of physical properties of substances.

6.2 State equations

The *equation of state* indicates the dependence between the state variables of a closed system. State variables are those that depend only on the current state of the system. For example, for gases, the equation of state provides the relationship between the temperature T, pressure P and volume V as

$$f(T,P,V) = 0.$$

In fluid dynamics, the form

$$f\left(T,P,\varrho\right) = 0 \tag{6.4}$$

is more appropriate. Relationship (6.4) together with the relationship between the specific internal energy E and temperature T allows closing the system of equations describing the flow (see section 3.10).

6.2.1 Equation of state of an ideal gas

The well known *ideal gas equation of state* has the form

$$PV = nRT,$$

where n is the molar amount of gas and R is the *universal (molar) gas constant* with the value

$$R \doteq 8.31446\ \mathrm{J\cdot mol^{-1}K}.$$

This equation can also be rewritten in a form related to a unit of volume

$$P = \frac{n}{V}RT = \frac{nM}{V}\frac{R}{M}T = \varrho R_{\mathrm{spec}}T, \tag{6.5}$$

where M is the molar mass of gas and $R_{\mathrm{spec}} = R/M$ is called the *specific gas constant*. According to the so-called Mayer's relation (proof can be found e.g. in [CB15, from p. 668]) it holds for the ideal gas that

$$c_P - c_V = R_{\mathrm{spec}}. \tag{6.6}$$

Substituting into (6.5) with the use of (6.3), we get the ideal gas equation of state in the form

$$P = \varrho\left(c_P - c_V\right)T = \left(\frac{c_P}{c_P} - 1\right)\varrho E = (\kappa - 1)\,\varrho E,\ \text{where}\ \kappa = \frac{c_P}{c_V}. \tag{6.7}$$

The coefficient κ is called the Poisson's constant of simply the *heat capacity ratio*.

6.2.2 Other forms of the equation of state

- EOS for mixtures etc.

6.3 Heat transfer

6.3.1 Heat transfer by radiation

- integro-differential equation for radiative heat transfer

CHAPTER

7 Formulation of problems in engineering practice

7.1 Boundary conditions for flow problems

- division of the boundary into inflow, outflow, and wall
- inlet and outlet conditions for viscous and inviscid flow
  - a range of possibilities that fit the PDR theory
  - e.g. in a pipe: speed or mass flow (momentum) at the inlet, pressure at the outlet,
  - other quantities are extrapolated from the flow field, i.e. the zero Neumann boundary condition applies to them
  - there are cases where all conditions can be prescribed at the input and none at the output (supersonic viscous flow, inviscid flow)
- wall conditions for viscous and inviscid flow ($\frac{\partial V}{\partial \boldsymbol{n}} = 0$ or no-slip condition $\boldsymbol{V} = 0$)
- Navier boundary condition: $\boldsymbol{v}$ is proportional to the component of $\mathbf{T}_D$ tangent to $\partial\Omega$
- No boundary condition is completely realistic (e.g. in reality, there will not always be a constant atmospheric pressure at the outflow of the pipe, as it will depend on what just blew out of the pipe.). By forcing an idealized boundary condition, oscillations and reflections can occur.
- resistance boundary condition
- pulsating flow - boundary conditions preventing reflection (Omer Rathore - contribution at NC2019)
- far field boundary conditions
- periodic boundary conditions and symmetry conditions (implementation: cells linked as if they continued beyond the domain boundary)
- boundary conditions for heat transfer
  - boundary conditions in 3D and source terms in 1D, Nusselt number
  - $$\lambda \frac{\partial}{\partial \boldsymbol{n}}(\varrho T) = A_{\text{conv}} \cdot (T - T_{\text{wall}}).$$

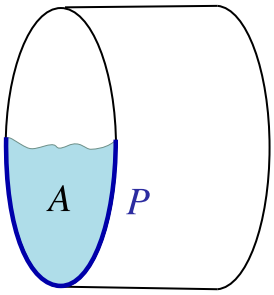

Figure 7.1: Flow area and wetted perimeter

7.2 Fluid flow in porous media

In this chapter, we briefly describe fluid flow in porous media. The porous environment is made up of a solid skeleton and a free, interconnected space (pores) through which fluids can flow. The presence of a rigid skeleton allows the law of conservation of linear momentum to be approximated by Darcy's law

$$\boldsymbol{V} = -\frac{1}{\mu}\mathbf{K}\left(\nabla P - \varrho \boldsymbol{g}\right), \tag{7.1}$$

where $\mathbf{K}$ $[m^2]$ is the permeability tensor of the environment.

Darcy's Law (7.1) can be further substituted into the continuity equation

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot \left(\varrho \boldsymbol{V}\right) = 0,$$

which gives us

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot \left(-\frac{\varrho}{\mu}\mathbf{K}\left(\nabla P - \varrho \boldsymbol{g}\right)\right) = 0. \tag{7.2}$$

When considering the equation of state for density $\varrho = \varrho(P)$, the dynamic description of fluid flow in a porous medium can be described by a single partial differential equation (7.2) for the unknown pressure P.

7.3 Dimensionless numbers characterizing the flow

- *Reynolds* number expressing the nature of the flow (laminar or turbulent)

$$\mathrm{Re} = \frac{\varrho\,|\boldsymbol{V}|\,D_\mathrm{H}}{\mu} = \frac{|\boldsymbol{V}|\,D_\mathrm{H}}{\nu},$$

where D_H is called the *hydraulic diameter* (of a pipe), or, in the general case, the so-called *characteristic distance*. The hydraulic diameter is the hypothetical diameter of a cylindrical pipe in which the flow would behave the same as in a real pipe with a general cross-sectional shape. Hydraulic *radius* is defined as a ratio of *cross-sectional flow area* to the *wetted perimeter*, see Figure 7.1 , and the hydraulic diameter as its quadruple (!), i.e.

$$R_\mathrm{H} = \frac{A}{P},\; D_\mathrm{H} = 4R_\mathrm{H}.$$

For example, for a completely filled pipe with a circular cross-section of radius R, it follows that

$$R_\mathrm{H} = \frac{\pi R^2}{2\pi R} = \frac{R}{2},\; D_\mathrm{H} = 2R\,(= D)\,.$$

For a tube with a rectangular cross-section with sides a, b, we get

$$D_{\mathrm{H}} = \frac{4ab}{2(a+b)} = \frac{2ab}{a+b}.$$

- *Mach* number indicating the ratio of the flow speed to the local speed of sound

$$M = \frac{|\boldsymbol{V}|}{A},$$

where the local speed of sound is generally given by equation [MMD16]

$$A = \sqrt{\kappa \left(\frac{\partial P}{\partial \varrho}\right)_T},$$

or, for an ideal gas satisfying the equation of state (6.5), one can write

$$A = \sqrt{\kappa R_{\mathrm{spec}} T},$$

where $\kappa = \frac{C_P}{C_V}$, see Section 6.2.1.

- *Prandtl* number indicating the relationship between momentum diffusivity (i.e. viscosity) and heat diffusivity

$$\mathrm{Pr} = \frac{\nu}{\alpha} = \frac{\mu/\varrho}{\lambda/(\varrho c_P)} = \frac{\mu c_P}{\lambda},$$

where

$$\alpha = \frac{\lambda}{\varrho c_P} \left[\mathrm{m}^2 \cdot \mathrm{s}^{-1}\right]$$

is the thermal diffusivity and $\lambda \left[\mathrm{W} \cdot \mathrm{m} \cdot \mathrm{K}^{-1}\right]$ is the thermal conductivity.

- *Schmidt* number indicating the ratio of diffusivity of momentum and mass

$$\mathrm{Sc} = \frac{\nu}{D} = \frac{\mu}{\varrho D},$$

where $D \left[\mathrm{m}^2 \cdot \mathrm{s}^{-1}\right]$ is the (mass) diffusion coefficient.

- *Péclet* number indicates the ratio of advective and diffusive transport of any quantity in free flow. It applies to mass tranfer in the form

$$\mathrm{Pe}_M = \frac{D_{\mathrm{H}} |\boldsymbol{V}|}{D} = \mathrm{ReSc}$$

and to heat tranfer as

$$\mathrm{Pe}_E = \frac{D_{\mathrm{H}} |\boldsymbol{V}|}{\alpha} = \mathrm{RePr}.$$

- *Nusselt* number indicating the ratio of convective and conductive heat transfer at the boundary (on the wall)

$$\mathrm{Nu} = \frac{h}{\lambda/L} = \frac{hL}{\lambda},$$

where on the pipe wall, the heat transfer is given by the convection coefficient

$$\dot{Q} = h(T_w - T_\infty),$$

where T_w is the pipe temperature and T_∞ is the free stream gas temperature.

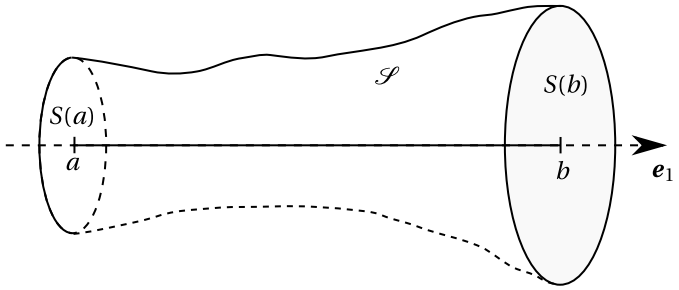

Figure 7.2: Control volume $\mathcal{V}$ in a pipe with a variable cross-section.

- *Sherwood* number indicating the ratio of convective and diffusive mass transfer at the interface of two substances, or phases

$$\mathrm{Sh} = \frac{u}{D/L} = \frac{uL}{D},$$

where L is the characteristic dimension and $u\ \left[\mathrm{m}\cdot\mathrm{s}^{-1}\right]$ is the convective mass transfer coefficient (de facto velocity). For example, for multiphase flow, it is the absolute value of the difference between individual phase velocities. It is used, for example, in modeling the rate of:

  - the transfer of water vapor to or from a water droplet during phase transitions,
  - access of oxygen to the surface of the burning particle.

  Characteristic dimension L is in that case equal to the diameter of the droplet or particle, respectively.

7.4 Quasi-1D flow

Consider the flow in a pipe V oriented parallel with the axis $x \equiv x_1$ with a variable internal cross-section $S(x)$ with surface area $|S(x)| = A(x)$ (shape doesn't matter). Let us now choose a control volume $\mathcal{V} \subset V$ as the inner segment of the tube for $x \in (a,b)$ (see Figure 7.2). Then

$$\mathcal{V} = \{S(x) \,|\, x \in (a,b)\}.$$

The mass conservation law in the form (2.17) expressed for this choice of $\mathcal{V}$ has the fom

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}} \varrho \mathrm{d}\boldsymbol{x} + \int_{\partial\mathcal{V}} \varrho \boldsymbol{V}\cdot\boldsymbol{n}\mathrm{d}S \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\int_a^b \mathrm{d}x \int_{S(x)} \varrho \mathrm{d}(x_2,x_3) + \int_{S(a)} \varrho \boldsymbol{V}\cdot\boldsymbol{n}\mathrm{d}S + \int_{S(b)} \varrho \boldsymbol{V}\cdot\boldsymbol{n}\mathrm{d}S + \int_{\mathscr{S}} \varrho \boldsymbol{V}\cdot\boldsymbol{n}\mathrm{d}S, \end{aligned} \tag{7.3}$$

where $\mathscr{S}$ is the surface surrounding $\mathcal{V}$ between the bases $S(a)$ and $S(b)$. Regardless of the choice of the boundary condition on the wall (see section 7.1),

$$\boldsymbol{V}\cdot\boldsymbol{n} = 0 \text{ on } \mathscr{S}$$

holds. Therefore, the last term in (7.3) drops out and further calculations yield

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}t}\int_a^b A(x)\,\varrho\left(t,\boldsymbol{\xi}_x\right)\mathrm{d}x + A(b)\,\varrho V_1\big|_{(t,\xi_b)} - A(a)\,\varrho V_1\big|_{(t,\xi_a)} \\ &= \int_a^b A(x)\frac{\partial}{\partial t}\varrho\left(t,\boldsymbol{\xi}_x\right)\mathrm{d}x + \int_a^b \frac{\partial}{\partial x}\left(A(x)\,\varrho V_1\big|_{(t,\xi_x)}\right)\mathrm{d}x, \end{aligned}$$

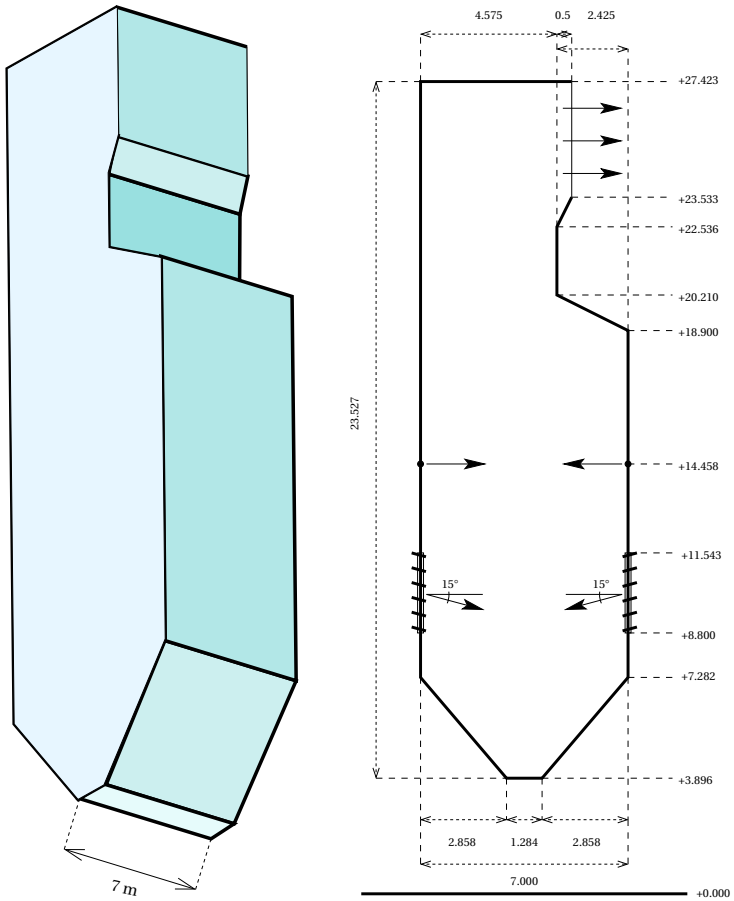

Figure 7.3: Three-dimensional geometry of the combustion chamber of an industrial boiler and its two-dimensional model.

where the mean value theorem was applied to the integral over $S(x)$ with $\boldsymbol{\xi}_x \in S(x)$. Given any choice of interval (a,b),

$$A(x)\frac{\partial}{\partial t}\varrho\left(t,\boldsymbol{\xi}_x\right)+\frac{\partial}{\partial x}\left(A(x)\,\varrho V_1\big|_{(t,\boldsymbol{\xi}_x)}\right)=0 \tag{7.4}$$

has to be satisfied. If we now introduce the functions $\bar{\varrho}(t,x)=\rho\left(t,\boldsymbol{\xi}_x\right)$, $\bar{V}_1(t,x)=V_1\left(t,\boldsymbol{\xi}_x\right)$, we can rewrite (7.4) to

$$\frac{\partial}{\partial t}\bar{\varrho}(t,x)+\frac{1}{A(x)}\frac{\partial}{\partial x}\left(A(x)\,\bar{\varrho}(t,x)\,\bar{V}_1(t,x)\right)=0. \tag{7.5}$$

Function values $\bar{\varrho}(t,x)$, $\bar{V}_1(t,x)$ can also be considered as average values of density, or x-velocity components taken over the cross-section $S(x)$ at time t.

7.5 Reacting multicomponent flow, combustion modeling

Finally, we present a the rather complicated problem of flow, combustion, heat transfer, and chemical reactions in the combustion chamber of an industrial pulverized coal-powered boiler. We will use it to demonstrate various aspects of mathematical and physical modeling of industrial processes. The model is based on the works [BSM+13b, BSM+13a], which were created as part of the joint project of FNSPE CTU in Prague and Honeywell.

The fuel in the boiler is a mixture of coal and biomass of generally different origin such as cereal bran or wood chips that are sold in in the form of pressed pellets. Biomass is represented only in

<table>
<tr><td colspan="7">as received basis</td></tr>
<tr><td>A</td><td colspan="3">C</td><td>H</td><td>O</td><td>N</td><td>S</td><td>W</td></tr>
<tr><td>ash (A)</td><td colspan="2">fixed carbon (FC)</td><td colspan="3">volatile matter (VM)</td><td colspan="2">moisture (W)</td></tr>
<tr><td colspan="2">char (coke)</td><td colspan="5">volatiles</td></tr>
</table>

Figure 7.4: Fuel composition from a chemical and physical point of view.

small fractions, as its higher share would have a negative effect on boiler operation (clogging of heat exchangers, etc.). Each fuel has a chemical composition with a certain representation of basic chemicals elements (*ultimate analysis*) and at the same time composition in terms of physical (*proximate analysis*) - see picture 7.4 . Chemical reactions during the combustion of a unit of fuel mass release the heat of combustion called *HHV – higher heating value*. However, moisture is present in the fuel, which evaporates during combustion. The latent heat consumed to evaporate the moisture reduces the amount of immediately available thermal energy. By subtracting it from the heat of combustion, we obtain the so-called calorific value or *LHV – lower heating value*. In devices that, as part of the work cycle, also ensure the condensation of flue gases (condensing boilers), the entire combustion heat is used and efficiency of these heat sources is higher than 100% of LHV.

A diagram of the nearly 30-meter-high combustion chamber is shown in Figure 7.3. In each corner of the combustion chamber, there are six burners, one above the other, which blow out a mixture of preheated primary air together with finely ground fuel. The stream of this mixture is still surrounded by the flow of secondary air. Above the burners is the entrance to the tertiary air or *OFA - Over Fire Air*, which can increase the oxygen concentration at the cost of reducing the flue gas temperature, and thereby ensure a more thorough combustion of the mixture. At the ceiling of the chamber, the flue gas is discharged into the chimney. Heat is transferred to the walls by radiation and convection. In the walls, there are vertical pipes in which steam is produced from liquid water under high pressure. The flow of steam is conducted from top to bottom, i.e. against the stream of flue gas to make the heat transfer more efficient. A heat exchanger is located in the upper part of the combustion chamber (so-called superheater) in which superheated steam is produced. The steam then drives a turbine to generate electricity and is further used after cooling down to distribute heat. In addition to the combustion chamber, the boiler also contains another heat exchanger, the so-called economizer, that uses already partially cooled flue gases for preheating the liquid water, and also a primary air preheater. In our model, however, only the combustion chamber itself is represented.

The model of the combustion chamber is two-dimensional, which in this case is not very appropriate. The flow in the chamber is heavily dependent on the spatial arrangement of the burners, which create a vortex in the central part of the chamber (see figure7.5). The flow in the chamber is highly turbulent, which contributes to mixing of fuel and air and thus also to nearly perfect combustion.

7.5.1 Fluid dynamics and energy balance equations

The system of equations describing 2D flow has the form

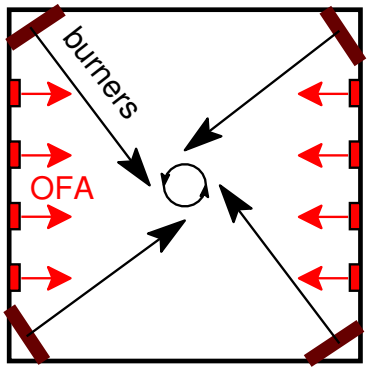

Figure 7.5: Top elevation of the combustion chamber with the arrangement of the burners indicated.

$$
\begin{aligned}
\frac{\partial}{\partial t}\varrho + \partial_{x_i}(\varrho V_i) &= 0, \\
\frac{\partial}{\partial t}(\varrho V_i) + \partial_{x_i}(P + \varrho V_i^2) &= \partial_{x_j}\left(\mu \partial_{x_j} V_i\right) + \frac{1}{3}\partial_{x_j}\left(\mu \partial_{x_i} V_j\right) - \frac{2}{3}\partial_{x_i}(\varrho k) + \varrho g_i, \\
c_P\left[\frac{\partial}{\partial t}(\varrho T) + \partial_{x_i}(\varrho T V_i)\right] &= \underbrace{-R_{\text{char}} h_{\text{char}} - R_{\text{vol}} h_{\text{vol}} - R_{\text{bms}} h_{\text{bms}}}_{\text{produkce tepla}} - \underbrace{\left(q_c + q_{rg} + q_{rw}\right)}_{\text{přestup tepla}} \\
&+ \partial_{x_j}\left[\left(\mu_L + \frac{\mu_T}{\sigma_k}\right)\partial_{x_j} k\right]
\end{aligned}
\tag{7.6}
$$

where the pressure P is calculated using the ideal gas equation of state

$$P = \varrho R_{\text{spec}} T. \tag{6.5}$$

The terms $R_{\text{char}}, R_{\text{vol}}, R_{\text{bms}}$ represent burning rates of solid coal components, volatile components coal, and biomass (see part 7.5.4), respectively. The terms q_c, q_{rg}, q_{rw} represent different methods of heat transfer, described later in Section 7.5.8.

The rate at which a particle burns depends on its size. The average coal particle size at a given point is calculated from the average count of particles per unit volume n, which is an intensive quantity subject to passive transport according to the equation

$$\frac{\partial}{\partial t} n + \partial_{x_i}(n V_i) = \underbrace{\partial_{x_i}\left(\frac{\mu_T}{\text{Sc}_t}\partial_{x_i} n\right)}_{\text{turbulentní difuze}}.$$

7.5.2 Modeling turbulence

Turbulence is modeled by to k-ε model , where k is the turbulent kinetic energy and ε is the rate of its dissipation. These quantities satisfy the equations

$$
\begin{aligned}
\frac{\partial}{\partial t}(\varrho k) + \partial_{x_i}(\varrho k V_i) &= \partial_{x_j}\left[\left(\mu_L + \frac{\mu_T}{\sigma_k}\right)\partial_{x_j} k\right] + G_k - G_b - Y_m - \varrho\varepsilon, \\
\frac{\partial}{\partial t}(\varrho \varepsilon) + \partial_{x_i}(\varrho \varepsilon V_i) &= \partial_{x_j}\left[\left(\mu_L + \frac{\mu_T}{\sigma_\varepsilon}\right)\partial_{x_j} \varepsilon\right] + C_{1\varepsilon}\frac{\varepsilon}{k}(G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon}\varrho\frac{\varepsilon^2}{k}
\end{aligned}
$$

where the friction coefficients satisfy

$$\mu_T = \varrho C_\mu \frac{k^2}{\varepsilon}, \quad \mu = \mu_L + \mu_T,$$

and turbulence production terms have the form

$$G_k = \left(\partial_{x_2} V_1 + \partial_{x_1} V_2\right)^2 + \partial_{x_1} V_1 \left[\frac{4}{3}\mu\partial_{x_1} V_1 - \frac{2}{3}\left(\varrho k + \mu\partial_{x_2} V_2\right)\right] + \partial_{x_2} V_2 \left[\frac{4}{3}\mu\partial_{x_2} V_2 - \frac{2}{3}\left(\varrho k + \mu\partial_{x_1} V_1\right)\right],$$
$$G_b = -g_i \frac{\mu}{\varrho \mathrm{Pr}_t}\partial_{x_i}\varrho,$$

where

$$C_{3\varepsilon} = \tanh\left|\frac{V_2}{V_1}\right|, \quad Y_m = 2\varrho\varepsilon M_t^2, \quad M_t = \sqrt{\frac{k}{a^2}}, \quad a = \sqrt{\gamma RT}.$$

7.5.3 Modeling of chemical reactions

7.5.3.1 Balance equation of chemical components

Reactions take place between the chemical compounds of the gas and between the gaseous components and fuel components. The individual chemical components satisfy the balance equations. On their right-hand side, source terms indicating the conversion rate of the respective component appear.

- For fixed carbon, volatile fuel components, and biomass, these are equations

$$\frac{\partial}{\partial t}\varrho_{\mathrm{char}} + \partial_{x_i}(\varrho_{\mathrm{char}} V_i) = \partial_{x_i}\left(\frac{\mu_T}{\mathrm{Sc}_t}\partial_{x_i}\varrho_{\mathrm{char}}\right) + R_{\mathrm{char}}, \tag{7.7}$$
$$\frac{\partial}{\partial t}\varrho_{\mathrm{vol}} + \partial_{x_i}(\varrho_{\mathrm{vol}} V_i) = \partial_{x_i}\left(\frac{\mu_T}{\mathrm{Sc}_t}\partial_{x_i}\varrho_{\mathrm{vol}}\right) + R_{\mathrm{vol}}, \tag{7.8}$$
$$\frac{\partial}{\partial t}\varrho_{\mathrm{bms}} + \partial_{x_i}(\varrho_{\mathrm{bms}} V_i) = \partial_{x_i}\left(\frac{\mu_T}{\mathrm{Sc}_t}\partial_{x_i}\varrho_{\mathrm{bms}}\right) \underbrace{+R_{\mathrm{bms}}}_{\text{vyhořívání paliva}}. \tag{7.9}$$

- For gas components, we have

$$\frac{\partial}{\partial t}(\varrho Y_*) + \partial_{x_i}(\varrho Y_* V_i) = \partial_{x_i}\left(-\frac{\mu_T}{\mathrm{Sc}_t}\partial_{x_i} Y_*\right) + \omega_*, \tag{7.10}$$

where $* \in \{\mathrm{O_2}, \mathrm{N_2}, \mathrm{NO}, \mathrm{HCN}, \mathrm{NH_3}, \mathrm{H_2O}, \mathrm{CO_2}\}$. As a representative of nitrogen oxides (NO_x), nitric oxide (NO) is included in this model.

7.5.3.2 Source terms and chemistry of nitrogen oxides

The source terms on the right-hand side of the equations (7.7)–(7.10) have the form

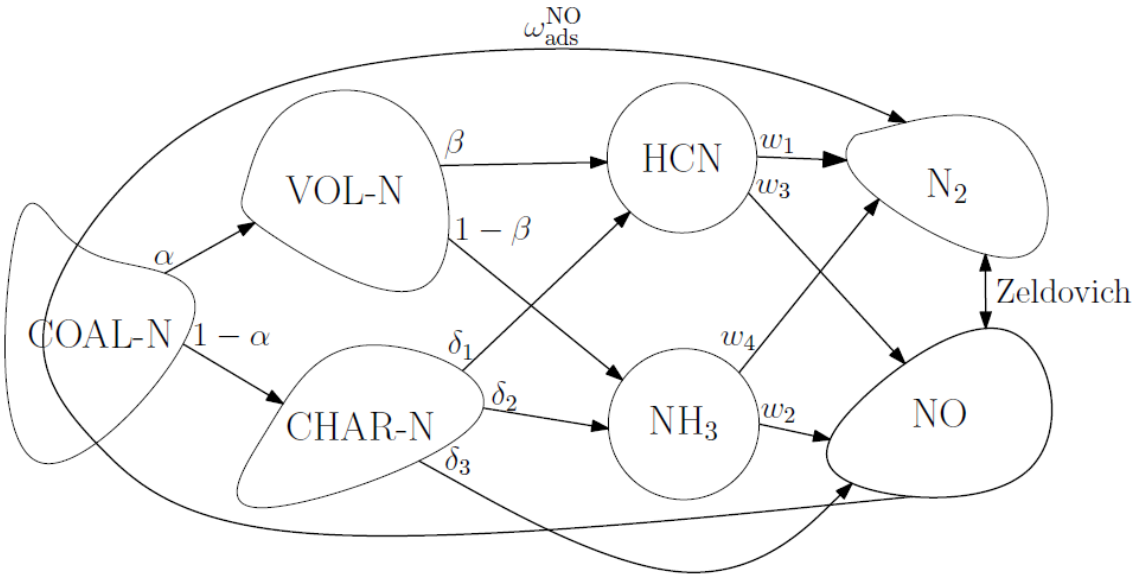

Figure 7.6: Mechanism and kinetics of nitrogen reactions (for coal only).

$$
\begin{aligned}
\omega_{O_2} &= \varrho_{O_2} V_{O_2}^{\circ} (R_{coal}^{char} + R_{coal}^{vol} + R_{bms}^{char} + R_{bms}^{vol}) + (-w_1 - w_3) \cdot \frac{M_{O_2} p}{RT} \\
\omega_{N_2} &= (w_2 + w_4) \cdot \frac{M_{N_2} p}{RT} + \omega_{ads}^{NO} \cdot \frac{M_{N_2}}{M_{NO}} \\
\omega_{NO} &= M_{NO} \cdot w_0 + (w_1 - w_2 + w_3 - w_4) \cdot \frac{M_{NO} p}{RT} - \omega_{ads}^{NO} \\
&+ \alpha \cdot \delta_3 \cdot \left(Y_{coal}^{N} (-R_{coal}^{char} - R_{coal}^{vol}) + Y_{bms}^{N} (R_{bms}^{char} - R_{bms}^{vol}) \right) \cdot \frac{M_{NO}}{M_N} \\
\omega_{HCN} &= (-w_1 - w_2) \frac{M_{HCN} p}{RT} - ((1-\alpha)\beta (Y_{coal}^{N} R_{coal}^{vol} + Y_{bms}^{N} R_{bms}^{vol}) - \delta_1 \alpha (Y_{coal}^{N} R_{coal}^{char} + Y_{bms}^{N} R_{bms}^{char})) \cdot \frac{M_{HCN}}{M_N} \\
\omega_{NH_3} &= (-w_3 - w_4) \cdot \frac{M_{NH_3} p}{RT} - ((1-\alpha)(1-\beta) (Y_{coal}^{N} R_{coal}^{vol} + Y_{bms}^{N} R_{bms}^{vol}) - \delta_2 \alpha (Y_{coal}^{N} R_{coal}^{char} + Y_{bms}^{N} R_{bms}^{char})) \cdot \frac{M_{NH_3}}{M_N} \\
\omega_{H_2O} &= \varrho_{H_2O} \cdot \left(11.1 \frac{H}{100} + 1.24 \frac{W}{100} \right) (-R_{coal}^{vol} - R_{bms}^{vol}) \\
\omega_{CO_2} &= \varrho_{CO_2} \cdot \left(-1.866 \cdot (R_{coal}^{char} + R_{bms}^{char}) - \frac{V_{CO_2} - 1.866 FC}{VM} (R_{coal}^{vol} + R_{bms}^{vol}) \right)
\end{aligned}
$$

where $\delta_1, \delta_2, \delta_3$ are the rates of conversion of nitrogen bound in solid fuel to HCN, NH_3, and NO, and coefficients w_k express the rate of reactions according to Arrhenius reaction kinetics. A simplified mechanism of nitrogen reactions is employed, which is shown schematically in Figure 7.6 . The relevant details follow below:

- Thermal NO, i.e. nitric oxide arising directly from the oxidation of nitrogen radicals in the flue gas at high temperatures is described by the Zeldovich [**?**] and the Bowman [**?**] mechanisms and the corresponding reaction rate is approximated by

$$
w_0 = 2k_1^+ \cdot X_O \cdot X_{N_2} \cdot \frac{1 - \frac{k_1^- k_2^- [NO]^2}{k_1^+ [N_2] k_2^+ [O_2]}}{1 + \frac{k_1^- \cdot [NO]}{k_2^+ [O_2] + k_3^+ [OH]}},
$$

where $k_1^{\pm}, k_2^{\pm}, k_3^{\pm}$ describe the velocities of the following forward (+) and reverse (−) reactions:

$$\begin{aligned} \mathrm{O} + \mathrm{N}_2 &\overset{k_1}{\rightleftharpoons} \mathrm{N} + \mathrm{NO}, \\ \mathrm{N} + \mathrm{O}_2 &\overset{k_2}{\rightleftharpoons} \mathrm{O} + \mathrm{NO}, \\ \mathrm{N} + \mathrm{OH} &\overset{k_3}{\rightleftharpoons} \mathrm{H} + \mathrm{NO}. \end{aligned}$$

Their approximation is given by

$$\begin{aligned} k_1^+ &= 1.8 \times 10^8 \cdot \exp\left(\frac{-38370}{T}\right), & k_1^- &= 3.8 \times 10^7 \cdot \exp\left(\frac{-425}{T}\right), \\ k_2^+ &= 1.8 \times 10^4 \cdot \exp\left(\frac{-4680}{T}\right), & k_2^- &= 3.8 \times 10^3 \cdot T \cdot \exp\left(\frac{-20820}{T}\right), \\ k_3^+ &= 7.1 \times 10^7 \cdot \exp\left(\frac{-450}{T}\right), & k_3^- &= 1.7 \times 10^8 \cdot \exp\left(\frac{-24560}{T}\right), \end{aligned}$$

as Arrhenius kinetics assume an exponential dependence reaction rates at temperature.

- The formation of NO by HCN oxidation occurs at a rate

$$w_1 = 1.0 \times 10^{10} X_{\mathrm{HCN}} X_{\mathrm{O}_2}^a \exp\left(-33732.5/T\right). \tag{7.11}$$

- Formation of NO by oxidation of NH_3 occurs at a rate

$$w_2 = 4.0 \times 10^6 X_{\mathrm{NH}_3} X_{\mathrm{O}_2}^a \exp\left(-16111.0/T\right). \tag{7.12}$$

- Consumption of NO by reduction to HCN occurs at a rate

$$w_3 = -3.0 \times 10^{12} X_{\mathrm{HCN}} X_{\mathrm{NO}} \exp\left(-30208.2/T\right). \tag{7.13}$$

- Consumption of NO by reduction to NH_3 occurs at a rate

$$w_4 = -1.8 \times 10^8 X_{\mathrm{NH}_3} X_{\mathrm{NO}} \exp\left(-13593.7/T\right). \tag{7.14}$$

- Heterogeneous reduction of NO on the surface of coal particles occurs at a rate

$$\omega_{\mathrm{ads}}^{\mathrm{NO}} = 2.27 \times 10^{-3} c_s A_{\mathrm{BET}} M_{\mathrm{NO}} p_{\mathrm{NO}} \exp\left(-17168.33/T\right). \tag{7.15}$$

In relationships (7.11)–(7.15), the symbol X represents the mole fraction a a is the order of the oxygen reaction.

Remark. Here it is important to note that the given wild values of the constants are **tied to a specific choice of physical units**. Absolute temperature T is given in Kelvin (K) and constants in exponentials have the dimension K^{-1}. When moving to other units, these very same constants will have a different numerical value!

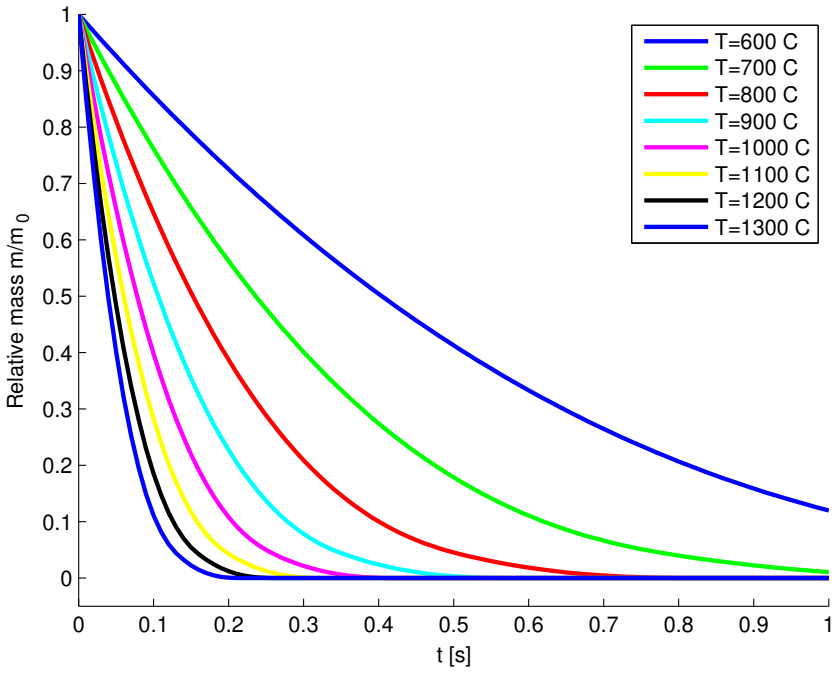

Figure 7.7: Burnout curves of fixed carbon in coal particles and their dependence on the temperature.

7.5.4 Fuel burnout

The terms $R_{\text{char}}, R_{\text{vol}}, R_{\text{bms}}$ in the energy equation (7.6) determine the burning rate of three fuel components (fixed carbon in coal, volatile substances from coal, biomass). For coal, the chemical and physical analysis is usually well known and therefore it is possible to consider the solid particles and volatile components separately and apply the known theory to them. However, it is not possible to monitor the gradual release of volatile components from the particles, and therefore due to the miniature size of the particles, it is assumed that the particles move together with the gas, and that complete devolatilization has already taken place before entering the combustion chamber. This is at least partly true, as the primary air is preheated.

A simple model [BSM+13a] for the burnout rate of both solid particles and volatile substances depending on their current concentration, or in terms of the mass of one particle, has the form

$$\frac{\mathrm{d}m_{\text{vol}}}{\mathrm{d}t} = -A_{\text{vol}} m_{\text{vol}}^{\alpha_{\text{vol}}} Y_{\text{O}_2}^{\beta_{\text{vol}}} \mathrm{e}^{-E_{\text{vol}}/(RT)}, \tag{7.16}$$

$$\frac{\mathrm{d}m_{\text{char}}}{\mathrm{d}t} = -A_{\text{char}} m_{\text{char}}^{\alpha_{\text{char}}} Y_{\text{O}_2}^{\beta_{\text{char}}} \mathrm{e}^{-E_{\text{char}}/(RT)}. \tag{7.17}$$

The so-called burnout curves for m_{char} depending on the temperature are shown in Figure 7.7.

The calorific value of the individual components is then given by the equation

$$h_{\text{char}} + h_{\text{vol}} = \text{LHV}_{\text{coal}},$$

where h_{char} is given by the reaction energy

$$\text{C} + \text{O}_2 \rightarrow \text{CO}_2$$

and LHV_{coal} is measured for a specific type of coal.

In the case of biomass, we use experimental data (such as [**?**, **?**] for spherical pinewood particles of initial radius 1 mm) on the weight loss of a biomass particle as a function of time. Again, we need to get the dependency in the form

$$\frac{\mathrm{d}m}{\mathrm{d}t} = f(m). \tag{7.18}$$

We proceed according to the following procedure:

1. Burnout curves are usually presented as the relative weight loss

$$m_{\mathrm{rel}}(t) = \frac{m(t)}{m(0)} \tag{7.19}$$

for a given initial particle mass $m(0)$. We fit the measured dependence with a smooth polynomial curve.

2. We approximate the derivative numerically

$$g(t) := \frac{\mathrm{d}m_{\mathrm{rel}}}{\mathrm{d}t}. \tag{7.20}$$

3. From the essence of the described phenomenon, the function $m_{\mathrm{rel}} = m_{\mathrm{rel}}(t)$ is sharply decreasing, and therefore it is possible to find (or numerically approximate) the inverse function $t = t(m_{\mathrm{rel}})$. Substituting into (7.20), we get

$$\frac{\mathrm{d}m_{\mathrm{rel}}}{\mathrm{d}t} = g(t(m_{\mathrm{rel}})) =: h(m_{\mathrm{rel}}).$$

4. Finally, we return to absolute weights. According to (7.19),

$$\frac{\mathrm{d}m}{\mathrm{d}t} = m(0)\frac{\mathrm{d}m_{\mathrm{rel}}}{\mathrm{d}t} = m(0)\,h\left(\frac{m}{m(0)}\right) =: f(m). \tag{7.21}$$

Values of f for $m \in [0, m(0)]$ can be sampled into a searchable table during the simulation. The whole process is shown in Figure 7.8 . The burnout curve here has two „stairs“, which correspond to the rapid release and combustion of volatile components and the slower burnout of the fixed carbon. There is therefore no need to model the burnout of both components of the fuel separately.

The following must also be resolved:

1. What happens if $m > m(0)$. It is easiest to put $m = m(0)$.

2. The dependence on temperature and oxygen concentration must be modeled. For example, we can use the model

$$\frac{\mathrm{d}m}{\mathrm{d}t} = f(m)\,F\left(T, Y_{\mathrm{O}_2}\right), \tag{7.22}$$

where

$$F\left(T, Y_{\mathrm{O}_2}\right) = \frac{Y_{\mathrm{O}_2}^{\beta}\,\mathrm{e}^{-E/(RT)}}{Y_{\mathrm{O}_2,0}^{\beta}\,\mathrm{e}^{-E/(RT_0)}}.$$

Constants β and E can be fitted from the knowledge of burning curves at different temperatures or concentrations. The resulting shape of the burning curve depending on the temperature can be like in Figure 7.9 .

Since the devolatilization of biomass is not modeled within the process of its combustion, we have only

$$h_{\mathrm{bms}} = \mathrm{LHV}_{\mathrm{bms}}.$$

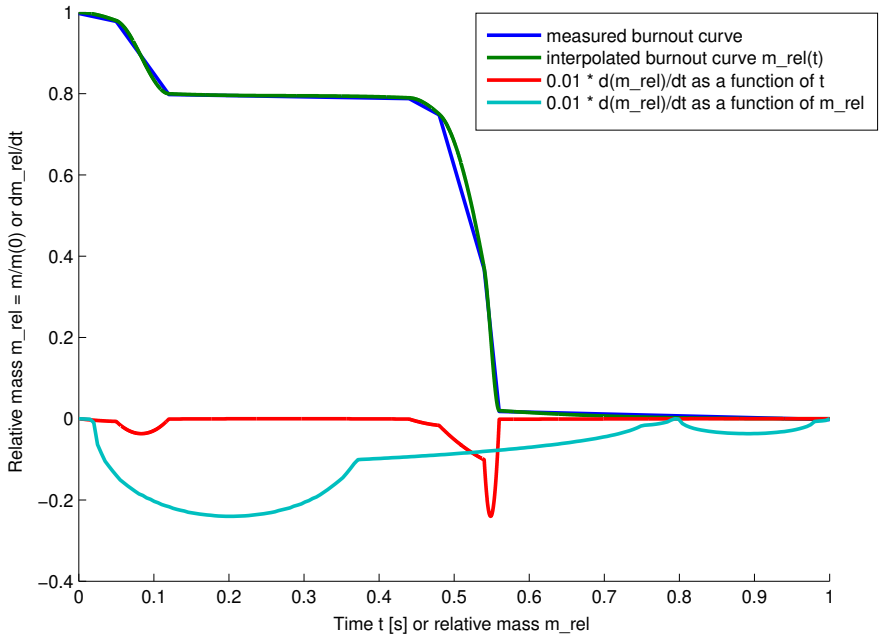

Figure 7.8: Construction of the function f given by the relation (7.21) from the measured burnout curve.

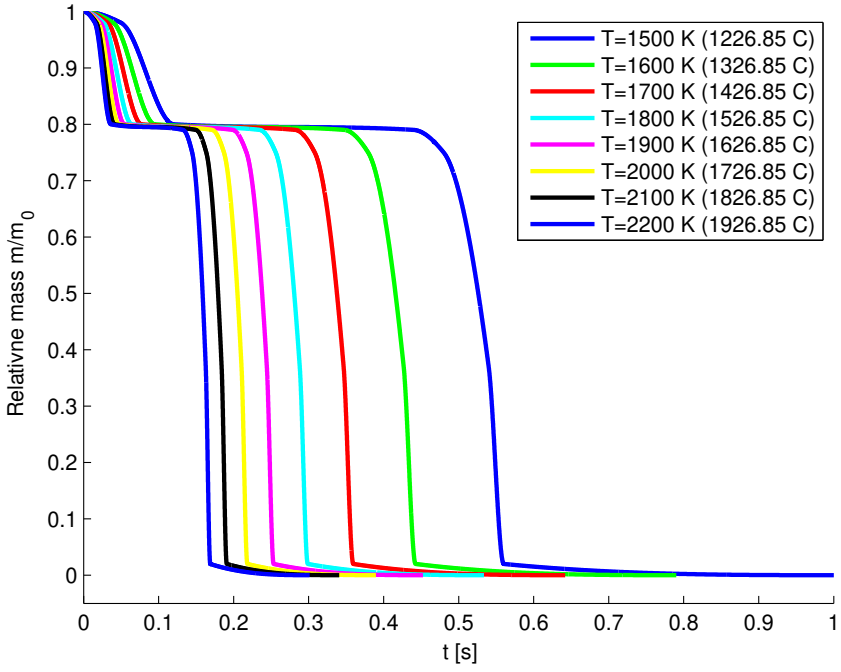

Figure 7.9: Dependence of the shape of biomass burning curves on temperature.

7.5.5 Remaining constants and expressions

This section summarizes the definitions of the remaining constants and expressions:

$$R^{\text{char}}_{\text{coal}} = R_{\text{char}},\ R^{\text{vol}}_{\text{coal}} = R_{\text{vol}},\ R^{\text{char}}_{\text{bms}} = (1-\text{vol}_{\text{bms}})\,R_{\text{bms}}, R^{\text{vol}}_{\text{bms}} = \text{vol}_{\text{bms}} R_{\text{bms}},$$

$$\begin{aligned} a_g &= \varepsilon_g(Y_{H_2O}, Y_{CO_2}, T_{\text{wall}}) \\ &= 1-\exp(-\sqrt{0.1(p_{H_2O}+p_{CO_2})}L(8+160\,p_{H_2O})(1-3.8\cdot 10^{-4}\,T_{\text{wall}})) \end{aligned}$$

$$p_{H_2O} = p\cdot[H_2O]\cdot 10^{-6}, \qquad p_{CO_2} = p\cdot[CO_2]\cdot 10^{-6}, \qquad L = 3.5\frac{V_{\text{furnace}}}{S_{\text{furnace}}},$$

$$\text{Sc}_t = 0.7, \qquad \text{Pr}_t = 0.85, \qquad \gamma = 1.4, \qquad \sigma_k = 1.0, \qquad \sigma_\varepsilon = 1.3, \qquad \sigma_s = 1.5,$$

$$\boldsymbol{g} = (0,-9.81,0), \qquad C_{1\varepsilon} = 1.44, \qquad C_{2\varepsilon} = 1.92, \qquad C_\mu = 0.09, \qquad \sigma = 5.67\cdot 10^{-8},$$

$$A_{\text{BET}} = 25000, \qquad p_{NO} = p\cdot[NO]\cdot 10^{-6}, \qquad c_s = c_s(n), \qquad X^a_{O_2} = X^a_{O_2}([O_2])$$

$$n_r = 1.7, \qquad \alpha = 0.5 \qquad \beta = 0.5 \qquad \delta_1 = 0.5 \qquad \delta_2 = \delta_3 = 0.25$$

7.5.6 Boundary conditions

The boundary conditions are defined as follows:

7.5.6.1 Boundary conditions on the walls

- **no-slip** boundary condition

$$V_1 = V_2 = 0,$$

- zero Neumann boundary condition for extrapolation of scalar quantities

$$\frac{\partial}{\partial \boldsymbol{n}}\varrho = \frac{\partial}{\partial \boldsymbol{n}}\varrho Y_* = \frac{\partial}{\partial \boldsymbol{n}}\varrho_{\text{char}} = \frac{\partial}{\partial \boldsymbol{n}}\varrho_{\text{vol}} = \frac{\partial}{\partial \boldsymbol{n}} n = 0,$$

- boundary condition for turbulent kinetic energy and its dissipation

$$\frac{\partial}{\partial \boldsymbol{n}}(\varrho k) = 0,$$

$$\varepsilon = 2\nu\left(\frac{\partial\sqrt{k}}{\partial \boldsymbol{n}}\right)^2,$$

- convective heat transfer to the walls assuming a constant wall temperature

$$\lambda\frac{\partial}{\partial \boldsymbol{n}}(\varrho T) = A_{\text{conv}}\cdot(T - T_{\text{wall}}). \tag{7.23}$$

7.5.6.2 Boundary conditions on burners

Setting the boundary conditions on the burners is as follows:

- burners:
  - fuel mass flow, mixture temperature
  - one of the following:
    - primary air velocity and excess air coefficient (excess air coefficient)
    - fresh air flow,
- boundary conditions for the $k-\varepsilon$ turbulence model

$$\varrho k = \rho_{\text{in}} \frac{3}{2} (|\boldsymbol{V}_{\text{in}}| I_{\text{in}})^2, \quad \rho\varepsilon = \rho_{\text{in}} \frac{C_\mu^{\frac{3}{4}} k^{\frac{3}{2}}}{0.007 D_h}$$

  where I_{in} represents the intensity of turbulent kinetic energy

$$I_{\text{in}} = 0.16 \left(\frac{\rho_{\text{in}} |\boldsymbol{V}_{\text{in}}| D_h}{\mu} \right)^{-\frac{1}{8}}.$$

- Secondary air and OFA nozzles are implemented as burners with zero fuel flow.

7.5.6.3 Recirculation of flue gases

In the fuel preparation system, the so-called *primary* mixture consists of

- recirculated flue gases that heat up the ground pulverized fuel,
- clean air, added to reduce the temperature of the mixture below the flash point of the fuel.

The resulting mixture is known to contain approx 10% of oxygen. This criterion is used to calculate the ratio of clean air to recirculated flue gas in the burners. The chemical composition of the recirculated gas does not correspond to the current values at the outflow from the combustion chamber, because this would require modeling the recirculation pipeline as well, or implement some non-local information transfer. Instead, this composition is prescribed as fixed based on previous simulations.

7.5.6.4 Boundary conditions at the outflow

The flue gas removal is *forced,* i.e., there is a fan at the outflow that drives the flue gases. This is because the pressure in the combustion chamber must be slightly below the atmospheric pressure. Otherwise, flue gases would escape through all leaks in the system. The boundary condition takes this into account by prescribing a fixed pressure value, which is related to the fan power.

7.5.7 Initial conditions

The initial conditions assume that there is clean air in the combustion chamber preheated to a temperature sufficient to ignite the fuel. The specific settings are as follows:

$$\begin{aligned}
\varrho &= \varrho_{\text{ini}} = 360.77819 \cdot T_{\text{ini}}^{-1.00336}, \\
\varrho Y_* &= \varrho_{\text{ini}} Y_{*,\text{ini}}, \\
\varrho_{\text{char}} &= 0, \quad \varrho_{\text{vol}} = 0, \quad n = 0, \\
\varrho V_1 &= \varrho_{\text{ini}} V_{1,\text{ini}}, \\
\varrho V_2 &= \varrho_{\text{ini}} V_{2,\text{ini}}, \\
\varrho T &= \varrho_{\text{ini}} T_{\text{ini}}, \\
\varrho k &= \varrho_{\text{ini}} \cdot 1.5 \left(I_{\text{ini}} \sqrt{V_{1,\text{ini}}^2 + V_{2,\text{ini}}^2} \right)^2, \\
\varrho \varepsilon &= \varrho_{\text{ini}} C_\mu^{0.75} \frac{k_{\text{ini}}^{1.5}}{0.07 D_h}.
\end{aligned}$$

Remark. During actual operation, each downtime is expensive and all efforts lead to operating the equipment without interruption for as long as possible. After shutdown, gas burners ensure preheating of the combustion chamber. However, after the start itself, the temperature in the combustion chamber stabilizes for several hours. Because we are only modeling the combustion chamber itself and prescribing the temperature of the wall as constant (and corresponding to the steady state), the time until steady state is reached takes only a few seconds of physical time.

7.5.8 Heat transfer modeling

The balance of heat production and consumption must be modeled particularly carefully because the rate of all chemical reactions, and thus the composition, fundamentally depends on the flue gas temperature, pollutant production, heat transfer efficiency, etc. The following approaches are included in the model:

- Heat conduction is given by standard Fourier's law (3.48), i.e. $q_c = -\nabla \cdot (\lambda \nabla T)$.
- *Convective* heat transfer on the walls is calculated algorithmically. Coefficient A_{conv} (7.23) is a function of
  - flue gas temperature T,
  - Reynolds numbers $\text{Re} = L \frac{\|V\| \varrho}{\mu}$, where L is the characteristic dimension (wall thickness),
  - thermal conductivity of the gas λ,
  - specific heat capacity of the gas c_P,
  - thermal conductivity of steel (wall material) $\lambda_{\text{wall}} = 44\ \text{J} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$ at temperature 300 °C,
  - specific heat capacities of steel $c_{P,\text{wall}} = 460\ \text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$.
- *Radiative* heat transfer $q_{rg} + q_{rw}$ in (7.6) consists of two parts. Radiation of type *gas-gas* is given by the Rosseland model
$$q_{rg} = -\nabla \cdot \left(16 \sigma \Gamma n_r^2 T^3 \nabla T \right)$$
where $n_r = 1.7$ is the index of refraction of flue gases (optically dense medium) and
$$\Gamma = \frac{1}{3\,(1.5 + \varepsilon\,(T))}.$$

Radiation of type *gas–wall* is given by the correlation

$$q_{rw} = \xi\sigma \cdot (\varepsilon(T)\, T^4 - \varepsilon(T_{\text{wall}})\, T_{\text{wall}}^4).$$

where $\xi = (1+0.9)\cdot 0.5$ is the correction parameter and the emissivity (and absorptivity) ε of the flue gas is evaluated based on the emissivity of its components H_2O and CO_2, with a possible incorporation of the emissivity of *ash* and *flames*. ε further depends on the mean beam length

$$L = 3.5\frac{V}{\zeta A}$$

where V is the volume of the combustion chamber and A is the total surface area of the walls. As the walls are wavy because of the pipes that run behind them, the formula is supplemented with a ripple factor ζ, which represents an increase in the real surface area of the walls.

- Important properties of materials (heat capacity, thermal conductivity, viscosity etc.) are temperature dependent. Correlations expressing the dependence of these quantities on temperature are usually available for the individual chemical components of the flue gas. The theoretical value for the mixture is then calculated from them according to the proportional representation of individual components.

7.6 Multiphase flow, fluidization

In this chapter, we formulate an Eulerian model for two-phase air flow and bulk solid material. In a chamber, into which air is blown from below at a sufficient velocity through a so-called *distributor* , solid particles rise and the resulting mixture behaves like a fluid, called a *fluidized bed*. The mass fraction of solid particles per unit volume is considered a continuous quantity, and therefore conservation laws can be formulated for their movement, analogous to the Navier-Stokes equations.

Fluidization is used for pneumatic transport of granular materials or in fluidized bed boilers [Bas06]. Depending on the air flow in them, they can be divided to

- bubbling fluidized bed, where solid particles only rise to a certain height in the combustion chamber and fall back again,
- circulating fluidized bed where the buoyancy is sufficient to allow the particles to leave the combustion chamber and return through the particle separator (cyclone).

Pneumatic transport occurs when the gas flow is further increased. In general, the fluidizing medium can be either a gas or a liquid.

Let $\Omega \subset \mathbb{R}^d$ where $d \in \{2,3\}$ be the domain representing the *fluidization chamber* and $\mathcal{J} = (0, t_{\max})$ be the time interval. For both phases (lower index g denotes gas and s denotes the solid phase), we consider the Navier-Stokes equations in the form

$$\frac{\partial}{\partial t}\begin{pmatrix} \varrho_g\varepsilon_g \\ \varrho_g\varepsilon_g \boldsymbol{V}_g \\ \varrho_s\varepsilon_s \\ \varrho_s\varepsilon_s \boldsymbol{V}_s \end{pmatrix} + \begin{pmatrix} \nabla\cdot(\varrho_g\varepsilon_g \boldsymbol{V}_g) \\ \nabla\cdot(\varrho_g\varepsilon_g \boldsymbol{V}_g \otimes \boldsymbol{V}_g) \\ \nabla\cdot(\varrho_s\varepsilon_s \boldsymbol{V}_s) \\ \nabla\cdot(\varrho_s\varepsilon_s \boldsymbol{V}_s \otimes \boldsymbol{V}_s) \end{pmatrix} = \begin{pmatrix} 0 \\ -\varepsilon_g\nabla P_g + \nabla\cdot(\varepsilon_g \mathbb{T}_g) \\ 0 \\ -G(\varepsilon_g)\nabla\varepsilon_s - \varepsilon_s\nabla P_g + \nabla\cdot(\varepsilon_s\mathbb{T}_s) \end{pmatrix} + \begin{pmatrix} 0 \\ \varrho_g\boldsymbol{g} + \beta_{gs}(\boldsymbol{V}_s - \boldsymbol{V}_g) \\ 0 \\ (\varrho_s - \varrho_g)\boldsymbol{g} + \beta_{gs}(\boldsymbol{V}_g - \boldsymbol{V}_s) \end{pmatrix}, \tag{7.24}$$

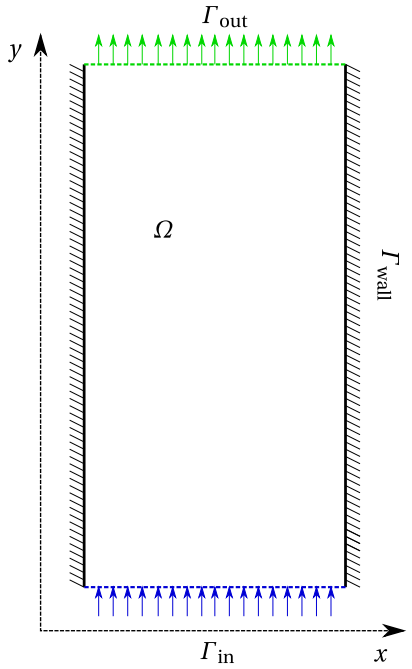

Figure 7.10: Simple example of the problem setup

Greatness	Unit	Range of values	Description
P_g	Bye	$\mathbb{R}$	gas phase pressure
T	TO	$\mathbb{R}^+$	temperature (constant)
ϱ_g	$\mathrm{kg}\cdot\mathrm{m}^{-3}$	$\mathbb{R}^+$	gas phase density
$\boldsymbol{V}_g$	$\mathrm{m}\cdot\mathrm{s}^{-1}$	$\mathbb{R}^d$	gas phase velocity
ε_g	-	$[0,1]$	volume fraction of the gas phase
ϱ_s	$\mathrm{kg}\cdot\mathrm{m}^{-3}$	$\mathbb{R}^+$	solid phase density (constant)
$\boldsymbol{V}_s$	$\mathrm{m}\cdot\mathrm{s}^{-1}$	$\mathbb{R}^d$	solid phase velocity
ε_s	-	$[0,1]$	solid phase volume fraction

Table 7.1: List of quantities describing two-phase flow during fluidization.

in $\mathscr{J} \times \Omega$, where individual unknown quantities are summarized in Table 7.1 . The term $G(\varepsilon_g)\nabla\varepsilon_s$ plays a role analogous to the theoretical pressure gradient of the solid phase ∇P_s and prevents excessive clumping of solid particles. Every granular material contains a significant proportion of free space (*voidage, void fraction*) $\varepsilon_{g,\min}$ between particles even when at rest. The corresponding maximum volume fraction of the solid phase (*packing limit*) is given by

$$\varepsilon_{s,\max} = 1 - \varepsilon_{g,\min}.$$

Function G is called *compressibility modulus* and according to [Gid94], it has an empirically determined form

$$G(\varepsilon_g) = 10^{-8.76\varepsilon_g + 5.43}. \tag{7.25}$$

Coefficient β_{gs} represents the transfer of momentum between the two phases, the so-called *drag*. The form of β_{gs} used in (7.24) is again according to [Gid94] given by

$$\beta_{gs} = \begin{cases} 150\frac{\varepsilon_s^2\mu_g}{(\varepsilon_g d_s\Phi_s)^2} + 1.75\frac{|V_g - V_s|\varrho_g\varepsilon_s}{\varepsilon_g d_s\Phi_s} & \varepsilon_s > 0.2, \\ \frac{4}{3}C_d\frac{|V_g - V_s|\varrho_g\varepsilon_s}{d_s\Phi_s} & \varepsilon_s \le 0.2, \end{cases} \tag{7.26}$$

$$C_d = \begin{cases} \frac{24}{Re_s}\left(1 + 0.15Re_s^{0.687}\right) & \mathrm{Re}_s \le 1000, \\ 0.44 & \mathrm{Re}_s > 1000, \end{cases} \tag{7.27}$$

$$\mathrm{Re}_s = \frac{\left|\boldsymbol{V}_g - \boldsymbol{V}_s\right| d_s\varrho_g\varepsilon_g}{\mu_g}. \tag{7.28}$$

The symbol $\boldsymbol{g}$ denotes the gravitational acceleration, d_s is the particle diameter and ϕ_s their sphericity.

Relationship

$$\varepsilon_g + \varepsilon_s = 1, \tag{7.29}$$

and ideal gas equation of state

$$P = \varrho R_{\mathrm{spec}} T. \tag{6.5}$$

close the system. The temperature T is considered constant and equal for both phases.

7.6.1 Initial conditions

The initial conditions are given as

$$\begin{aligned} P_g(0,\boldsymbol{x}) &= P_{g,\mathrm{ini}}(\boldsymbol{x}), \\ \boldsymbol{V}_g(0,\boldsymbol{x}) &= \boldsymbol{V}_{g,\mathrm{ini}}(\boldsymbol{x}), \\ \varepsilon_s(0,\boldsymbol{x}) &= \varepsilon_{s,\mathrm{ini}}(\boldsymbol{x}), \\ \boldsymbol{V}_s(0,\boldsymbol{x}) &= \boldsymbol{V}_{s,\mathrm{ini}}(\boldsymbol{x}), \end{aligned} \tag{7.30}$$

from which other quantities such as

$$\begin{aligned} \varrho_g(0,\boldsymbol{x}) &= \frac{P_{g,\mathrm{ini}}(\boldsymbol{x})}{R_{\mathrm{spec}}T}, \\ \varepsilon_g(0,\boldsymbol{x}) &= 1 - \varepsilon_{s,\mathrm{ini}}(\boldsymbol{x}) \end{aligned} \tag{7.31}$$

are calculated.

7.6.2 Boundary conditions

We consider three types of boundary conditions on the boundary divided to the inflow Γ_{in}, the outflow Γ_{out} and the wall Γ_{wall}, where $\partial\Omega = \Gamma_{\text{in}} \cup \Gamma_{\text{out}} \cup \Gamma_{\text{wall}}$.

- On the wall (for $\boldsymbol{x} \in \Gamma_{\text{wall}}$), we consider no-slip boundary conditions for both speeds, i.e.

$$\boldsymbol{V}_s(t,\boldsymbol{x}) = \boldsymbol{V}_g(t,\boldsymbol{x}) \quad = \quad 0 \quad \forall t \in \mathscr{J}, \tag{7.32}$$

  and zero Neumann boundary conditions for ϱ_g and ε_s, i.e.

$$\frac{\partial \varrho_g(t,\boldsymbol{x})}{\partial \boldsymbol{n}} = \frac{\partial \varepsilon_s(t,\boldsymbol{x})}{\partial \boldsymbol{n}} = 0 \quad \forall t \in \mathscr{J}, \tag{7.33}$$

  where $\boldsymbol{n}$ is the outer normal vector to $\partial\Omega$.

- At the inflow (for $\boldsymbol{x} \in \Gamma_{\text{in}}$), the velocity of both phases and the volume fraction of the solid phase are prescribed by

$$\boldsymbol{V}_g(t,\boldsymbol{x}) \quad = \quad \boldsymbol{V}_{g,\text{in}}(t,\boldsymbol{x}), \tag{7.34}$$
$$\boldsymbol{V}_s(t,\boldsymbol{x}) \quad = \quad \boldsymbol{V}_{s,\text{in}}(t,\boldsymbol{x}), \tag{7.35}$$
$$\varepsilon_s(t,\boldsymbol{x}) \quad = \quad \varepsilon_{s,\text{in}}(t,\boldsymbol{x}). \tag{7.36}$$

  Furthermore, zero Neumann condition for the gas density

$$\frac{\partial \varrho_g(t,\boldsymbol{x})}{\partial \boldsymbol{n}} = 0 \tag{7.37}$$

  is considered

- At the outflow (for $\boldsymbol{x} \in \Gamma_{\text{out}}$), gas pressure is prescribed by

$$P_g(t,\boldsymbol{x}) \quad = \quad P_{g,\text{out}}(t,\boldsymbol{x}). \tag{7.38}$$

  For other quantities, zero Neumann condition applys, i.e.,

$$\frac{\partial \boldsymbol{V}_g(t,\boldsymbol{x})}{\partial \boldsymbol{n}} = \frac{\partial \boldsymbol{V}_s(t,\boldsymbol{x})}{\partial \boldsymbol{n}} = \boldsymbol{0}, \tag{7.39}$$
$$\frac{\partial \varepsilon_s(t,\boldsymbol{x})}{\partial \boldsymbol{n}} = 0. \tag{7.40}$$

7.7 Flow with a free boundary, phase transitions

- flow with a free boundary
  - *volume of fluid* method
- phase transitions, Stefan problem
- phase-field formulation
- phase transitions with flow
- *fluid-structure interaction*

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