

A BRIEF INTRODUCTION INTO HYDRODYNAMICS

Variational point of view

DENYS DUTYKH
CNRS INSMI – LAMA UMR 5127
Université Savoie Mont Blanc



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To my parents.

ABSTRACT

In this manuscript we present some basic notions of Hydrodynamics in view of free surface flows modeling. The text is composed of 11 Chapters. We start the exposition with the brief description of classical Lagrangian and Hamiltonian mechanics. Then, we move to the continuous case where we present the governing equations of the incompressible fluid mechanics in the Eulerian description. The variational structure is highlighted for irrotational flows. Finally, we present the Lagrangian (fluid particle) description of incompressible flows along with some exact solutions. Throughout this manuscript we make a particular emphasis on the variational structures arising in classical and fluid mechanics. Finally, this manuscript contains an Appendix containing a brief description of the main mathematical tools needed in the main part of the text.

ACKNOWLEDGMENTS

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The hospitality of the Johannes Kepler Universität Linz (Austria) and of the Basque Center for Applied Mathematics (BCAM) is also acknowledged, where some parts of this manuscript were prepared. Of course, the main part of this work was done at my home laboratory — LAMA UMR #5127 at the University of Savoie Mont Blanc, France. The constant support of my friends and colleagues Dr. Marx CHHAY, Dr. Marguerite GISCLON, Dr. Michel RAIBAUT and many others is also greatly acknowledged. I would like to thank also my collaborators, especially Prof. Didier CLAMOND (University of Nice Sophia Antipolis, France), Prof. Dimitrios MITSOTAKIS (Victoria University of Wellington, New Zealand) and Dr. Ashkan RAFIEE (Carnegie Wave Energy, Australia), from whom I learnt a lot.

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PREFACE

In order to unveil the general philosophy of the book, the Author would like to quote some passages from the appendix “*Mathematical formalities and style*” to the book by E. JAYNES [Jay03], published posthumously as “*Probability Theory: The Logic of Science*”:

[...] Obviously, mathematical results cannot be communicated without some decent standards of precision in our statements. But a fanatical insistence on one particular form of precision and generality can be carried so far that it defeats its own purpose; XXth century mathematics often degenerates into an idle adversary game instead of a communication process.

The fanatic is not trying to understand your substantive message at all, but only trying to find fault with your style of presentation. He will strive to read nonsense into what you are saying, if he can possibly find any way of doing so. In self-defense, writers are obliged to concentrate their attention on every tiny, irrelevant, nit-picking detail of how things are said rather than on what is said. The length grows; the content shrinks.

Mathematical communication would be much more efficient and pleasant if we adopted a different attitude. For one who makes the courteous interpretation of what others write, the fact that x is introduced as a variable already implies that there is some set X of possible values. Why should it be necessary to repeat that incantation every time a variable is introduced, thus using up two symbols where one would do? (Indeed, the range of values is usually indicated more clearly at the point where it matters, by adding conditions such as $(0 < x < 1)$ after an equation.)

For a courteous reader, the fact that a writer differentiates $f(x)$ twice already implies that he considers it twice differentiable; why should he be required to say everything twice? If he proves proposition A in enough generality to cover his application, why should he be obliged to use additional space for irrelevancies about the most general possible conditions under which A would be true?

A scourge as annoying as the fanatic is his cousin, the compulsive mathematical nitpicker. We expect that an author will define his technical terms, and then use them in a way consistent with his definitions. But if any other author has ever used the term with a slightly different shade of meaning, the nitpicker will be right there accusing you of inconsistent terminology. The writer has been subjected to this many times; and colleagues report the same experience.

Nineteenth century mathematicians were not being non rigorous by their style; they merely, as a matter of course, extended simple civilized courtesy to others, and expected to receive it in return. This will lead one to try to read sense into what others write, if it can possibly be done in view of the whole context; not to pervert our reading of every mathematical work into a witch-hunt for deviations from the Official Style. [...]

The Author of this manuscript subscribes to every single word of this quotation.

INTRODUCTION

Physics is, hopefully, simple. Physicists are not.

— Edward Teller

Mechanics as a science was established mainly during the XVIIth century. COPERNICUS introduced the reference system in 1543 and Galileo GALILEI stated the principle of inertia in 1638 in his *“Discorsi e dimostrazioni mathematiche, intorno a due nove scienze alla meccanica ed i movimenti locali”*. This period was finished in 1687 when Isaac NEWTON published his book *“Philosophiæ Naturalis Principia Mathematica”*.

The beginning of the variational era is due to Pierre DE FERMAT, a judge in Toulouse, who proposed the principle least time in geometrical optics. It is interesting to note that Fermat is particularly known for his works in Mathematics. This discovery resulted from the criticism about René DESCARTES's chapter *“Dioptrique”*, a part of his celebrated *“Discours de la Méthode”*. During this quarrel Fermat criticized in 1637 the lack of rigor in Descartes's *“pseudo proof”*. To resolve this controversy, Fermat in 1661 formulated his principle of *least time*. In his original work it was named the *principle of natural economy*.

The principle of *least action* in mechanics was stated for the first time by Pierre-Louis Moreau DE MAUPERTUIS in 1744, who was a popularizer of Newton's ideas in France. He understood that Newton's equations are equivalent to the minimality conditions of a quantity that he called the *action*. However, the mathematical proof of Maupertuis's principle was given later by Leonhard EULER in his treatise *“Methodus inveniendi lineas curvas maximi minimive proprietate gaudens”*. The understanding that the laws of nature can be viewed as optimization principles had a great impact in the XVIIIth century.

The application of variational principles is not restricted exclusively to mechanics and optics. For example, the electric current is distributed in an electrical network such that the energy loss by Joule heating is minimal. Mathematically it is expressed as the celebrated Kirchhoff's laws.

Leonhard EULER, Joseph-Louis LAGRANGE and William R. HAMILTON in their subsequent works set the foundations of modern theoretical physics

For instance, since Galilei we know that a linear uniform motion is a state and not a process!

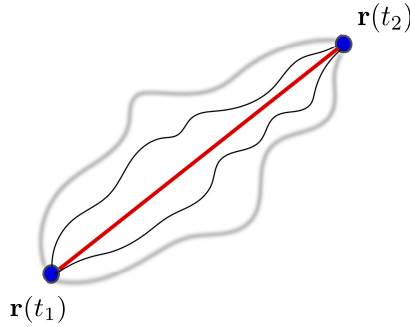


Figure 0.1.: Optimal trajectory (in red) joining two points in space-time $\mathbf{r}(t_1)$ and $\mathbf{r}(t_2)$.

with consequences which can be found today in general relativity, gauge theory of fundamental interactions and many other fields.

The main mathematical tool developed by Euler is the calculus of variations. The major contributions of Lagrange in statics as well as in dynamics were published in 1788 in his *“Mécanique Analytique”*. In this work Lagrange changed the paradigm of considering a mechanical problem. Instead of finding instantaneous values of the position $\mathbf{r}(t)$ and velocity $\mathbf{v}(t)$ of a particle, given its initial state $\{\mathbf{r}(t_0), \mathbf{v}(t_0)\}$, Lagrange proposed to seek the global trajectory of the particle starting at $\{\mathbf{r}(t_1), \mathbf{v}(t_1)\}$ and arriving at $\{\mathbf{r}(t_2), \mathbf{v}(t_2)\}$, in analogy to Fermat’s reasoning in geometric optics.

Hamilton spent all his life in Dublin, Ireland where he served as a Professor of Astronomy and as an Astronomer in Dunsink Observatory. Hamilton noticed the similarity between the Maupertuis’s principle in mechanics and Fermat’s principle in optics. In 1830 he made a profound observation that Newtonian mechanics corresponds to the same limit as the geometrical optics derives from the wave optics. His remark did not attract much attention until 1890 when Felix KLEIN made it widely known. Thus, Hamilton’s mechanics can be considered as a precursor of quantum mechanics.

Variational principles are universal. All physical laws can be recast in the variational form which leads the usual local form (*i.e.* Euler–Lagrange equations). However, the global form is richer and more powerful. In these lecture notes we shall show how these ideas found applications in Hydrodynamics.

These Lecture Notes are based on several sources. The first two Chapters were greatly inspired by the excellent book of J.-L. BASDEVANT [Bas07] and

lectures of John C. BAEZ on Classical Mechanics [BWS05]. A few geometrical remarks were inspired by [Fero6]. The classical book of LANDAU & LIFSHITZ (volume 1) [LL76] is also highly recommended.

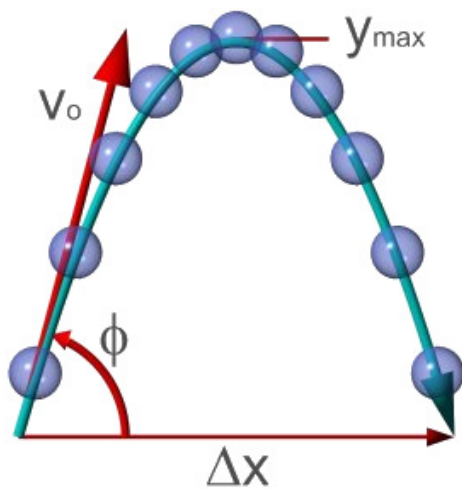
EXERCISES

1. Find in the neighbourhood of Dublin the bridge, under which Sir Hamilton wrote his formulas of quaternions multiplication.

Part I

CLASSICAL MECHANICS

Classical mechanics is a part of classical physics dealing with deterministic systems of point particles or rigid bodies. Sometimes the systems with infinitely many degrees of freedom are also included (e.g. infinite arrays of particles). The equations of motions are expressed as systems of Ordinary Differential Equations (ODEs). Non-dissipative systems may be described geometrically using the formalism of *symplectic manifolds*, or more generally *Poisson manifolds*. Classical mechanics can be conventionally divided into three parts — *statics*, *kinematics* and *dynamics*. Statics studies the balance of forces in states of equilibria. Kinematics describes the relation between the position, velocity and acceleration, without reference to the causes of motion. Finally, Dynamics studies the forces as causes of motion and as the mean of mechanical interaction between bodies.



1

LAGRANGIAN MECHANICS

In the beginning there was the Action.

— Johann Wolfgang Goethe

Nature always acts by the shortest paths.

— Pierre de Fermat

1.1 LEAST ACTION PRINCIPLE

The variational principle presented below was actually formulated by Hamilton in 1834 and we use, since it is simpler than the original one.

Any conservative mechanical system can be characterized by the Lagrangian density \mathcal{L} . For an idealized system consisting of a single particle the Lagrangian $\mathcal{L} = \mathcal{L}(x, \dot{x}, t)$, where $x(t)$ is the particle's position and $\dot{x}(t) := \frac{dx}{dt}$. The quantities (x, \dot{x}) are the state variables of the particle. For this system the Lagrangian \mathcal{L} takes the form

$$\mathcal{L} := \frac{1}{2} m \dot{x}^2 - V(x, t),$$

where m is the particle's mass, $V(x, t)$ is the potential which determines the forces acting on the particle $f(x, t) := -\frac{\partial V}{\partial x}$.

For an arbitrary trajectory $x(t)$ we can define the *action* \mathcal{L} as the following integral

$$\mathcal{L} := \int_{t_1}^{t_2} \mathcal{L}(x, \dot{x}, t) dt.$$

The *least action principle* states that the trajectory realized in physics will be such that the action \mathcal{L} has an extremum. In other words, the physical trajectories are stationary points of the Lagrangian functional.

The choice of the Lagrangian function is non-unique and it will be discussed below.

1.2 EULER–LAGRANGE EQUATIONS

1.2.1 Beltrami identity

1.3 FORM OF THE LAGRANGIAN

1.3.1 Maupertuis's action

The action \mathcal{A} of Maupertuis is the product of three terms: the mass, the velocity and the distance

$$\mathcal{A} := \int_{x_1}^{x_2} m v \, dl.$$

By assuming that the energy E is the integral of motion.

2

HAMILTONIAN MECHANICS

2.1 A GEOMETRICAL PARENTHESIS

The field of the modern geometry which studies the phase space of Hamiltonian systems is the symplectic geometry [Sou97]. A symplectic manifold \mathcal{M} is a usual manifold equipped with a symplectic (i.e. closed, non-degenerate, 2-form) ω . Darboux's theorem states that in the neighbourhood of any point $x \in \mathcal{M}$ there exist local coordinates (q_i, p_i) such that the symplectic form ω takes the standard form [MS98]. Consequently, all symplectic manifolds, at least locally, have the same structure.

A different interpretation of Hamiltonian equations leads to the so-called Poisson Geometry. In analogy to the symplectic manifolds, a Poisson manifold \mathcal{P} is a manifold equipped with a Poisson bracket $\{\cdot, \cdot\}$ (i.e. a Lie bracket on the algebra of smooth functions $C^\infty(\mathcal{P})$ which satisfies the Leibniz identity). Then, the following result can be proven [Wei83]

Theorem 2.1. *Let $(\mathcal{P}, \{\cdot, \cdot\})$ be a Poisson manifold. For every $x \in \mathcal{P}$ there exist coordinates $(q_1, \dots, q_n, p_1, \dots, p_n, y_1, \dots, y_l)$ centered at x such that*

$$\{F, G\} = \sum_{i=1}^n \left(\frac{\partial F}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial G}{\partial q_i} \right) + \sum_{j,k=1}^l \pi_{jk}(y) \frac{\partial F}{\partial y_j} \frac{\partial G}{\partial y_k},$$

where $\pi_{jk}(y) = -\pi_{kj}(y)$ are certain functions of the (y_1, \dots, y_l) alone which vanish at 0.

Therefore, contrary to the symplectic geometry, in Poisson geometry it is important to understand the local structure as well.

Contrary to one's intuition, the letter \mathcal{H} in the Hamiltonian functional comes from the name of a Dutch mathematician Christiaan HUYGENS (1629 – 1695).

Part II

CONTINUUM MECHANICS: EULERIAN DESCRIPTION

Continuum mechanics is a branch of classical physics which studies the mechanical properties of continuous media such as fluids or deformable solid bodies. Continuum mechanics is related to the mechanics of point particles by various limiting processes. Equations of motions are expressed as systems of Partial Differential Equations (PDEs) describing the classical fields such as the velocities, displacements, deformations, strains, *etc.*



A vortex created by this agricultural plane' wing. © Wikimedia Commons.

3

FLUID DYNAMICS EQUATIONS

*We absolutely must leave room for doubt or there is no progress and no learning.
There is no learning without posing a question. And a question requires
doubt. . . Now the freedom of doubt, which is absolutely essential for the
development of science, was born from a struggle with constituted authorities.*

— Richard Feynmann (1964)

In this book we consider the Fluid Mechanics only. For the introduction into the Solid Mechanics theory the reader will have to consult the more specific literature, e.g. [LL86, MH94].

Fluid dynamics is a branch of continuum mechanics which studies the motion of liquids and gases (or fluids in general). A fluid is in general a material which deforms constantly even when it is released from any action of the force. In contrast, an elastic solid recovers to its original state, once it is released from the force, while the fluid will keep deforming. Common examples of fluids include water and air.

The ultimate goal of this discipline is to study and predict the fluid motion or at least some of its main characteristics (for turbulent flows, for example). In this Chapter we present an elementary derivation of basic equations of the Fluid Dynamics. The reader can refer to almost any classical book on this topic if more details are needed. We can recommend the book of A. CHORIN & J. MARSDEN [CM93] for its conciseness and mathematical clarity. The exposition below will follow the great lines of this reference.

3.1 DERIVATION OF THE GOVERNING EQUATIONS

For the sake of clarity all the derivations given below will be performed in Cartesian coordinates. A special care has to be used in other (curvilinear) coordinate systems. We would like to mention that it is possible to develop intrinsic coordinate free formulas valid in any system of coordinates. We refer to [AMR88] for more information on this approach.

3.1.1 Choice of the coordinate system

Consider the standard Euclidean space with a Cartesian coordinates system $Oxyz$ and let Ω be a domain (bounded or unbounded) in \mathbb{R}^d ($d = 2, 3$) filled with a fluid. Let $\mathbf{x} = (x, y, z) \in \Omega$ be a point of the fluid domain. We assume that a *continuum assumption* holds. This means that physical properties such as the density $\rho(\mathbf{x}, t)$, velocity $\mathbf{u}(\mathbf{x}, t)$, pressure $p(\mathbf{x}, t)$, etc. can be well-defined in every geometrical point $\mathbf{x} \in \Omega$. For most macroscopic phenomena this physical assumption is very accurate.

Let $\rho(\mathbf{x}, t)$ and $\mathbf{u}(\mathbf{x}, t)$ denote respectively the density and velocity fields in the fluid at the time instance $t \in \mathbb{R}^+$. From the physical sense the density function $\rho(\mathbf{x}, t) > 0, \forall t \geq 0$ has to be positive in the fluid domain. For each fixed time $t \geq 0$ the velocity $\mathbf{u}(\mathbf{x}, t)$ defines a vector field on Ω . Below we shall assume that the functions $\rho(\mathbf{x}, t)$ and $\mathbf{u}(\mathbf{x}, t)$ are smooth enough in order to perform the standard calculus operations (e.g. integration, differentiation, etc.) on them.

The derivation of Fluid Mechanics equations is based on three basic principles:

- Mass is neither created nor destroyed
- The rate of change of momentum of the fluid parcel equals the sum of all forces applied to it
- Energy is neither created nor destroyed

3.1.2 Mass conservation

Let us take a (bounded) elementary volume $V \subseteq \Omega$, which does not change with time (for the illustration see Figure 3.1). The mass $m_V(t)$ of the fluid contained in V is then given by¹

$$m_V(t) = \int_V \rho(\mathbf{x}, t) dV,$$

where dV is a volume element. The rate of change (in time) of the fluid mass contained in a region V is given by the time derivative

$$\frac{d m_V}{dt} = \frac{d}{dt} \int_V \rho(\mathbf{x}, t) dV = \int_V \frac{\partial \rho(\mathbf{x}, t)}{\partial t} dV,$$

where the time derivative could be put under the integral sign since the integration domain is time-independent. The change of mass inside V can be possible only due to the fluid transport through the boundary ∂V by the velocity field $\mathbf{u}(\mathbf{x}, t)$ (see Figure 3.2 for the illustration). Since the

For instance, this assumption is not verified for the rarefied gases in the stratosphere, where the Boltzmann mesoscopic description is more appropriate.

The mass conservation principle was formulated for the first time independently by M. LOMONOSOV (1748) in Russia and thirty years later by A. LAVOISIER (1774) in France.

¹ Normally one has to write triple \iiint and double \iint integrals in this Section. However, we do not do it for the sake of brevity. It will become clear from the context and from the differentials dV and $d\sigma$ which integral is being considered.

The rate of volume flow across ∂V per unit area is $\mathbf{u} \cdot \mathbf{n}$, while the mass flow rate per unit area is $\rho \mathbf{u} \cdot \mathbf{n}$.

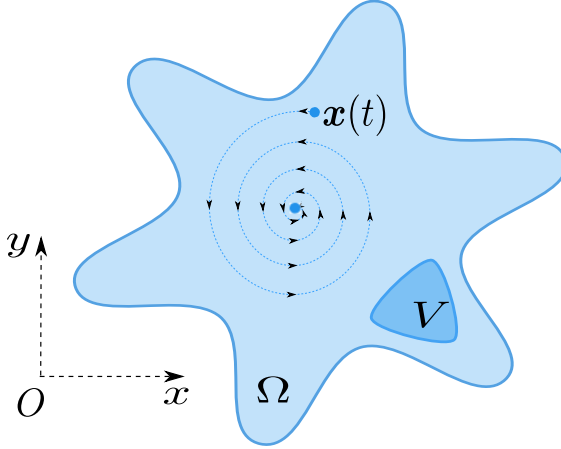


Figure 3.1.: Sketch of the flow domain Ω along with a possible particle trajectory and a control volume dV .

mass is neither being generated nor destroyed, both rates of change have to be equal

$$\frac{d}{dt} \int_V \rho(\mathbf{x}, t) dV = - \int_{\partial V} \rho \mathbf{u} \cdot \mathbf{n} d\sigma, \quad (3.1)$$

where $d\sigma$ is the element of surface. The sign $-$ comes from the convention that the positive normal \mathbf{n} to ∂V points in the outward direction. Thus, the incoming mass flux is negative. By applying the Gauß–Ostrogradsky theorem (see Section A.3.7.3) to equation (3.1), one obtains

$$\int_V \left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) \right] dV = 0.$$

Since the control volume $V \subseteq \Omega$ is arbitrary, the last integral equation is equivalent to the following differential equation of continuity, which expresses the conservation of mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0. \quad (3.2)$$

Both equations (3.1) and (3.2) express the same physical fact. The former is the integral form, while the latter is the differential one. In cases where one of the functions $\rho(\mathbf{x}, t)$ or $\mathbf{u}(\mathbf{x}, t)$ has discontinuities (*i.e.* shock waves), the integral form (3.1) has to be used.

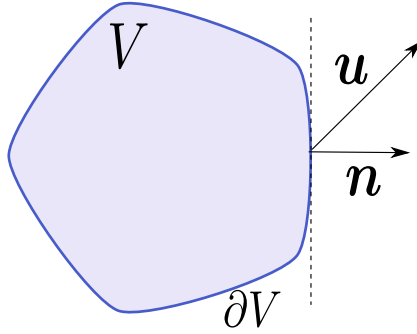


Figure 3.2.: An elementary volume V with an outward normal \mathbf{n} and fluid particle velocity \mathbf{u} at this point on the boundary. The mass flux is positive since $\mathbf{u} \cdot \mathbf{n} > 0$.

3.1.3 Momentum conservation

The balance of momentum states that the amount of momentum contained inside a given volume cannot change unless some forces cause it. In other words, the momentum rate of change inside a volume has to be in equilibrium with the forces applied to it.

Consider a fluid particle trajectory $\mathbf{x}(t) = (x(t), y(t), z(t))$. We shall assume that there exists a so-called *flow map* $\mathbf{a} \mapsto \mathbf{x}(t) = \phi_t(\mathbf{a})$, which gives the particle position at time t provided that initially it was located at $\mathbf{a} = \mathbf{x}(0)$ ². The flow map is intrinsically associated to the vector field (fluid velocity) $\mathbf{u}(\mathbf{x}, t)$ which advects fluid particles. Given a particle label \mathbf{a} the set $\{\phi_t(\mathbf{a}) | t \in \mathbb{R}^+\}$ is called the orbit of \mathbf{a} under the flow ϕ . Physically speaking, an orbit corresponds to a particle trajectory (see Figure 3.3 for an illustration). The flow map is used extensively in the Lagrangian description of fluid flows. See Chapter 7 for more details.

Remark 3.1. The existence and regularity of the flow map can be shown under quite generic assumptions on the flow field $\mathbf{u}(\mathbf{x}, t)$. For example, it is sufficient to assume that \mathbf{u} is Lipschitz continuous in \mathbf{x} and just continuous in t . Then, the application of Picard–Lindelöf–Cauchy–Lipschitz³ theorem to the following system of ODEs

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{u}(\mathbf{x}(t), t), \quad \mathbf{x}(0) = \mathbf{a}, \quad (3.3)$$

The index t in $\phi_t(\mathbf{a})$ should not be confused with a derivative operator in time. Here it means that the flow map depends on time as on the parameter.

In mathematics a flow is a group action of an additive group of real numbers.

² Variable \mathbf{a} is called in general a particle label

³ This theorem is named after Émile Picard (1856 – 1941), Ernst Lindelöf (1870 – 1946), Rudolf Lipschitz (1832 – 1903) and Augustin-Louis Cauchy (1789 – 1857).

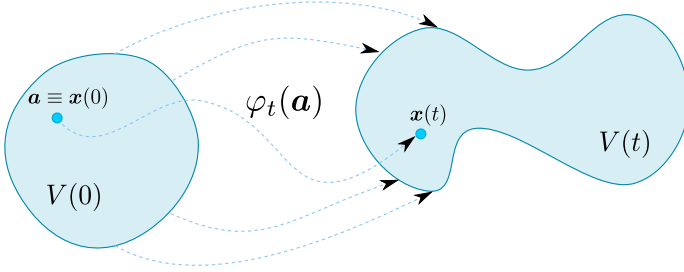


Figure 3.3.: Action of the flow map on an elementary volume $V(0)$.

gives us the existence and uniqueness of the flow map locally in time. A(n) (analytical or more often a numerical) solution to the ODE system (3.3) provides us with a practical way of computing the flow map $\phi_t(\mathbf{a})$.

Remark 3.2 (Semi-group property). The flow map ϕ_t generates the semi-group structure on the fluid domain. Namely, the identity element is given by $\mathbb{I} \equiv \phi_0$, since $\phi_0(\mathbf{a}) = \mathbf{a}$. Then one can show that the composition of flow maps is well defined and $\phi_s(\phi_t(\mathbf{a})) = \phi_{t+s}(\mathbf{a})$. Thus, we have the group operation

$$\phi_t \circ \phi_s = \phi_{t+s}.$$

The associativity follows immediately from the corresponding property of the map composition \circ operation. In some cases the inverse mapping ϕ_{-t} exists as well and we obtain the group structure:

$$\phi_t \circ \phi_{-t} = \mathbb{I}.$$

We can compute a particle velocity and acceleration using the flow map $\phi_t(\mathbf{a})$. For instance, the velocity follows directly from the system (3.3), since

$$\frac{d\phi_t(\mathbf{a})}{dt} \equiv \frac{d\mathbf{x}(t)}{dt} = \mathbf{u}(\mathbf{x}(t), t) \equiv \mathbf{u}(\phi_t(\mathbf{a}), t). \quad (3.4)$$

The acceleration of fluid particles is given by the second derivative of the particle trajectory $\mathbf{x} = \mathbf{x}(t)$. Namely,

$$\begin{aligned} \frac{d^2\mathbf{x}(t)}{dt^2} &= \frac{d}{dt}\mathbf{u}(\phi_t(\mathbf{a}), t) = \partial_t\mathbf{u} + \frac{dx}{dt}\partial_x\mathbf{u} + \frac{dy}{dt}\partial_y\mathbf{u} + \frac{dz}{dt}\partial_z\mathbf{u} = \\ \partial_t\mathbf{u} + \mathbf{u}\partial_x\mathbf{u} + v\partial_y\mathbf{u} + w\partial_z\mathbf{u} &= \partial_t\mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} =: \frac{D\mathbf{u}}{Dt}. \end{aligned}$$

In the last equality we introduced the *material derivative* operator:

$$\frac{D}{Dt} := \frac{\partial}{\partial t} + (\mathbf{u} \cdot \nabla). \quad (3.5)$$

Thus, we just showed that the acceleration of fluid particles is given by

Remark 3.3. We would like to underline that the notation $(\mathbf{u} \cdot \nabla)$ means the scalar product of vectors $\mathbf{u} = (u, v, w)$ and $\nabla = (\partial_x, \partial_y, \partial_z)$. As a result we obtain an operator (not a function)

$$\mathbf{u} \cdot \nabla = u \partial_x + v \partial_y + w \partial_z.$$

The notation $(\mathbf{u} \cdot \nabla)$ is not to be confused with $\nabla \cdot \mathbf{u}$ which gives the divergence (see, for example, Lemma 3.1 below).

The general integral form of balance of momentum states that the rate of change of momentum inside a flowing elementary volume $V(t)$ is equal to the sum of forces acting on this volume and on its surface $\partial V(t)$:

$$\frac{d}{dt} \int_{V(t)} \rho \mathbf{u} dV = \int_{\partial V(t)} \boldsymbol{\sigma} \cdot \mathbf{n} d\sigma + \int_{V(t)} \rho \mathbf{g} dV, \quad (3.6)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor [MH94] and \mathbf{g} is the vector representing the volume (body) force per unit mass. In most practical situations $\mathbf{g} = (0, 0, -g)$, where $g = 9.80665 \text{ m/s}^2$ is the standard gravity acceleration. The stress tensor $\boldsymbol{\sigma}$ can be easily computed by *ideal* (or perfect) fluids.

Definition 3.1. A fluid is called *ideal* if there exists a scalar function $p(\mathbf{x}, t)$ called the pressure such that the stress tensor $\boldsymbol{\sigma}$ inside the fluid is equal to

$$\boldsymbol{\sigma} = \begin{pmatrix} -p & 0 & 0 \\ 0 & -p & 0 \\ 0 & 0 & -p \end{pmatrix}.$$

In this case the force per unit area acting on an elementary surface neighbourhood S of a point $\mathbf{x} \in S$ is given by

$$\boldsymbol{\sigma} \cdot \mathbf{n} = -p(\mathbf{x}, t) \mathbf{n},$$

where \mathbf{n} is the exterior unit normal to the surface S in the point \mathbf{x} . The total force \mathcal{F} applied to the surface of a closed compact volume V can be obtained by computing the following surface integral

$$\mathcal{F}_{\partial V} = \int_{\partial V} \boldsymbol{\sigma} \cdot \mathbf{n} d\sigma = - \int_{\partial V} p \mathbf{n} d\sigma.$$

The value of the constant g given in the text is prescribed by current standards. However, the local gravity acceleration varies with the position on the Earth.

In order to differentiate under the first integral sign in (3.6), one has to change the variables to work on a fixed integration domain (which is time independent, in other words). For this purpose we shall use the flow map $\mathbf{x} = \phi_t(\mathbf{a})$ to come back to the initial positions of fluid particles⁴ (see Figure 3.3 for illustration):

$$\frac{d}{dt} \int_{V(t)} \rho \mathbf{u} \, dV = \frac{d}{dt} \int_{V(0)} (\rho \mathbf{u})(\phi_t(\mathbf{a}), t) J(\mathbf{a}, t) \, dV,$$

where $J(\mathbf{a}, t)$ is the determinant of the Jacobian matrix of the map ϕ_t . Even if the expression under the integral on the right hand side became more complex, the integration domain is fixed, which allows to pull the derivative into the integral sign. By the product rule we have to differentiate the functions $(\rho \mathbf{u})(\phi_t(\mathbf{a}))$ and $J(\mathbf{a}, t)$. The former can be differentiated by applying the material derivative operator (3.5):

$$\frac{d}{dt} (\rho \mathbf{u})(\phi_t(\mathbf{a}), t) = \frac{D(\rho \mathbf{u})}{Dt}(\phi_t(\mathbf{a}), t),$$

while the derivative of the latter is given by the following

Lemma 3.1.

$$\frac{d}{dt} J(\mathbf{a}, t) = \nabla \cdot \mathbf{u}(\phi_t(\mathbf{a}), t) J(\mathbf{a}, t).$$

Proof. In the proof we shall extensively use the well-known fact that a determinant is a multilinear function of its columns. By denoting the components of the map ϕ_t by $(\phi_t^1, \phi_t^2, \phi_t^3)$ and the components of \mathbf{a} by (a, b, c) , we have by definition of the determinant:

$$J(\mathbf{a}, t) = \frac{1}{3!} \sum_{\tau \in S_3} (-1)^{\deg(\tau)} \phi_{ta}^{\tau(1)}(\mathbf{a}, t) \phi_{tb}^{\tau(2)}(\mathbf{a}, t) \phi_{tc}^{\tau(3)}(\mathbf{a}, t),$$

where S_3 is the symmetric group of permutations of 3 symbols $(1, 2, 3)$ and $\tau \in S_3$ is an arbitrary permutation. The subscripts a, b and c denote partial derivatives with respect to these independent variables. Now we can differentiate the determinant $J(\mathbf{a}, t)$ with respect to time by using the usual product rule:

$$\begin{aligned} \frac{\partial J}{\partial t} = \frac{1}{3!} \sum_{\tau \in S_3} (-1)^{\deg(\tau)} & \left[\frac{\partial \phi_{ta}^{\tau(1)}(\mathbf{a}, t)}{\partial t} \phi_{tb}^{\tau(2)}(\mathbf{a}, t) \phi_{tc}^{\tau(3)}(\mathbf{a}, t) + \right. \\ & \phi_{ta}^{\tau(1)}(\mathbf{a}, t) \frac{\partial \phi_{tb}^{\tau(2)}(\mathbf{a}, t)}{\partial t} \phi_{tc}^{\tau(3)}(\mathbf{a}, t) + \\ & \left. \phi_{ta}^{\tau(1)}(\mathbf{a}, t) \phi_{tb}^{\tau(2)}(\mathbf{a}, t) \frac{\partial \phi_{tc}^{\tau(3)}(\mathbf{a}, t)}{\partial t} \right]. \quad (3.7) \end{aligned}$$

⁴ It is always possible since the flow map is a one-to-one correspondence. Otherwise it would contradict the unicity result for the system (3.3). In other words, the particles trajectories cannot cross.

By using the chain rule and equation (3.4), one can compute the partial derivatives with respect to time (for the sake of illustration we take the first element of the first column):

$$\begin{aligned} \frac{\partial \phi_{ta}^1(\mathbf{a}, t)}{\partial t} &= \frac{\partial}{\partial \mathbf{a}} \left(\underbrace{\frac{\partial \phi_t^1(\mathbf{a}, t)}{\partial t}}_{=u(\phi(\mathbf{a}, t), t) \text{ by (3.4)}} \right) = \frac{\partial u(\phi(\mathbf{a}, t), t)}{\partial \mathbf{a}} = \\ &u_x \frac{\partial \phi_t^1}{\partial \mathbf{a}} + u_y \frac{\partial \phi_t^2}{\partial \mathbf{a}} + u_z \frac{\partial \phi_t^3}{\partial \mathbf{a}}. \end{aligned}$$

Substituting similar expressions into (3.7), many terms will vanish, since the determinant of a matrix with repeating columns is zero. What is left is summarized below

$$\frac{\partial J}{\partial t} = u_x J + v_y J + w_z J = (\nabla \cdot \mathbf{u}) J.$$

□

Now we can return to our integral and continue its differentiation with respect to time:

$$\begin{aligned} \frac{d}{dt} \int_{V(t)} \rho \mathbf{u} \, dV &= \\ &= \int_{V(0)} \left[\frac{D(\rho \mathbf{u})}{Dt} + (\nabla \cdot \mathbf{u})(\rho \mathbf{u}) \right] J \, dV = \\ &= \int_{V(t)} \left[\frac{D(\rho \mathbf{u})}{Dt} + \rho(\nabla \cdot \mathbf{u})\mathbf{u} \right] dV = \\ &= \int_{V(t)} \left[\frac{D\rho}{Dt} \mathbf{u} + \rho \frac{D\mathbf{u}}{Dt} + \rho(\nabla \cdot \mathbf{u})\mathbf{u} \right] dV = \\ &= \int_{V(t)} \left[\underbrace{\left(\frac{D\rho}{Dt} \mathbf{u} + \rho(\nabla \cdot \mathbf{u})\mathbf{u} \right)}_{=0 \text{ by (3.2)}} + \rho \frac{D\mathbf{u}}{Dt} \right] dV = \\ &= \int_{V(t)} \rho \frac{D\mathbf{u}}{Dt} \, dV. \end{aligned}$$

In these computations we actually showed the following important

Theorem 3.1 (Reynolds transport theorem).

$$\frac{d}{dt} \int_{V(t)} \rho f \, dV = \int_{V(t)} \rho \frac{Df}{Dt} \, dV.$$

One can derive another form of the Reynolds transport theorem, which does not involve the mass density:

$$\frac{d}{dt} \int_{V(t)} f \, dV = \int_{V(t)} \left(\frac{\partial f}{\partial t} + \nabla \cdot (f \mathbf{u}) \right) dV.$$

Remark 3.4. For instance, the mass conservation equation (3.2) can be readily obtained from the last integral identity by setting $f = \rho(\mathbf{x}, t)$.

However, the main goal of this section is to derive the momentum conservation equation. Indeed, we have assembled all necessary ingredients. After pulling the time derivative under the integral sign in (3.6) and taking into account that the volume $V(t)$ is arbitrary, we obtain the following balance of momentum:

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \rho \mathbf{g}. \quad (3.8)$$

In situations where the regularity of solutions is low, it is interesting to have the integral form of momentum balance in a fixed volume V . We give it here without the proof (which can be found in [CM93]):

$$\frac{d}{dt} \int_V \rho \mathbf{u} \, dV = - \int_{\partial V} (p \mathbb{I} + \rho \mathbf{u} \otimes \mathbf{u}) \cdot \mathbf{n} \, d\sigma + \int_V \rho \mathbf{g} \, dV,$$

where \mathbb{I} is the identity matrix and \otimes is the tensorial product, *i.e.*

$$\mathbf{u} \otimes \mathbf{u} = \begin{pmatrix} u^2 & uv & uw \\ vu & v^2 & vw \\ wu & wv & w^2 \end{pmatrix}.$$

3.1.4 Energy conservation

A fluid moving in a domain Ω has a kinetic energy K given by

$$K = \frac{1}{2} \int_{\Omega} \rho |\mathbf{u}|^2 \, dV.$$

In order to obtain the total energy E , one has to add also the internal energy ϵ

$$E = K + \epsilon.$$

The internal energy ϵ , as its name indicates it, comes from internal sources such as intermolecular potentials and molecular motion/vibrations. This

Please, note that ϵ does not have to be small ☺

energy cannot be measured (at the macroscopic level), but it can be deduced from the laws of Thermodynamics (see Section 3.1.5.3) and measurable macroscopic quantities (e.g. volume V , temperature T and pressure p).

The rate of change of the kinetic energy can be computed by applying the Reynolds transport theorem 3.1 and the momentum conservation equation (3.8):

$$\begin{aligned} \frac{dK}{dt} &= \frac{d}{dt} \frac{1}{2} \int_{\Omega} \rho |\mathbf{u}|^2 dV = \frac{1}{2} \int_{\Omega} \rho \frac{D|\mathbf{u}|^2}{Dt} dV \\ &= \int_{\Omega} \rho \frac{D\mathbf{u}}{Dt} \cdot \mathbf{u} dV \\ &= - \int_{\Omega} \nabla p \cdot \mathbf{u} dV + \int_{\Omega} \rho \mathbf{g} \cdot \mathbf{u} dV. \end{aligned}$$

The first term on the right hand side is the mechanical work done by pressure forces, while the second one is the work of body forces.

If additionally we assume the flow to be incompressible, then the integral involving the pressure can be integrated by parts:

$$\frac{dK}{dt} = - \int_{\Omega} p \mathbf{u} \cdot \mathbf{n} dV + \int_{\Omega} \rho \mathbf{g} \cdot \mathbf{u} dV,$$

where we used the Gauss–Ostrogradsky theorem and the following relation:

$$\nabla \cdot (p\mathbf{u}) = \nabla p \cdot \mathbf{u} + p \underbrace{\nabla \cdot \mathbf{u}}_{=0}.$$

3.1.5 Special flows

3.1.5.1 Incompressible flows

Definition 3.2. A fluid flow is called incompressible if the measure of any elementary volume $V(t)$ is preserved by the flow, i.e.

$$\int_{V(t)} dV \equiv \int_{V(0)} dV = \text{const}, \quad \forall t > 0.$$

The mass is always conserved. The volume conservation is an additional condition for the incompressibility.

The following conditions are just avatars of the flow incompressibility:

1. $\nabla \cdot \mathbf{u} = 0, \quad \forall \mathbf{x} \in \Omega(t), \quad \forall t > 0,$
2. $J(\mathbf{a}, t) \equiv 1, \quad \forall \mathbf{a} \in \Omega(0), \quad \forall t > 0,$
3. $\frac{D\rho}{Dt} = 0, \quad \forall \mathbf{x} \in \Omega(t), \quad \forall t > 0.$

The equivalence of first two conditions (1), (2) follows from the following simple computation valid for an arbitrary fluid volume $V(t)$:

$$0 = \frac{d}{dt} \int_{V(t)} dV = \frac{d}{dt} \int_{V(0)} J dV = \int_{V(0)} (\nabla \cdot \mathbf{u}) J dV = \int_{V(t)} \nabla \cdot \mathbf{u} dV.$$

The last avatar (3) readily follows from the mass conservation and the divergence-free condition (1).

The following set of equations describes an incompressible flow of an ideal fluid:

$$\begin{aligned} \rho \frac{D\mathbf{u}}{Dt} &= -\nabla p + \rho \mathbf{g}, \quad (\mathbf{x}, t) \in \Omega \times \mathbb{R}^+ \\ \frac{D\rho}{Dt} &= 0, \quad (\mathbf{x}, t) \in \Omega \times \mathbb{R}^+ \\ \nabla \cdot \mathbf{u} &= 0, \quad (\mathbf{x}, t) \in \Omega \times \mathbb{R}^+, \end{aligned}$$

along with appropriate boundary conditions. On a wall one can require that fluid particles do not penetrate the solid boundary, *i.e.* the normal component of the velocity vanishes

$$\mathbf{u} \cdot \mathbf{n} = 0, \quad \mathbf{x} \in \partial\Omega.$$

Boundary conditions will be discussed in Section 3.4.

Incompressible flows are very important in applications since most of the flows we encounter in nature are incompressible. For instance, the usual water under normal conditions is fairly incompressible. A general criterium to decide whether the flow is compressible or not consists in estimating the Mach number, *i.e.* the ratio between the speed of sound c_s (in this medium) to the characteristic flow speed u_0 :

$$\text{Ma} := \frac{u_0}{c_s}.$$

It is considered that if the Mach number is roughly $\text{Ma} \lesssim 0.1$ then the flow can be assumed to be incompressible.

3.1.5.2 Flows of homogeneous fluids

Definition 3.3. *A fluid is called homogeneous if its mass density ρ is constant in space.*

A homogeneous fluid is also incompressible if and only if the density ρ is also constant in time (not only in space as require by the definition 3.3). Note, that a fluid which is initially homogeneous remains so if and only if the flow is also incompressible. Otherwise, the density variations will appear due to compressible effects.

3.1.5.3 *Isentropic flow*

Definition 3.4. A flow is called *isentropic* if it is not accompanied by any change in entropy.

If a flow is taking place in mild periodic conditions (e.g. a very gradual compression followed by a gradual expansion), the flow variables may return to their original values. In Physics such processes are called *reversible*. According to the Second law of Thermodynamics, a reversible flow implies a constant value of the entropy. In other words, such flows are called *isentropic*. According to Gibbs relation

$$Tds = d\epsilon + pdV,$$

where T is the absolute temperature, ϵ is the internal energy per unit mass and s is the entropy. Since, the flow is *isentropic*, $ds = 0$ and we have

$$d\epsilon = \frac{p}{\rho^2} d\rho.$$

Thus, by integrating the last relation from 0 to ρ one obtains the expression of the internal energy for isentropic flows:

$$\epsilon = \int_0^\rho \frac{p(\rho)}{\rho^2} d\rho.$$

The notion of entropy was introduced for the first time by Rudolf CLAUDIUS

In Greek “iso” means the same.

3.2 NAVIER–STOKES EQUATIONS

So far we worked with ideal fluids only. In such fluids the forces acting across an internal surface are always normal to this surface. In this Section we shall consider more general fluids which involve some tangential (frictional) forces as well. These effects are important for the description of shear flows, for example.

The mass conservation is obviously not affected by tangential stresses. However, we have to review the momentum balance equation (3.6). Previously we assumed that the stress σ reduces only to normal components (i.e. the pressure p) in an ideal fluid. In viscid fluids we have to include also the tangential forces across an arbitrary material surface:

$$\sigma = -p\mathbb{I} + \tau,$$

where τ is the *tangential stress tensor*. Consequently, the momentum balance equation (3.6) takes the following form:

$$\frac{d}{dt} \int_{V(t)} \rho \mathbf{u} dV = - \int_{\partial V(t)} p \mathbf{n} d\sigma + \int_{\partial V(t)} \tau \cdot \mathbf{n} d\sigma + \int_{V(t)} \rho \mathbf{g} dV.$$

By conservation of angular momentum we necessarily have that this tensor is symmetric, i.e. $\tau^T = \tau$.

Moreover, if we assume the fluid to be *Newtonian*, the symmetric tensor $\boldsymbol{\tau}$ has the following form

$$\boldsymbol{\tau} = \lambda(\boldsymbol{\nabla} \cdot \mathbf{u})\mathbf{I} + 2\mu\mathbf{D}, \quad (3.9)$$

where λ, μ are viscosity coefficients⁵ and $\mathbf{D} = \frac{1}{2}(\boldsymbol{\nabla}\mathbf{u} + {}^T(\boldsymbol{\nabla}\mathbf{u}))$ is the *deformation tensor*. The coefficient λ is called the *bulk viscosity* and μ is the *dynamic viscosity*. By applying the Reynolds transport theorem 3.1 and taking into account that the volume V is arbitrary we obtain the following local form of the Cauchy momentum equation:

$$\rho \frac{D\mathbf{u}}{Dt} = -\boldsymbol{\nabla}p + \boldsymbol{\nabla} \cdot \boldsymbol{\tau} + \rho\mathbf{g}.$$

The divergence of the tangential stress tensor can be easily computed taking into account (3.9) (it is easier to perform the computations in tensorial notations):

$$\begin{aligned} \boldsymbol{\nabla} \cdot \boldsymbol{\tau} &= \partial_j \tau_{ij} = \\ &= \partial_j [\lambda(\partial_k u_k) \delta_{ij} + 2\mu \frac{1}{2}(\partial_i u_j + \partial_j u_i)] = \\ &= \lambda \partial_i (\partial_k u_k) + \mu [\partial_i \partial_j u_j + \partial_j^2 u_i] = \\ &= (\lambda + \mu) \partial_i (\partial_k u_k) + \mu \partial_{jj} u_i. \end{aligned}$$

δ_{ij} is the Kronecker symbol, i.e. $\delta_{ii} = 1$ and $\delta_{ij} = 0$, if $i \neq j$.

As a result, the momentum balance in Navier–Stokes equations can be written as

$$\rho \frac{D\mathbf{u}}{Dt} = -\boldsymbol{\nabla}p + (\lambda + \mu)\boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \mathbf{u}) + \mu \nabla^2 \mathbf{u} + \rho\mathbf{g},$$

the operator $\nabla^2 = \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is the celebrated Laplace operator. The last equation can be simplified for incompressible flows to give a more conventional form of the Navier–Stokes equations:

$$\frac{D\rho}{Dt} = 0, \quad (3.10)$$

$$\boldsymbol{\nabla} \cdot \mathbf{u} = 0, \quad (3.11)$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \boldsymbol{\nabla})\mathbf{u} + \frac{1}{\rho} \boldsymbol{\nabla}p = \nu \nabla^2 \mathbf{u} + \mathbf{g}, \quad (3.12)$$

where $\nu := \frac{\mu}{\rho}$ is the kinematic viscosity.

⁵ We can assume λ, μ to be constant in the first approximation. For more complex and especially compressible fluids the viscosity coefficients may depend on the local fluid density, i.e. $\lambda = \lambda(\rho)$, $\mu = \mu(\rho)$.

3.2.1 Dimensionless equations

In this Section we shall obtain the scaled version of Navier–Stokes equations, where all variables are replaced by their dimensionless counterparts. A general approach to the dimensional analysis will be presented in Section 3.5. Here we just provide an application to the particular case of incompressible Navier–Stokes equations.

The process of obtaining dimensionless equations allows to derive the relevant physical scaling parameters which determine properties of the solution. Consider a flow of an incompressible fluid past a long cylinder of radius R as it is schematically depicted on Figure 3.6. This flow is described by incompressible Navier–Stokes equations (3.11), (3.12). The body force is taken to be the gravity acceleration $\mathbf{g} = (0, 0, -g)$. We assume that the scales in all directions x , y and z are the same. In order to obtain dimensionless equations one has to choose the characteristic values of all dependent and independent physical variables in order to introduce their dimensionless counterparts (denoted with an asterisk *):

$$\mathbf{x}^* = \frac{\mathbf{x}}{\ell}, \quad t^* = \frac{t}{t_0}, \quad \mathbf{u} = \frac{\mathbf{u}}{U}, \quad p^* = \frac{p}{P},$$

where ℓ , t_0 , U and P are some scales of the length, time, speed and pressure correspondingly. In our problem it is reasonable to take the cylinder radius R as the typical length scale⁶, i.e. $\ell = R$. The fluid velocity at infinity can be chosen as a typical flow speed U . Since we have the length and velocity scales, we can compose a consistent time scale by taking their ratio $t_0 = \ell/u = R/u$. The choice of a typical pressure value P will become clear from the computations below.

The continuity equation in scaled variables reads:

$$\frac{U}{R} \nabla^* \cdot \mathbf{u}^* = 0 \implies \nabla^* \cdot \mathbf{u}^* = 0.$$

Consequently, it remains invariant due to its linearity. For the sake of convenience in the following we shall drop out the asterisk *, since all variables will be dimensionless. The momentum balance equation (3.12) will read

$$\frac{U^2}{R} \frac{\partial \mathbf{u}}{\partial t} + \frac{U^2}{R} (\mathbf{u} \cdot \nabla) \mathbf{u} + \frac{P}{\rho R} \nabla p = \frac{\nu U}{R^2} \nabla^2 \mathbf{u} - g \mathbf{e}_3,$$

with $\mathbf{e}_3 = (0, 0, 1)$. Multiplying the last equation by R/U^2 yields

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \frac{P}{\rho U^2} \nabla p = \frac{\nu}{RU} \nabla^2 \mathbf{u} - \frac{gR}{U^2} \mathbf{e}_3.$$

⁶ If there is no solid object present in the flow, one can take the size of a typical eddy, for example.

Now one can see that the most reasonable choice for the pressure scale is $P := \rho U^2$. Finally, we can introduce two dimensionless combinations which characterize our flow

$$\text{Re} := \frac{RU}{\nu}, \quad \text{Fr} := \frac{U}{\sqrt{gR}}.$$

These parameters are called the Reynolds and Froude numbers after O. REYNOLDS and W. FROUDE. The fully dimensionless version of incompressible Navier–Stokes equations reads

$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0, \\ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p &= \frac{1}{\text{Re}} \nabla^2 \mathbf{u} + \frac{1}{\text{Fr}^2} \mathbf{e}_3. \end{aligned}$$

By definition the Froude number measures the relative importance of the inertial to gravitational force and the Reynolds number is the ratio of the inertial to the viscous force. The former plays an important rôle in Hydraulics, while the latter controls essentially the transition to turbulence as it was shown experimentally in historical experiments on transient flows in pipes by REYNOLDS (see Figure 3.4 for an illustration). He was the first to find this scaling parameter Re and to fully recognize its rôle in Fluid Dynamics.

As it often happens, the celebrated Reynolds number was discovered first by G. STOKES (1851). O. REYNOLDS proposed it only in 1883.

3.3 VORTICITY

Consider a velocity field $\mathbf{u}(\mathbf{x}, t)$ defined on an open domain $\Omega \subseteq \mathbb{R}^3$. Let us study how this field changes locally around any interior point $\mathbf{x} \in \Omega$. By applying the Taylor formula up to the 2nd order in the vicinity of \mathbf{x} we obtain (in this Section we shall consider the velocity field $\mathbf{u}(\mathbf{x})$ to be stationary to just simplify the notation):

$$\mathbf{u}(\mathbf{y}) = \mathbf{u}(\mathbf{x}) + \nabla \mathbf{u}(\mathbf{x}) \cdot \Delta \mathbf{x} + \mathcal{O}(\|\Delta \mathbf{x}\|^2), \quad (3.13)$$

where $\Delta \mathbf{x} := \mathbf{y} - \mathbf{x} = (\Delta x_1, \Delta x_2, \Delta x_3)$. The Jacobian matrix $\nabla \mathbf{u}(\mathbf{x})$, as any other second order tensor, can be decomposed into the sum of its symmetric \mathbb{D} and skew-symmetric \mathbb{A} parts

$$\begin{aligned} \mathbb{D} &:= \frac{1}{2} (\nabla \mathbf{u} + {}^T(\nabla \mathbf{u})), \\ \mathbb{A} &:= \frac{1}{2} (\nabla \mathbf{u} - {}^T(\nabla \mathbf{u})). \end{aligned}$$

The tensor \mathbb{D} was called above the deformation tensor. So, the Taylor expansion (3.13) becomes:

$$\mathbf{u}(\mathbf{y}) = \mathbf{u}(\mathbf{x}) + \mathbb{D}(\mathbf{x}) \cdot \Delta \mathbf{x} + \mathbb{A}(\mathbf{x}) \cdot \Delta \mathbf{x} + \mathcal{O}(\|\Delta \mathbf{x}\|^2).$$

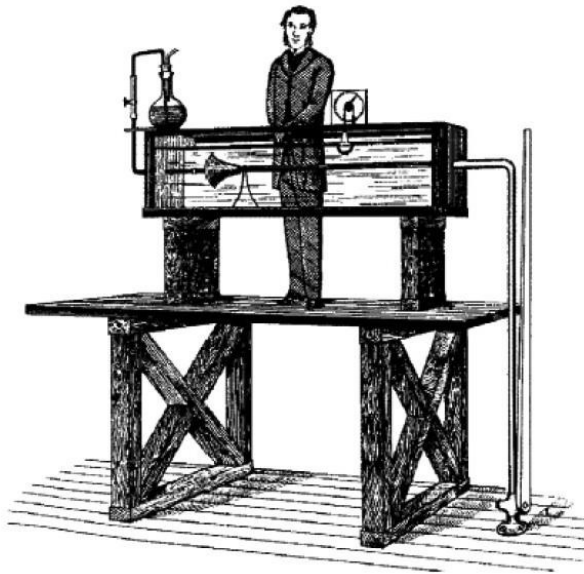


Figure 3.4.: *Osborne Reynolds (1893) observing transition from laminar to turbulent flow in a pipe.*

By performing some simple algebraic computations the anti-symmetric part can be transformed as follows

$$\begin{aligned}
 \mathbb{A}(\mathbf{x}) \cdot \Delta \mathbf{x} &= \frac{1}{2} \begin{pmatrix} 0 & \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} & \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} \\ \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} & 0 & \frac{\partial v}{\partial z} - \frac{\partial w}{\partial y} \\ \frac{\partial w}{\partial x} - \frac{\partial u}{\partial z} & \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} & 0 \end{pmatrix} \cdot \begin{pmatrix} \Delta x_1 \\ \Delta x_2 \\ \Delta x_3 \end{pmatrix} \\
 &= \frac{1}{2} \begin{pmatrix} \left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}\right) \Delta x_2 + \left(\frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}\right) \Delta x_3 \\ \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right) \Delta x_1 + \left(\frac{\partial v}{\partial z} - \frac{\partial w}{\partial y}\right) \Delta x_3 \\ \left(\frac{\partial w}{\partial x} - \frac{\partial u}{\partial z}\right) \Delta x_1 + \left(\frac{\partial w}{\partial y} - \frac{\partial v}{\partial z}\right) \Delta x_2 \end{pmatrix} \\
 &= \frac{1}{2} \begin{pmatrix} \left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}\right) \Delta x_3 - \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right) \Delta x_2 \\ \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right) \Delta x_1 - \left(\frac{\partial w}{\partial y} - \frac{\partial v}{\partial z}\right) \Delta x_3 \\ \left(\frac{\partial w}{\partial x} - \frac{\partial u}{\partial z}\right) \Delta x_2 - \left(\frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}\right) \Delta x_1 \end{pmatrix} \\
 &= \frac{1}{2} \begin{pmatrix} \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} \\ \frac{\partial v}{\partial z} - \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial x} - \frac{\partial w}{\partial y} \end{pmatrix} \times \begin{pmatrix} \Delta x_1 \\ \Delta x_2 \\ \Delta x_3 \end{pmatrix} = \frac{1}{2} (\nabla \times \mathbf{u}) \times \Delta \mathbf{x} = \frac{1}{2} \boldsymbol{\omega} \times \Delta \mathbf{x},
 \end{aligned}$$

where we defined the so-called vorticity vector $\boldsymbol{\omega} := \nabla \times \mathbf{u}$. Consequently, the local change of the velocity field around a fixed location \mathbf{x} can be represented as

$$\mathbf{u}(\mathbf{y}) - \mathbf{u}(\mathbf{x}) = \mathbb{D}(\mathbf{x}) \cdot \Delta \mathbf{x} + \boldsymbol{\omega}(\mathbf{x}) \times \Delta \mathbf{x} + \mathcal{O}(\|\Delta \mathbf{x}\|^2).$$

The last formula has a simple physical interpretation: the local change of the velocity field $\mathbf{u}(\mathbf{x})$ is the superposition of deformation with rate $\mathbb{D}(\mathbf{x})$ and a rigid rotation with vector $\boldsymbol{\omega}(\mathbf{x})$ given by the rotor (or curl) operator applied to the velocity field at this point \mathbf{x} . Please notice that this transformation preserves the volume for incompressible fields.

3.3.1 Irrotational flows

Definition 3.5. A flow is called irrotational if the velocity field $\mathbf{u}(\mathbf{x}, t)$ satisfies $\boldsymbol{\omega}(\mathbf{x}, t) = \nabla \times \mathbf{u} = 0$, $\forall t \geq 0$.

From the geometrical sense of vorticity $\boldsymbol{\omega}$ it is clear now why such flows are called irrotational.

As it is known from the vector calculus, an irrotational vector field \mathbf{u} can be expressed as the gradient of a scalar field $\phi(\mathbf{x}, t)$ called the *velocity potential*:

$$\mathbf{u}(\mathbf{x}, t) = \nabla \phi(\mathbf{x}, t).$$

Conversely, when a velocity potential exists, i.e. $\mathbf{u} = \nabla \phi$, the flow is necessarily irrotational. This fact follows from the following well-known vector identity:

$$\boldsymbol{\omega}(\mathbf{x}, t) = \nabla \times \mathbf{u}(\mathbf{x}, t) = \nabla \times \nabla \phi(\mathbf{x}, t) \equiv 0.$$

It is for this reason that irrotational flows are often referred to in the literature as the *potential flows*. Irrotational (or potential) flows are particularly suitable for the description of waves on the surface of a fluid layer. The water wave problem will be discussed in more details in Chapter 4.

3.4 BOUNDARY CONDITIONS

So far we did not discuss at all the question of boundary conditions. In the theory of (partial or ordinary) differential equations these extra conditions have to be imposed to obtain a well-posed problem. In this way we can hope to have the unicity property of the solution. However, the unicity for Boundary-Value Problems (BVP) is rather an exceptional situation.

The number and nature of boundary conditions in Fluid Mechanics depends whether the fluid is viscous or perfect. The former is described by (parabolic) Navier–Stokes equations, while the latter by (hyperbolic) Euler equations. So, the number of boundary conditions cannot be the same. We shall consider only the simplest case of solid (or wall) boundaries. So, in the case of Navier–Stokes equations the so-called “no-slip” condition is imposed

$$\mathbf{u}(\mathbf{x}, t) = 0, \quad \mathbf{x} \in \partial\Omega.$$

We underline that above we have three scalar conditions in \mathbb{R}^3 . In the inviscid case described by Euler equations we impose only one “no-penetration” condition

$$\mathbf{u}(\mathbf{x}, t) \cdot \mathbf{n} = 0, \quad \mathbf{x} \in \partial\Omega.$$

where \mathbf{n} being the exterior normal. The last condition can be easily interpreted from the physical point of view: it simply says that fluid particles cannot penetrate a solid boundary. This condition written for potential flows becomes the classical homogeneous Neumann condition

$$\mathbf{u}(\mathbf{x}, t) \cdot \mathbf{n} = \nabla\phi \cdot \mathbf{n} = \frac{\partial\phi}{\partial\mathbf{n}} = 0, \quad \mathbf{x} \in \partial\Omega.$$

In general, the Euler equations describe fairly well the flows relatively far⁷ from the boundaries. However, the difference between the nature of boundary conditions in Navier–Stokes and Euler equations is responsible of the important *boundary layer* phenomenon.

⁷ The precise meaning of “farness” depends on the Reynolds number. It can be shown that the boundary layer size scales with $\text{Re}^{-\frac{1}{2}}$.

3.5 DIMENSIONAL ANALYSIS

The methods of dimensional analysis have been proved to be very useful in Physics in general and they can be also successfully applied to Fluid Mechanics problems. That is why we include this Section into the Chapter devoted to Fluid Dynamics equations. Moreover, it allows in some cases to answer on physical questions without solving the initial problem.

Theorem 3.2 (π -theorem). *Let a physical problem involves n dimensional variables v_1, v_2, \dots, v_n*

$$F(v_1, v_2, \dots, v_n) = 0,$$

which depend only on r different independent dimensional units u_1, u_2, \dots, u_r . Then, the problem can be recast in the form

$$G(\pi_1, \pi_2, \dots, \pi_{n-r}) = 0,$$

where $\{\pi_k\}_{k=1}^{n-r}$ are $n-r$ dimensionless variables which describe the physics of the problem:

$$\pi_k = v_1^{\mu_{k1}} \cdot v_2^{\mu_{k2}} \cdot \dots \cdot v_n^{\mu_{kn}},$$

where $\mu_{kj} \in \mathbb{Q}$ are some rational numbers which make the product π_k dimensionless.

The π -theorem was first proved by a French mathematician Joseph BERTRAND in 1878. However, in Anglo-Saxons literature it is often called Buckingham π theorem, named after Edgar BUCKINGHAM.

Proof. The proof of this theorem relies on some basic facts of the Linear Algebra. In particular, one has to construct the *dimension matrix* of the problem. So, any dimensional quantity v_i can be expressed as a product of fundamental units u_1, u_2, \dots, u_r :

$$v_k = u_1^{a_{1k}} \cdot u_2^{a_{2k}} \cdot \dots \cdot u_r^{a_{rk}}, \quad k = 1, 2, \dots, n. \quad (3.14)$$

The dimensional matrix $A = (a_{ik})$, $1 \leq i \leq r$, $1 \leq k \leq n$ is composed of the exponents a_{ik} written in columns. By assumptions of the π -theorem the rank of this matrix A is equal to r (the number of different independent fundamental units), i.e. $\text{rank}(A) = r$. Now let us compose an arbitrary dimensionless combination π_k in the framework of our physical problem:

$$\pi_k = v_1^{\mu_{k1}} \cdot v_2^{\mu_{k2}} \cdot \dots \cdot v_n^{\mu_{kn}}.$$

Substituting the representation (3.14) into the last formula and after equating all the exponents to zero (since the result has to be dimensionless), we

obtain the following system of equations with respect to the unknown vector $\{\mu_{kj}\}_{j=1}^n$:

$$\sum_{j=1}^n a_{ij} \mu_{kj} = 0, \quad i = 1, 2, \dots, r.$$

Under the assumptions of our theorem the dimension of null space of this linear system is equal to $n - r$. \square

Remark 3.5. The π -theorem 3.2 does not guarantee the unicity of the set of dimensionless parameters. Basically, the non-unicity comes from the fact that the choice of the null space basis is not unique. However, in every problem the choice of the “most meaningful” dimensionless numbers is usually guided by the physical intuition and some other considerations. They should help the reader to avoid an awkward set of dimensionless products.

This theorem should be considered as a recipe to compute the sets dimensionless variables for a given physical problem in hand. Notice that dimensionless parameters can be computed even if the equations are unknown (one such example will be given in Section 3.5.4). One has just to know the physical variables involved in the problem.

Two physical problems which share the same set of dimensionless parameters are called *similar* and they form similarity classes with respect to this equivalence relation. In fact, such problems are completely equivalent from the mathematical point of view, while being possibly situated at very different scales in the real world (e.g. dynamite and nuclear blast explosion). The good side of it is that it is sufficient to solve one representative physical problem to know the solutions for the whole similarity class. Indeed, the solutions to *all* other *similar* problems can be obtained by a simple *rescaling* of variables.

This similarity transposes the notion of homothety transformation of geometrical figures to physical problems.

The following examples illustrate how to use the π theorem 3.2 in three physical problems coming from different physical horizons (e.g. Classical Mechanics, Fluid Mechanics and Detonation).

3.5.1 Harmonic oscillator

A *harmonic oscillator* is one of the most fundamental objects in Theoretical Physics. It refers to a linear undamped oscillator described by the following equation written in dimensionless variables

$$\ddot{\theta} + k\theta = 0, \quad k = \text{const} > 0, \quad \theta(0) = \theta_0$$

where $\theta(t)$ is the angle. In contrast, a *mathematical oscillator* refers to a nonlinear oscillator described by the following equation

$$\ddot{\theta} + k \sin \theta = 0, \quad \theta(0) = \theta_0$$

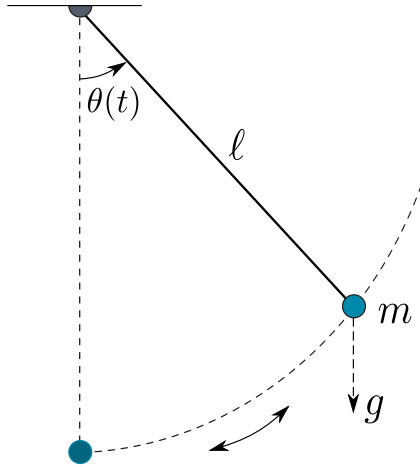


Figure 3.5.: A simple pendulum as an illustration of a mathematical oscillator.

It is easy to see that the former equation is obtained from the latter by applying the small angle approximation $\sin \theta \approx \theta$, $|\theta| \ll 1$. The mechanical model of an oscillator is given by a simple pendulum depicted in Figure 3.5. It can be equally given by a mass attached to a spring, electrical circuits, *etc.* The goal of the present Section is to obtain some physical conclusions about a harmonic (or even a mathematical) oscillator without solving any ODEs. So, we shall forget now the governing equations given above.

Consider a simple pendulum of mass m at the end of a rope of length ℓ and we would like to describe its motion parametrized by the rope deviation angle $\theta(t)$ from the stable equilibrium position $\theta = 0$. The initial position of the pendulum is $\theta_0 = \theta(0)$. In total there are six variables which describe the state of this physical system:

θ : deviation angle, [1] (dimensionless)

θ_0 : initial angle, [1] (dimensionless)

g : gravity acceleration, [m/s^2]

m : pendulum mass, [kg]

ℓ : rope length, [m]

t : time, [s]

There are only three fundamental independent units kg , m and s which are involved in physical variables listed above. So, according to the π -theorem the problem can be described by three ($6 - 3 = 3$) dimensionless parameters $\pi_{1,2,3}$. Please notice, that the pendulum mass m is the only variable containing the mass unit kg . So, it cannot cancel with any other multiplier and in the dimensionless combinations m can appear only with zero exponent since $m^0 = 1$. A closer inspection suggests the following dimensionless variables:

$$\pi_1 = \theta_0, \quad \pi_2 = \theta(t), \quad \pi_3 = \frac{g}{\ell} t^2.$$

So, common sense suggests that we can write our problem in the form $\pi_2 = \Lambda(\pi_1, \pi_3)$, or equivalently

$$\theta(t) = \Lambda(\theta_0, \frac{g}{\ell} t^2).$$

The motion is periodic with period say T , thus, we can write the periodicity condition $\theta(T) = \theta(0)$ as

$$\Lambda(\theta_0, \frac{g}{\ell} T^2) - \Lambda(\theta_0, 0) = 0.$$

If we assume that the last equation can be solved with respect to T , we obtain

$$T = \sqrt{\frac{g}{\ell}} \Upsilon(\theta_0).$$

To make a conclusion, we just showed using simple dimensional arguments that the pendulum period T depends in general on the initial pendulum inclination θ_0 and T scales with $\sqrt{g/\ell}$.

Remark 3.6. *The reader can notice that the search of dimensionless quantities is guided by close inspection and physical intuition. The brute force should be used only when everything else has been failed.*

3.5.2 Viscous drag

In Fluid Dynamics the *drag* (or fluid/air resistance) is a force exerted on a moving body surrounded by a fluid, which acts in the direction opposite to its relative motion. The drag belongs to frictional forces and it appears essentially because of the viscous friction effects. It explains why this Section is called “Viscous drag”. Examples of drag include a component of the aerodynamic force acting on a car in the direction opposite to its motion. Notice that drag can act also in the same direction of motion. This effect is used for sailing, for example. In this Section we apply the

Even though the drag is ultimately caused by the viscosity, the turbulent drag turns out to be independent of it.

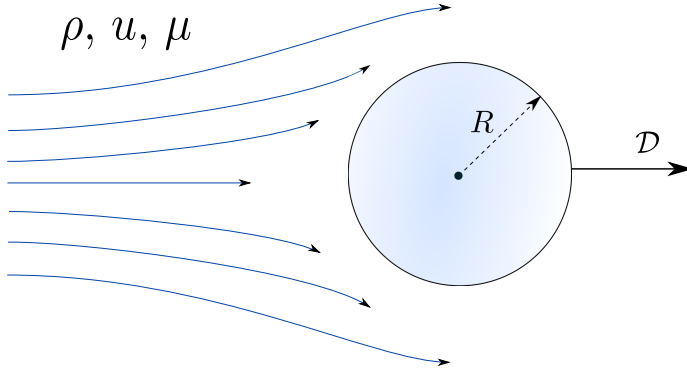


Figure 3.6.: An infinitely long cylinder in a steady flow of a viscous fluid.

π -theorem 3.2 to analyze the problem of viscous steady flow around an infinitely long cylinder of radius R . The sketch of this problem is shown on Figure 3.6.

Remark 3.7 (d'Alembert paradox). *Jean Le Rond d'ALEMBERT showed in 1752 that the potential steady flow around a disk (in 2D) predicted exactly zero drag force. This theoretical prediction was in clear contradiction with experimental evidences. This fact became generally known as d'Alembert paradox. Later there were some attempts to remove the irrotationality assumption, but steady solutions to Euler equations with vorticity did not result in realistic predictions. Finally, this paradox was solved in 1904 by L. PRANDTL who introduced the boundary layer theory and explained the origins of drag even at high Reynolds number, where Navier–Stokes equations approach the inviscid Euler.*

Geometrically the similarity is satisfied automatically since the cylinder radius R is the only length scale involved in this problem. The physical quantities which govern this problem are

\mathcal{D} : drag⁸, $[\text{N/m}] = [\text{kg/s}^2]$

U : fluid velocity, $[\text{m/s}]$

R : cylinder radius, $[\text{m}]$

ρ : fluid density, $[\text{kg/m}^3]$

μ : dynamic viscosity, $[\text{kg/m}\cdot\text{s}]$

⁸ In our simplified 2D problem the drag is the force per unit length.

Let us express the drag \mathcal{D} as a product of other physical quantities:

$$\mathcal{D} = R^\alpha \cdot U^\beta \cdot \rho^\gamma \cdot \mu^\delta, \quad (3.15)$$

or in dimensional units:

$$\text{kg} \cdot \text{s}^{-2} = \text{m}^\alpha \cdot (\text{m/s})^\beta \cdot (\text{kg/m}^3)^\gamma \cdot (\text{kg/m}\cdot\text{s})^\delta$$

After some algebraic simplifications we obtain

$$\text{kg}^1 \cdot \text{m}^0 \cdot \text{s}^{-2} = \text{kg}^{\gamma+\delta} \cdot \text{m}^{\alpha+\beta-3\gamma-\delta} \cdot \text{s}^{-\beta-\delta}.$$

By equating the exponents on the left and on the right we obtain a linear system of equations:

$$\begin{aligned} \gamma + \delta &= 1, \\ \alpha + \beta - 3\gamma - \delta &= 0, \\ -\beta - \delta &= -2. \end{aligned}$$

So, we have three equations for four unknown exponents α , β , γ and δ . We can express the first three exponents in terms of δ , $\delta \in \mathbb{Q}$:

$$\begin{aligned} \alpha &= 1 - \delta, \\ \beta &= 2 - \delta, \\ \gamma &= 1 - \delta. \end{aligned}$$

So, the initial guess (3.15) for the drag can be written now in a more specific form

$$\mathcal{D} = \rho U^2 R \left(\frac{\mu}{R U \rho} \right)^\delta,$$

or equivalently

$$\underbrace{\frac{\mathcal{D}}{\rho U^2 R}}_{C_{\mathcal{D}}} = \left(\underbrace{\frac{\mu}{R U \rho}}_{1/\text{Re}} \right)^\delta.$$

The dimensionless quantity on the left is the so-called drag coefficient $C_{\mathcal{D}}$, while on the right one can recognize⁹ the inverse of the Reynolds number introduced above in Section 3.2.1. Our dimensional analysis shows that the drag coefficient $C_{\mathcal{D}}$ is related to the Reynolds number by the following relation

$$C_{\mathcal{D}} = \text{Re}^{-\delta}, \quad \delta \in \mathbb{Q}.$$

⁹ We remind that the kinematic viscosity ν is related to the dynamic one by this relation $\nu = \mu/\rho$.

Unfortunately the dimensional analysis cannot provide the numerical value of the exponent δ . However, from the experiments we know that $\delta \propto -1$ for laminar flow and $\delta \propto 0$ for turbulent ones¹⁰.

In order to check our conclusions let us compose formally also the dimensional matrix described in the π -theorem¹¹:

$$\begin{pmatrix} \text{kg} & 1 & 0 & 0 & 1 & 1 \\ \text{m} & 0 & 1 & 1 & -3 & -1 \\ \text{s} & -2 & 0 & -1 & 0 & -1 \end{pmatrix}$$

$$\begin{matrix} & \mathcal{D} & R & U & \rho & \mu \end{matrix}$$

The rank of this matrix is equal to three and the number of physical variables is equal to five. Consequently, according to the π -theorem there are two dimensionless quantities which govern the physics of this problem. At this stage we already know that they are the drag coefficient $C_{\mathcal{D}}$ and the Reynolds number Re .

3.5.3 Falling particle

As another illustration of the power of dimensional analysis we consider briefly the problem of a spherical particle falling in a viscous fluid. This situation is schematically depicted on Figure 3.7. The relevant physical variables are

R : particle radius, [m]

U : particle velocity, [m/s]

ρ^+ : particle density, [kg/m³]

ρ^- : fluid density, [kg/m³]

g : gravity acceleration, [m/s²]

μ : dynamic viscosity, [kg/m·s]

In total it makes six variables with three fundamental units (kg, m and s). So, the problem should be described by three dimensionless quantities. After a close inspection one can write down the following set dimensionless products:

$$\pi_1 = \frac{\rho^+}{\rho^-}, \quad \pi_2 = \frac{U^2}{Rg}, \quad \pi_3 = \frac{UR}{\mu/\rho^-}.$$

¹⁰ It means that the drag coefficient $C_{\mathcal{D}}$ does not depend on the viscosity for a fully developed turbulent flow.

¹¹ In fact, we already did it implicitly while deriving the linear system for the exponents α , β , γ and δ from the representation (3.15).

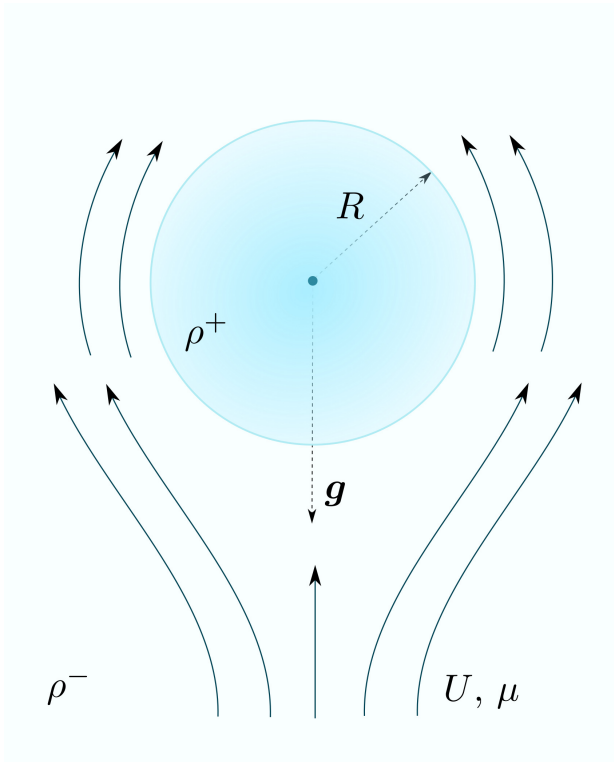


Figure 3.7.: Spherical particle fall into a viscous fluid.

The physical sense to these scaled variables can be easily given: π_1 is the ratio of densities, π_2 is the squared Froude number and π_3 is the Reynolds number. We can assume that our problem is described by the following relation

$$\pi_2 = \Lambda(\pi_1, \pi_3) \iff \frac{U^2}{Rg} = \Lambda\left(\frac{\rho^+}{\rho^-}, \frac{\rho^- UR}{\mu}\right).$$

Experiments suggest that the function $\Lambda(\pi_1, \pi_3)$ has a particular structure $\Lambda(\pi_1, \pi_3) = \pi_3 \Upsilon(\pi_1)$, or in physical variables it reads:

$$U = \frac{\rho^- g R^2}{\mu} \Upsilon\left(\frac{\rho^+}{\rho^-}\right).$$

Since we are dealing with buoyancy, when the two densities are equal $\rho^+ = \rho^-$ (or $\pi_1 = 1$) the particle has to remain motionless, *i.e.* $U = 0$. This can be achieved in the simplest way if the function $\Upsilon(\pi_1) = \pi_1 - 1$. We can write the final result

$$U = C \frac{\rho^- g R^2}{\mu} \left(\frac{\rho^+}{\rho^-} - 1\right),$$

where C is a constant. From more detailed computations it follows that for a spherical particle $C = \frac{2}{9}$. The obtained formula is called Stokes's drag law after Sir George Gabriel STOKES (1819 – 1903).

3.5.4 Nuclear explosion

As the final illustration of the π -theorem we shall analyze the nuclear blast problem. This example is probably the most famous, but its scientific aspect is not necessarily widely known.

The atomic bomb was tested by United States in Alamogordo, New Mexico on July 16, 1945. During the test (known as Trinity test) a several number of high speed photographs were taken. However, they were published only in 1947 in an issue of Life Magazine after the World War II. The yield (energy) of this atomic bomb was obviously classified, since this information is of primary military importance. Nevertheless, based only on published pictures (see Figure 3.8) Soviet scientists could obtain a fairly good estimate of the energy.

First of all, let us make two simplifications:

- The total amount of energy E was instantaneously released into a small volume
- The explosion results in a shock wave of radius $R(t)$ which expands into the undisturbed surrounding air of density ρ_a .

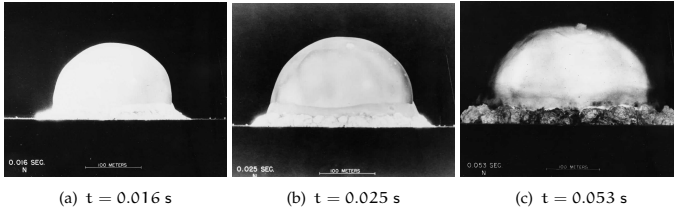


Figure 3.8.: Time laps of the Trinity test on July 16, 1945. © Atomic Heritage Foundation

In total, there are four physical parameters involved in this problem:

E : explosion energy, $[\text{kg} \cdot \text{m}^2 / \text{s}^2]$

t : time elapsed from the explosion, $[\text{s}]$

ρ_a : air density, $[\text{kg} / \text{m}^3]$

R : shock wave radius, $[\text{m}]$

There are three fundamental units (kg, m and s). So, according to the π -theorem there is only one dimensionless parameter in this problem. After a closer inspection we can find that the required dimensionless combination is

$$\pi_1 = C \frac{E t^2}{\rho_a R^5(t)}.$$

Henceforth, π_1 should be invariant during the expansion of the shock wave. Assuming the proportionality constant C is simply one and using time and distances thoroughly indicated by US Army on published photographs, one could estimate that the energy of the Trinity test was about 25 kilotons of TNT. A better estimate would require a test with dynamite in your garden thanks to the *similarity*¹² between these two problems.

3.5.5 Conclusions

To make an overall conclusion to this Section we would like to underline that the dimensional consistency of mathematical equations is the first test which allows to see whether the model derivation is correct. A straightforward dimensional analysis can provide us with an impressive amount information about the problem without solving (exactly or approximatively) any equations. Finally, understanding the relationship

¹² In the sense of similarity introduced in this Section just above.

among dimensionless parameters and their physical sense is of capital importance in studying a physical problem.

3.6 FLOW VISUALIZATION

In general there are four main types of characteristic curves, which can be used to visualize better a fluid flow. In this Section we describe briefly these curves, which appear regularly in CFD literature.

Suppose that a vector field $\mathbf{u}(\mathbf{x}, t) = (u(\mathbf{x}, t), v(\mathbf{x}, t), w(\mathbf{x}, t))$ is defined in a domain $\Omega \subseteq \mathbb{R}^3$. We assume that for any fixed time instant t this vector field is smooth enough to ensure the existence and unicity of integral curves. Then, a *stream line* $\mathbf{x}(s) = (x(s), y(s), z(s))$ passing through the point $\mathbf{x}(0) = \mathbf{a}$ is a solution to the following system of ODEs:

$$\frac{d\mathbf{x}}{ds} = \mathbf{u}(\mathbf{x}, t), \quad \mathbf{x}(0) = \mathbf{a}. \quad (3.16)$$

In the last system the time variable t is regarded as a parameter, which prescribes a continuous family of vector fields $\mathbf{u}(\mathbf{x}, t)$. By specifying various initial conditions $\mathbf{x}(0)$ distributed more or less uniformly in the domain Ω , one obtains a family of curves at each instant t . Notice that a stream line corresponds to a particle's trajectory in an autonomous vector field $\mathbf{u}(\mathbf{x})$.

A *path line* (or *particle path*) is the trajectory of a massless particle in a time-dependent vector field. Path lines are represented by solutions to the following system of ODEs:

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t), \quad \mathbf{x}(0) = \mathbf{a}. \quad (3.17)$$

One can notice that the systems (3.16) and (3.17) are identical for autonomous ODEs. It implies that stream lines and path lines are identical for steady fields. By the way, this system realizes also the connection between the Eulerian and Lagrangian descriptions of fluid flows (see Chapter 7 for more details).

A *streak line* is the locus of fluid particles which pass through a fixed location over time. In other words, a streak line is not a trajectory, but rather a collection of particles which passed by the same (specific) point. If we denote this point by \mathbf{a} , the streak-line will be represented parametrically as $\mathbf{x}(s) = \mathbf{x}(t - s; \mathbf{a})$, where $\mathbf{x}(t; \mathbf{a})$ solves the system (3.17). In experiments the streak lines can be visualized by releasing constantly the dye (or smoke in aerodynamics) into the flow in a constant point.

For steady flows, the stream, path and streak lines coincide and all give the same "portrait" of the flow. This is in contrast to *time lines*, which differ

CFD stands for the
Computational Fluid
Dynamics. Sometimes
to joke it is also called
Coloured Fluid
Dynamics ☺

from the other characteristic curves in both steady and unsteady vector fields. A *time line* is the collection of fluid particles advected over time starting from a fixed line arbitrarily chosen in the flow domain. So, a time line is not seeded at a point location, but along a line. The analogy in the real world experiment would consist in putting a perfectly flexible massless wire in the flow and watching its transport over the time. However, in contrast to the wire, a time line can change its length (become shorter or longer) depending on the flow configuration. For the computational recipes, but also to see some beautiful examples of how these concepts can be used in practice to visualize complex fluid flows, we refer to [WT12].

EXERCISES

1. Prove the following identities for the material derivative:

$$\begin{aligned}\frac{D(f+g)}{Dt} &= \frac{Df}{Dt} + \frac{Dg}{Dt} && \text{(linearity),} \\ \frac{D(f \cdot g)}{Dt} &= f \frac{Dg}{Dt} + g \frac{Df}{Dt} && \text{(product rule),} \\ \frac{D(f \circ g)}{Dt} &= (f' \circ g) \frac{Dg}{Dt} && \text{(chain rule),}\end{aligned}$$

where f' stands for the first derivative of function $f(\cdot)$ with respect to its argument.

2. (1 000 000\$ exercise ☺) Prove the *global existence* of 3D Navier–Stokes equations. To claim the reward, the reader has to publish his/her proof in a peer-reviewed journal and address it to the Clay Institute. For more details, please, consult this URL address:

<http://www.claymath.org/millennium-problems/>

4

WATER WAVE PROBLEM



Sunset and the surf wave at Andaman Sea. © Vitaliy Sokol

5

LAGRANGIAN VARIATIONAL PRINCIPLE

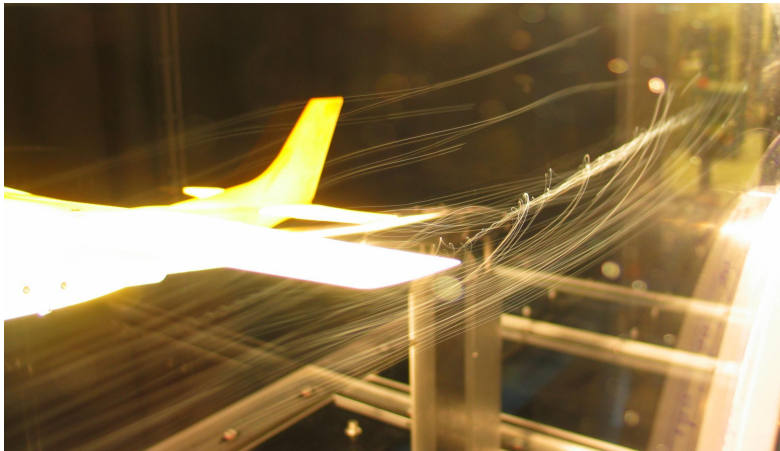
6

HAMILTONIAN FORMULATION

Part III

CONT. MECHANICS: LAGRANGIAN DESCRIPTION

There are at least two different descriptions of the flow field: Lagrangian and Eulerian (and all the mixed approaches). In the Lagrangian framework the observer follows individual fluid parcels. This can be visualized as sitting in a boat and drifting down a river. On the other hand, the Eulerian description focuses on specific locations in space as the fluid flows. It corresponds to sitting on the bank of a river and watching the water pass the fixed location. The Lagrangian formulation is analogue to Heisenberg's representation in Quantum Mechanics, while the Eulerian description is similar to Schrödinger's one. The names Eulerian/Lagrangian are completely conventional since both descriptions were proposed by Leonhard EULER (see a few historical remarks in Section [7.1](#) below).



A wind tunnel model of a Cessna 182 showing a wingtip vortex. Tested in the Rensselaer Polytechnic Institute Subsonic Wind Tunnel. © Wikimedia Commons

7

LAGRANGIAN FLUID DYNAMICS

One owes to Euler the first general formulas for fluid motion. . . presented in the simple and luminous notation of partial differences. . . By this discovery, all fluid mechanics was reduced to a single point analysis, and if the equations involved were integrable, one could determine completely, in all cases the motion of a fluid moved by any forces.

— J.-L. Lagrange (*Mécanique analytique*, 1788)

The Lagrangian description of fluid flows seems to be more natural than the Eulerian one since it is related directly to the motion of fluid particles (see Section 7.2 for the definition of fluid particle). The topics for which the Lagrangian description is particularly appropriate include various *transport* and *mixing* phenomena. The main applications include (but not limited to) geophysical flows (e.g. pollutant transport), combustion, microfluidics, etc. The main reason is that the advection of passive scalars can be treated without any numerical diffusion inherent to Eulerian methods.

The governing equations derived in Lagrangian setting (especially for viscous flows) seem to be intractable (so far). Consequently, nowadays the Eulerian formulation is used to determine the velocity field. Then, in the second time, the kinematic equations are integrated to obtain the trajectory of any fluid particle.

The relation between the Eulerian and Lagrangian formulations is really subtle. It seems that the Lagrangian equations have a potential to generate a much richer dynamics. There are clear experimental evidences [KO92] which show Lagrangian turbulence for simple Eulerian velocity fields at Reynolds numbers $Re \propto 1$. In other words, when a velocity field is turbulent in the Eulerian setting, it is also turbulent in the Lagrangian one. However, one can have a purely kinematic Lagrangian turbulence, which has no Eulerian counterpart (since the velocity field is laminar). It is manifested in experiments by a very complex structure of the passive tracer field, while the corresponding velocity field can be quite simple.

The reason for it is the following: the Eulerian turbulence is a dynamical phenomenon, while the Lagrangian one may be a purely kinematic one. We shall not discuss deeper the question of Lagrangian/Eulerian turbulence, since it is out of scope of the present manuscript. For this topic the interested reader can refer to [Tsi09].

Unfortunately, there is a very limited literature available on this topic. For instance, the classical monograph by H. LAMB [Lam32] (1932) contains a few sections on the Lagrangian formulation of Fluid Dynamics equations. The later monographs LANDAU & LIFSHITZ [LL87] (the 1st edition in 1959) and by G. BATCHELOR [Bat67] (1967) do not even provide the governing equations in the Lagrangian form. We are aware of only two modern books entirely devoted to the Lagrangian fluid mechanics: by A. BENNETT [Ben06] and by A. ABRASHKIN & E. YAKUBOVICH [AY06] (in Russian). Below we shall mainly follow the latter reference.

7.1 HISTORICAL REMARKS

The names Eulerian/Lagrangian are completely conventional since both descriptions were proposed by Leonhard EULER about 30 years before Joseph-Louis LAGRANGE. Moreover, there was a correspondence between L. EULER and J.-L. LAGRANGE and EULER communicated these ideas to LAGRANGE. For example, in the monograph of LAMB [Lam32] the name Lagrangian is written in quotes: “*Lagrangian*” *form of the equations of motion and of the equation of continuity*. There is a more complete discussion of this misnomer by C. TRUESDELL in [Tru54] (see pages 30–32 partially quoted here):

By the middle nineteenth century the history of fluid dynamics in the eighteenth century had apparently sunk into obscurity. Euler’s papers were not often read, of his results which were not forgotten several were attributed to more recent authors who had appropriated them without acknowledgement or discovered them afresh, and indeed his supreme achievements in mathematics, mechanics, and mathematical physics were undervalued then, though not so much as now. The erroneous terminology still current was introduced in the posthumous memoir of Dirichlet [1860, 1, Introd.], edited by Dedekind, where [1757, 2] was quoted as the source of the “Eulerian” method, while it was stated that Lagrange in the *Mécanique Analytique* [1788, 1, Part II, Sect. II, ¶4–7] had introduced the “Lagrangian” method, but had immediately converted the resulting equations to “Eulerian” form.

[...] The whole matter is easily clarified, however. In a letter, written to Lagrange under the date 27 October 1759, Euler after expressing his admiration for Lagrange's first memoir on the propagation of sound stated that one had reason to doubt that propagation in two or three dimensions would follow the same law as in the one dimensional case, since he has already found the fundamental equations to be of different form. The equations he gives are the linearized equations of plane flow of a perfect fluid expressed in terms of the variables X, Y .

The beginning of the modern vortex dynamics can be associated with the pioneering paper of H. HELMHOLTZ (1858) [Hel58]. The "golden age" of the study of vortex dynamics using the Lagrangian description can be ascribed approximatively to 1870 – 1920 when important results were obtained starting from the important work of G. KIRCHOFF (1876) [Kir76]. The application of Lagrangian methods for the study of water waves in the presence of vorticity starts with the work of F. GERSTNER (1809) [Ger09] and continues with important contributions by M.-L. DUBREIL-JACOTIN [DJ34] and R. GOUYON [Gou58]. In general, exact solutions obtained in Lagrangian description are much more precious than those obtained in the Eulerian one since a Lagrangian solution provides also the history of all particle trajectories in addition to the velocity field, given by the Eulerian solutions.

7.2 ON THE NOTION OF A FLUID PARTICLE

When a fluid flow is considered, it is assumed to be continuous. However, it is useful to introduce a discrete concept to develop a different point of view. This concept is usually referred to as the *fluid particle*. However, the term *fluid parcel* would be more accurate, but it is not generally accepted. So, a fluid particle in Fluid Mechanics has nothing to do with water H_2O or air O_2 molecules. A fluid particle is the fluid mass contained in a small volume dV whose size is small enough from the macroscopic point of view. On the other hand, this volume dV has to be large enough from the microscopic (*i.e.* intermolecular distance) viewpoint. The main constraint is that the number of molecules has to be sufficient to give sense to the statistical description, since we would like to get rid of local fluctuations. For example, if intermolecular distances scale with 10^{-6} mm under normal conditions, the fluid particle "*diameter*" will scale with 10^{-3} mm or even larger. Again, under the same normal conditions (*e.g.* 0° C and 760 mm Hg) a cube with a side equal to 10^{-3} mm contains about 10^7 molecules. It is considered to be enough to have stable statistical aver-

ages over this ensemble. Of course, for rarefied gases all these estimations have to be readjusted.

7.3 DERIVATION OF EQUATIONS

The basic idea of Lagrangian description consists in following the motion of fluid particles marked with some labels $\mathbf{a} = (a, b, c) \in \mathbb{R}^3$. If in the Eulerian description the spatial coordinates $\mathbf{x} = (x, y, z)$ are considered as independent variables, in Lagrangian description they become unknown functions of particle labels \mathbf{a} and time $t \in \mathbb{R}^+$. To underline this fact we will use capital letters to denote this functional dependence, *i.e.*

$$\mathbf{x} = \mathbf{X}(\mathbf{a}, t), \quad t \geq 0. \quad (7.1)$$

Let us describe how these labels appear in the fluid flow description. As before, the components of the velocity field are denoted with $\mathbf{u}(\mathbf{x}, t)$ and by definition we have

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t).$$

A general solution to this system of ODEs can be formally written as

$$\mathbf{x} = \mathbf{X}(t; \mathbf{a}),$$

where $\mathbf{X} = (X, Y, Z)$ are some functions of t and $\mathbf{a} = (a, b, c)$. The parameters (a, b, c) are three arbitrary integration constants, which have to be determined from the initial conditions:

$$\mathbf{X}(0; \mathbf{a}) = \mathbf{x}_0 \implies \mathbf{a} = \mathbf{X}^{-1}(0; \mathbf{x}_0).$$

It can happen that integration constants coincide with the initial positions of fluid particles $\mathbf{x}(0) = \mathbf{a}$, but in general it does not have to be the case. If they coincide, then the components (X, Y, Z) constitute the *flow map* introduced in Section 3.1.3.

So, these integration constants (a, b, c) can be viewed as a curvilinear coordinate system defined in the fluid domain. However, the “fluid” coordinate axes $\{(a, 0, 0) \mid a \in \mathbb{R}\}$, $\{(0, b, 0) \mid b \in \mathbb{R}\}$ and $\{(0, 0, c) \mid c \in \mathbb{R}\}$ can become quite stretched when represented in the original Euclidean space $(x, y, z) \in \mathbb{R}^3$ as the time (and flow) evolves. It is unnecessary to say that this coordinate system is in general *non-orthogonal* and *non-stationary*. In the rest of this Chapter we shall denote the arguments of particle trajectories on equal footing, *i.e.* $\mathbf{x} = \mathbf{X}(\mathbf{a}, t)$. In other words we forget what is the argument and what is the parameter. Particle labels \mathbf{a} and time t will be both the arguments.

The relation between two ways of fluid description is given by the following equation

$$\frac{\partial \mathbf{X}(\mathbf{a}, t)}{\partial t} = \mathbf{u}(\mathbf{X}(\mathbf{a}, t), t). \quad (7.2)$$

In the last equation the Lagrangian velocity field $\mathbf{V}(\mathbf{a}, t) = \frac{\partial \mathbf{X}(\mathbf{a}, t)}{\partial t}$ is related to the Eulerian velocity $\mathbf{u}(\mathbf{x}, t)$ by the nonlinear relation (7.2). We can summarize now. In order to pass from Lagrangian to Eulerian coordinates, one has to do three steps:

- Differentiate the function $\mathbf{X}(\mathbf{a}, t)$ with respect to time in order to obtain the velocity field as a function of labels $\mathbf{V}(\mathbf{a}, t) = \frac{\partial \mathbf{X}(\mathbf{a}, t)}{\partial t}$
- Invert relations (7.1) in order to express particle labels \mathbf{a} as functions of Eulerian coordinates, *i.e.* $\mathbf{a} = \mathbf{X}^{-1}(\mathbf{x}, t)$
- Substitute these expressions $\mathbf{a} = \mathbf{X}^{-1}(\mathbf{x}, t)$ into the Lagrangian velocity field $\mathbf{V}(\mathbf{a}, t)$ in order to obtain the Eulerian velocities $\mathbf{u}(\mathbf{x}, t) = \mathbf{V}(\mathbf{X}^{-1}(\mathbf{x}, t), t)$.

However, these transformations can be performed analytically only in some exceptional cases.

7.3.1 Mass conservation

Consider a domain $\Omega \in \mathbb{R}^3$ filled continuously with a fluid. Let us choose an arbitrary compact volume $V(t) \subseteq \Omega$ which evolves with the flow. Moreover we assume that its boundary $\partial V(t)$ always remains a closed surface (*i.e.* it does not undergo any topological changes). Then, a fluid particle \mathbf{a} situated initially in the point $\mathbf{x}_0 = \mathbf{X}(\mathbf{a}, t_0)$ will move to a new position $\mathbf{x} = \mathbf{X}(\mathbf{a}, t)$ when time changes from t_0 to t . This transformation applies to every particle of the volume $V(t_0)$, *i.e.*

$$V(t) = \phi_t(V(t_0), t),$$

where ϕ_t is the flow map defined in Section 3.1.3 (see also Figure 3.3 for an illustration). Similarly, the density of a fluid particle will change from $\rho(\mathbf{a}, t_0)$ to $\rho(\mathbf{a}, t)$. By using the conservation of mass principle, we can write the following identity

$$\int_{V(t_0)} \rho(\mathbf{a}, t_0) dV = \int_{V(t)} \rho(\mathbf{a}, t) dV, \quad (7.3)$$

where $dV = dx dy dz$ is the volume element. Let us make a change of

It would be more correct to write
 $dV = dx \wedge dy \wedge dz$.
See Appendix A.3 for more details.

variables in the last integral in order to integrate on the same domain \mathcal{T} parametrized¹ by particle labels $\mathcal{T} = \mathbf{X}^{-1}(\mathbf{V}(\mathbf{t}), \mathbf{t})$:

$$\int_{\mathbf{V}(\mathbf{t})} \rho(\mathbf{a}, \mathbf{t}) d\mathbf{V} = \int_{\mathcal{T}} \rho(\mathbf{a}, \mathbf{t}) J(\mathbf{a}, \mathbf{t}) d\mathbf{V}_a, \quad d\mathbf{V}_a = da db dc,$$

where $J(\mathbf{a}, \mathbf{t})$ is the determinant of the Jacobian matrix of the transformation $\mathbf{X}(\cdot, \mathbf{t}) : \mathbf{a} \mapsto \mathbf{x}(\mathbf{t})$, *i.e.*

$$J(\mathbf{a}, \mathbf{t}) = \frac{D\mathbf{X}(\mathbf{a}, \mathbf{t})}{D\mathbf{a}} \equiv \begin{vmatrix} X_a & Y_a & Z_a \\ X_b & Y_b & Z_b \\ X_c & Y_c & Z_c \end{vmatrix}(\mathbf{a}, \mathbf{t}),$$

where the subscripts a, b and c denote the partial derivatives. Below we shall use quite often the Jacobian matrix (not only its determinant $J(\mathbf{a}, \mathbf{t})$), which will be denoted as $\mathcal{J}(\mathbf{a}, \mathbf{t})$, *i.e.*

$$\mathcal{J}(\mathbf{a}, \mathbf{t}) := \begin{pmatrix} X_a & Y_a & Z_a \\ X_b & Y_b & Z_b \\ X_c & Y_c & Z_c \end{pmatrix}(\mathbf{a}, \mathbf{t}), \quad J(\mathbf{a}, \mathbf{t}) \equiv \det(\mathcal{J}(\mathbf{a}, \mathbf{t})).$$

In other words, the matrix \mathcal{J} gives the connection between an infinitely small change in Lagrangian labels $d\mathbf{a}$ and the change of the fluid element $d\mathbf{X}$ by this linear relation $d\mathbf{X} = \mathcal{J} d\mathbf{a}$.

After the last change of variables the condition (7.3) can be rewritten as

$$\int_{\mathcal{T}} (\rho(\mathbf{a}, t_0) J(\mathbf{a}, t_0) - \rho(\mathbf{a}, \mathbf{t}) J(\mathbf{a}, \mathbf{t})) d\mathbf{V}_a = 0.$$

Since the volume $\mathbf{V}(\mathbf{t})$ is completely arbitrary, the expression under the integral sign has to be equal to zero, which is equivalent to

$$\rho(\mathbf{a}, \mathbf{t}) J(\mathbf{a}, \mathbf{t}) = \rho(\mathbf{a}, t_0) J(\mathbf{a}, t_0), \quad \forall \mathbf{t} \in \mathbb{R}^+. \quad (7.4)$$

The last equality is the continuity equation written in Lagrange variables. For incompressible flows we have additionally the volume conservation property which can be expressed as

$$J(\mathbf{a}, \mathbf{t}) = J(\mathbf{a}, t_0), \quad \forall \mathbf{t} \in \mathbb{R}^+. \quad (7.5)$$

It shows that for incompressible flows the determinant $J(\mathbf{a}, \mathbf{t})$ does not depend on time, but only on Lagrangian variables \mathbf{a} .

¹ In mathematical terms we would say that the domain \mathcal{T} is the pre-image of the volume $\mathbf{V}(\mathbf{t})$ under the map $\mathbf{X}(\cdot, \mathbf{t}) : \mathbf{a} \mapsto \mathbf{x}(\mathbf{t})$, *i.e.* $\mathbf{X}(\mathcal{T}, \mathbf{t}) = \mathbf{V}(\mathbf{t})$.

Equation (7.4) can be further simplified if the particle labels \mathbf{a} are chosen as initial positions of fluid particles, i.e. $\mathbf{a} = \mathbf{x}(t_0)$, then

$$\begin{vmatrix} X_a & Y_a & Z_a \\ X_b & Y_b & Z_b \\ X_c & Y_c & Z_c \end{vmatrix} (\mathbf{a}, t_0) = \begin{vmatrix} \frac{\partial x(t_0)}{\partial a} & \frac{\partial y(t_0)}{\partial a} & \frac{\partial z(t_0)}{\partial a} \\ \frac{\partial x(t_0)}{\partial b} & \frac{\partial y(t_0)}{\partial b} & \frac{\partial z(t_0)}{\partial b} \\ \frac{\partial x(t_0)}{\partial c} & \frac{\partial y(t_0)}{\partial c} & \frac{\partial z(t_0)}{\partial c} \end{vmatrix} = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} = 1.$$

With this particular choice of labels, the continuity equation (7.4) reads

$$\rho(\mathbf{a}, t_0) = \rho(\mathbf{a}, t) J(\mathbf{a}, t).$$

Finally, under the same assumptions on the choice of particle labels, the continuity equation for incompressible flows (7.5) simply becomes:

$$J(\mathbf{a}, t) = \begin{vmatrix} X_a & Y_a & Z_a \\ X_b & Y_b & Z_b \\ X_c & Y_c & Z_c \end{vmatrix} (\mathbf{a}, t) = 1.$$

7.3.2 Momentum conservation

In order to obtain the momentum balance equation in Lagrangian variables, we start from the derived above momentum balance equation (3.8) in Eulerian iscid setting, where we replace the fluid velocity $\mathbf{u}(\mathbf{x}, t)$ by $\frac{d\mathbf{x}}{dt}$:

$$\frac{d^2 \mathbf{X}}{dt^2} = -\frac{1}{\rho} \nabla p + \mathbf{g}. \quad (7.6)$$

In many papers the last equation is claimed to have the Lagrangian form. However, it is not the case yet, since the pressure term contains the derivatives with respect to unknown functions $\mathbf{X}(\mathbf{a}, t)$. In order to eliminate this operation we shall multiply (in the sense of the scalar product) the vectorial equation (7.6) by \mathbf{X}_a , \mathbf{X}_b and \mathbf{X}_c to obtain

$$\begin{aligned} \frac{d^2 \mathbf{X}}{dt^2} \cdot \mathbf{X}_a &= -\frac{1}{\rho} \nabla p \cdot \mathbf{X}_a + \mathbf{g} \cdot \mathbf{X}_a, \\ \frac{d^2 \mathbf{X}}{dt^2} \cdot \mathbf{X}_b &= -\frac{1}{\rho} \nabla p \cdot \mathbf{X}_b + \mathbf{g} \cdot \mathbf{X}_b, \\ \frac{d^2 \mathbf{X}}{dt^2} \cdot \mathbf{X}_c &= -\frac{1}{\rho} \nabla p \cdot \mathbf{X}_c + \mathbf{g} \cdot \mathbf{X}_c. \end{aligned}$$

By noticing that $\nabla p \cdot \mathbf{X}_a = p_a$ (by the chain rule) and the same holds for derivatives with respect to b and c we obtain the required equations written in the vectorial form

$$\frac{d^2 \mathbf{X}}{dt^2} \cdot \nabla_a \mathbf{X} = -\frac{1}{\rho} \nabla_a p + \mathbf{g} \cdot \nabla_a \mathbf{X}, \quad (7.7)$$

The viscid case will be considered below in Section 7.5.

where $\nabla_{\mathbf{a}} = (\frac{\partial}{\partial a}, \frac{\partial}{\partial b}, \frac{\partial}{\partial c})$. The same equation can be rewritten also in scalar form for the sake of clarity:

$$\begin{aligned} X_{tt}X_a + Y_{tt}Y_a + Z_{tt}Z_a &= -\frac{1}{\rho}p_a + \mathbf{g} \cdot \mathbf{X}_a \\ X_{tt}X_b + Y_{tt}Y_b + Z_{tt}Z_b &= -\frac{1}{\rho}p_b + \mathbf{g} \cdot \mathbf{X}_b \\ X_{tt}X_c + Y_{tt}Y_c + Z_{tt}Z_c &= -\frac{1}{\rho}p_c + \mathbf{g} \cdot \mathbf{X}_c. \end{aligned}$$

Finally, it is not difficult to see that we can provide also a matrix form to the governing equations using the Jacobian matrix \mathcal{J} :

$${}^T \mathcal{J} \left(\frac{d^2 \mathbf{X}}{dt^2} - \mathbf{g} \right) = -\frac{1}{\rho} \nabla_{\mathbf{a}} p.$$

7.3.3 Weber transformation

If it turns out that the exterior body force \mathbf{g} is potential, *i.e.* there exists a scalar function $G(\mathbf{x})$, defined on the fluid domain, such that

$$\mathbf{g} = \nabla_{\mathbf{x}} G(\mathbf{x}),$$

where the gradient is taken with respect to Eulerian variables $\mathbf{x} = \mathbf{X}(\mathbf{a}, t)$. Such forces are also called conservative. For a conservative body force the momentum conservation equation (7.7) becomes:

$$\frac{d^2 \mathbf{X}}{dt^2} \cdot \nabla_{\mathbf{a}} \mathbf{X} = -\frac{1}{\rho} \nabla_{\mathbf{a}} p + \nabla_{\mathbf{a}} G.$$

These equations can be integrated in time from 0 to t to give:

$$\frac{d\mathbf{X}}{dt} \cdot \nabla_{\mathbf{a}} \mathbf{X} - \frac{d\mathbf{X}_0}{dt} \cdot \nabla_{\mathbf{a}} \mathbf{X}_0 = -\nabla_{\mathbf{a}} \Upsilon, \quad (7.8)$$

where $\mathbf{X}_0 = \mathbf{X}(\mathbf{a}, 0)$, $\frac{d\mathbf{X}_0}{dt} = \mathbf{X}_t(\mathbf{a}, 0)$ and the function Υ is defined as

$$\Upsilon = \int_0^t \left[G + \int \frac{d\mathbf{p}}{\rho} - \frac{1}{2} |\mathbf{X}_t|^2 \right] dt.$$

$\int \frac{d\mathbf{p}}{\rho}$ is a primitive function which satisfies the identity $\nabla_{\mathbf{a}} \int \frac{d\mathbf{p}}{\rho} = \frac{1}{\rho} \nabla_{\mathbf{a}} p$.

These equations were proposed for the first time by Max WEBER in 1868. In deriving equation (7.8) we used the following identity

$$\int_0^t \frac{d^2 \mathbf{X}}{dt^2} \cdot \nabla_{\mathbf{a}} \mathbf{X} dt = \frac{d\mathbf{X}}{dt} \cdot \nabla_{\mathbf{a}} \mathbf{X} - \frac{d\mathbf{X}_0}{dt} \cdot \nabla_{\mathbf{a}} \mathbf{X}_0 - \frac{1}{2} \nabla_{\mathbf{a}} \int_0^t |\mathbf{X}_t|^2 dt.$$

7.4 CHANGE OF VARIABLES

We saw in previous sections that the passage from Eulerian to Lagrangian form requires replacing the derivatives with respect to Eulerian variables $\mathbf{x} = \mathbf{X}(\mathbf{a}, t)$ by derivatives on Lagrangian labels \mathbf{a} . In this Section we derive the general transformation formulas.

Consider a function $f(\mathbf{x}, t)$ of Eulerian variables which might depend on time but it depends also on Lagrangian labels through particle trajectories $\mathbf{x} = \mathbf{X}(\mathbf{a}, t)$:

$$f(\mathbf{a}, t) = f(\mathbf{X}(\mathbf{a}, t), t).$$

We compute the gradient of $f(\mathbf{a}, t)$ with respect to labels using the chain rule:

$$\begin{aligned}\frac{\partial f}{\partial \mathbf{a}} &= \frac{\partial f}{\partial \mathbf{x}} X_{\mathbf{a}} + \frac{\partial f}{\partial y} Y_{\mathbf{a}} + \frac{\partial f}{\partial z} Z_{\mathbf{a}}, \\ \frac{\partial f}{\partial \mathbf{b}} &= \frac{\partial f}{\partial \mathbf{x}} X_{\mathbf{b}} + \frac{\partial f}{\partial y} Y_{\mathbf{b}} + \frac{\partial f}{\partial z} Z_{\mathbf{b}}, \\ \frac{\partial f}{\partial \mathbf{c}} &= \frac{\partial f}{\partial \mathbf{x}} X_{\mathbf{c}} + \frac{\partial f}{\partial y} Y_{\mathbf{c}} + \frac{\partial f}{\partial z} Z_{\mathbf{c}}.\end{aligned}$$

The last identities can be seen as a system of linear algebraic equations with respect to Eulerian derivatives $\frac{\partial f}{\partial \mathbf{x}}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$ as unknowns. The system matrix is precisely the Jacobian $\mathcal{J}(\mathbf{a}, t)$:

$$\mathcal{J} \cdot \nabla_{\mathbf{x}} f = \nabla_{\mathbf{a}} f.$$

From Linear Algebra we know that the solution to this system can be obtained analytically using, for example, the Cramer's rule:

$$\frac{\partial f}{\partial \mathbf{x}} = \frac{1}{J} \begin{vmatrix} f_{\mathbf{a}} & Y_{\mathbf{a}} & Z_{\mathbf{a}} \\ f_{\mathbf{b}} & Y_{\mathbf{b}} & Z_{\mathbf{b}} \\ f_{\mathbf{c}} & Y_{\mathbf{c}} & Z_{\mathbf{c}} \end{vmatrix}, \quad J = \det(\mathcal{J}),$$

provided that the transformation $\mathbf{x} = \mathbf{X}(\mathbf{a}, t)$ is non-singular, i.e. $J(\mathbf{a}, t) \neq 0, \forall t \in \mathbb{R}^+$. Similar expressions can be written for other partial derivatives. To shorten the notation, it is convenient to introduce a shorthand notation for the above determinant situated in the nominator $[f, Y, Z]$, where the gradient $\nabla_{\mathbf{a}}$ of each vector is taken and written in the corresponding column of the determinant. Please, note that *the value of the determinant does not change under a circular rotation of its columns* (and rows as well, by the way). The other derivatives read

$$\frac{\partial f}{\partial y} = \frac{1}{J} [X, f, Z], \quad \frac{\partial f}{\partial z} = \frac{1}{J} [X, Y, f].$$

One can give a general formula using the index notation:

$$\frac{\partial f}{\partial x_i} = \frac{1}{J} [X_j, X_k, f], \quad (7.9)$$

where (i, j, k) is a cyclic permutation of $(1, 2, 3)$. The expressions for second order derivatives will be given in the following Section.

7.5 VISCOUS FLUIDS

In this Section we shall give the Navier–Stokes equations in Lagrangian variables. The momentum balance equation for an incompressible Newtonian fluid was given above in (3.12). It will be our starting point of the derivation:

$$\frac{d^2 X}{dt^2} = -\frac{1}{\rho} \nabla p + \mathbf{g} + \nu \nabla^2 \mathbf{u}, \quad (7.10)$$

where we just replaced $\frac{D\mathbf{u}}{Dt}$ by $\frac{d^2 X}{dt^2}$. As it was already the case for inviscid flows, we cannot say that the momentum balance equation above is written in the Lagrangian form since the right-hand side contains the derivatives with respect to Eulerian variables $\mathbf{x} = \mathbf{X}(\mathbf{a}, t)$. So, we have to express in terms of derivatives with respect to Lagrangian labels \mathbf{a} . The pressure gradient ∇p is readily obtained by applying formula (7.9):

$$\frac{\partial p}{\partial x_i} = \frac{1}{J} [X_j, X_k, p], \quad i = 1, 2, 3.$$

In order to express the Laplace operator in terms of derivatives with respect to particle labels, we have to know how to compute the second order partial derivatives. Let us take a function $f(\mathbf{x}, t)$ and apply two times the formula (7.9):

$$\frac{\partial^2 f}{\partial x_i^2} = J^{-1} [X_j, X_k, J^{-1} [X_j, X_k, f]], \quad i = 1, 2, 3.$$

Then, the Laplace operator ∇^2 will be given by the sum of three partial derivatives. Finally, the momentum balance equation (7.10) in Lagrangian form written for the component X_i will read [Ger49]

$$\frac{d^2 X_i}{dt^2} = -(\rho J)^{-1} [X_j, X_k, p] + \mathbf{g} + \nu J^{-1} \left\{ [X_2, X_3, J^{-1} [X_2, X_3, X_i]] + [X_3, X_1, J^{-1} [X_3, X_1, X_i]] + [X_1, X_2, J^{-1} [X_1, X_2, X_i]] \right\}, \quad i = 1, 2, 3.$$

The last equation may look very cumbersome. However, some further simplification can be achieved if we choose the particle labels according to their initial locations. By using the continuity equation it will yield $J \equiv 1$.

It is worth to mention that in the Eulerian formulation the advection operator is nonlinear ($\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u}$), while viscous terms are linear. This situation is completely inverse in the Lagrangian description. Namely, the advection becomes linear, while the dissipative term becomes of the fifth order in nonlinearity (please, check it) and fortunately the second order in derivatives (as in the Eulerian description).

8

VARIATIONAL STRUCTURE

9

LONG WAVES

10 | SOME EXACT SOLUTIONS

10.1 GERSTNER WAVE

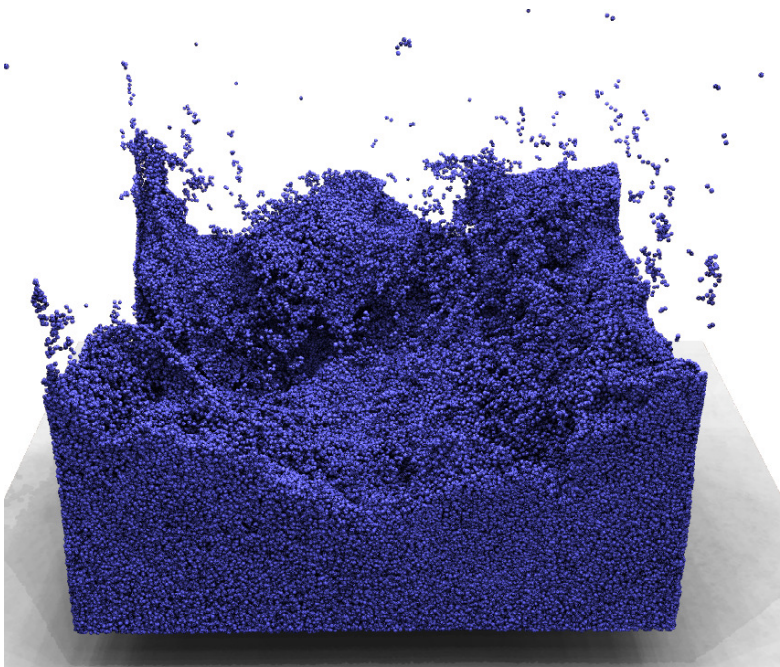
11

SMOOTHED PARTICLE HYDRODYNAMICS

In this Chapter we shall describe a numerical method which is situated in between the Eulerian and Lagrangian descriptions. Namely, the underlying formulation is Eulerian, strictly speaking. However, the idea to describe the flow in terms of fluid parcels (*i.e.* “particles”) is borrowed from the Lagrangian description.

The Smoothed Particle Hydrodynamics (SPH) method was proposed by L. LUCY [Luc77] & R. GINGOLD & J. MONAGHAN [GM77] in Astrophysics to simulate star and galaxy formation. Much later it was applied to the simulation of free surface flows in a seminal paper of J. MONAGHAN [Mon94]. Some key ideas of this method (without the numerical implementation) can be also found in works of R. SALMON [Sal88], before it has become one of the standard methods in hydrodynamics.

As general comprehensive references on the SPH method we could probably suggest the review paper by J. MONAGHAN [Mon05]. An extension to MHD is explained in [Pri12b]. For Russian-speaking readers we could recommend the review paper by A. ALIEV & G. TARNAVSKY [AT07]. Below we shall follow the great lines of these excellent expositions.



SPH fluid simulation. © Frank Zimmer

11.1 WHY PARTICLE METHODS?

There are well-established grid-based methods such as finite differences, finite volumes and finite elements. So, what is the motivation to develop particle-based (or meshless) methods? It turns out that the absence of a rigid topological structure of the mesh is beneficial in situations where topological changes may occur. An emblematic example is the wave breaking phenomenon. So, the main advantages of particle-based methods over mesh-based ones are summarized here:

- Treatment of large deformations is easy
- The advection is solved exactly (without any numerical diffusion)
- Identifying the free surface or another interface is easy
- Atomization (e.g. splashing) and other topological changes (e.g. fragmentation, collision) are seamless.

From this description particle-based methods appear to be the ideal choice for most free surface flows simulations. However, some drawbacks of the SPH method will be discussed below in Section 11.4.

We would like to stress out one more time that the particles used in the SPH method are purely numerical concepts which are introduced in order to discretize the governing equations. These “particles” have nothing to do with the fluid particles discussed in Section 7.2.

11.2 PARTICLE INTERPOLATION

The Smoothed Particle Hydrodynamics (SPH) method starts with the following applied mathematical question: given an arbitrary distribution of particles, carrying some physical quantities, how to reconstruct a continuous field? One answer on this question passes through the integral interpolation methods. For any function $g(\mathbf{x}) : \Omega \rightarrow \mathbb{R}$ defined in a domain $\Omega \in \mathbb{R}^d$, $d = 1, 2, 3$. This function can be represented as an integral using the Dirac δ -function:

$$g(\mathbf{x}) = \int_{\Omega} g(\mathbf{y}) \delta(\mathbf{x} - \mathbf{y}) dV_{\mathbf{y}}.$$

However, due to the nature of the Dirac function, this identity would produce a discrete approximation of the continuous field, i.e. all the information is concentrated in particle locations. Consequently, we shall regularize the δ -function by replacing it with a suitable smoothing kernel $W(\mathbf{x}, h)$, where h is a parameter which characterizes the smoothing

The function $g(\mathbf{x})$ can be, for example the pressure, velocity, temperature or any other quantity appearing in the description of a fluid flow.

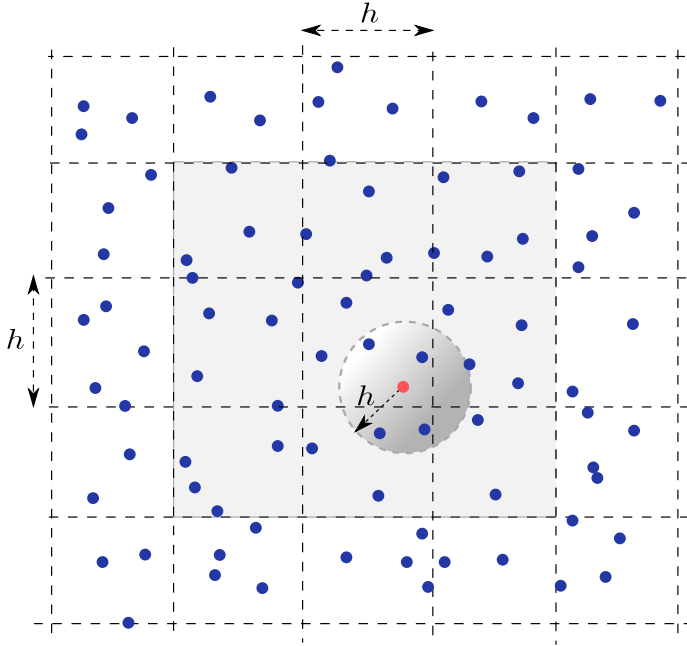


Figure 11.1.: Interpolation in the SPH method. The active particle is shown in Red. The underlying grid is used only to locate the candidates of neighbouring particles. The surrounding cells are shown in Grey. By h we denote the compact support length of the SPH kernel $W(\mathbf{r}, h)$.

length. This function has to satisfy at least two following natural conditions:

$$\int_{\Omega} W(\mathbf{x} - \mathbf{y}, h) dV_{\mathbf{y}} = 1, \quad \lim_{h \rightarrow 0} W(\mathbf{x} - \mathbf{y}, h) = \delta(\mathbf{x} - \mathbf{y}).$$

Now we can define a smoothed variant of the integral interpolation by taking a convolution with the smoothing kernel $W(\mathbf{x}, h)$:

$$\hat{g}(\mathbf{x}) = \int_{\Omega} g(\mathbf{y}) W(\mathbf{x} - \mathbf{y}, h) dV_{\mathbf{y}}. \quad (11.1)$$

Even if the initial function $g(\mathbf{x})$ was not smooth enough, after the convolution operation against a smooth kernel, we can easily differentiate the resulting function $\hat{g}(\mathbf{x})$ under the integral sign:

$$\nabla \hat{g}(\mathbf{x}) = \int_{\Omega} g(\mathbf{y}) \nabla_{\mathbf{x}} W(\mathbf{x} - \mathbf{y}, h) dV_{\mathbf{y}},$$

Notice that the smoothed function $\hat{g}(\mathbf{x})$ is different from $g(\mathbf{x})$, but hopefully not too different as the smoothing length $h \rightarrow 0$. In fact, the application of the convolution operation results in a *blurred* (or smoothed) version of $g(\mathbf{x})$. It is this smoothing property which is responsible of the first 'S' in the name of the SPH method. The smoothing kernels appeared already in works of Russian/Soviet mathematicians Vladimir A. STEKLOV and Sergei L. SOBOLEV much time before the introduction of the SPH method.

Now we have to discretize the convolution formula (11.1) using N_p discrete particles. It turns out that the way to express $\hat{g}(\mathbf{x})$ is

$$\hat{g}(\mathbf{x}) = \sum_{i=1}^{N_p} g(\mathbf{x}_i) W(\mathbf{x} - \mathbf{x}_i, h) \Delta V_i = \sum_{i=1}^{N_p} \frac{m_i}{\rho_i} g_i W(\mathbf{x} - \mathbf{x}_i, h), \quad (11.2)$$

where $g_i \equiv g(\mathbf{x}_i)$; $m_i, \rho_i, i = 1, \dots, N_p$ are correspondingly masses and densities of fluid "particles". In the formula above we used the relation $\Delta V_i = \frac{m_i}{\rho_i}$, which gives the volume of an SPH particle i . We need precisely the volume (in 3D), since the integral (11.1) is taken with respect to volume and not the mass.

The resulting representation (11.2) is very useful since it provides us with a smooth function $\hat{g}(\mathbf{x})$ from knowing the initial function $g(\mathbf{x})$ in a set of discrete locations $\mathbf{x}_i, i = 1, \dots, N_p$. Please, notice also that we do not guarantee that $\hat{g}(\mathbf{x}_i) = g(\mathbf{x}_i)$, but hopefully the difference will not be too big.

Remark 11.1 (Shepard correction). *In order to improve the consistency of the SPH representation (11.2) close to boundaries, one can adopt an improved version which takes the following form proposed by Donald SHEPARD [She68]:*

$$\dot{g}(\mathbf{x}) = \frac{\sum_{i=1}^{N_p} \frac{m_i}{\rho_i} g_i W(\mathbf{x} - \mathbf{x}_i, h)}{\sum_{i=1}^{N_p} \frac{m_i}{\rho_i} W(\mathbf{x} - \mathbf{x}_i, h)}.$$

By taking $g(\mathbf{x}) = \rho(\mathbf{x})$, we can obtain an important application of formula (11.2):

$$\dot{\rho}(\mathbf{x}) = \sum_{i=1}^{N_p} m_i W(\mathbf{x} - \mathbf{x}_i, h).$$

The last representation provides us with a smoothed form of the density in any point $\mathbf{x} \in \Omega$ of the fluid domain. For instance, the representation (11.2) can be also differentiated to compute numerically the derivatives of the function $g(\mathbf{x})$:

$$\nabla \dot{g}(\mathbf{x}) = \sum_{i=1}^{N_p} \frac{m_i}{\rho_i} g_i \nabla_{\mathbf{x}} W(\mathbf{x} - \mathbf{x}_i, h), \quad (11.3)$$

where the gradient of the smoothing kernel can be easily computed

$$\nabla_{\mathbf{x}} W(\mathbf{x} - \mathbf{x}_i, h) = \frac{\mathbf{x} - \mathbf{x}_i}{|\mathbf{x} - \mathbf{x}_i|} \frac{\partial W(r, h)}{\partial r}.$$

The last derivation formula (11.3) is slightly too straightforward. Below we shall propose an alternative version which has better numerical conservation and thus properties.

Historically, the first smoothing kernel function employed by GINGOLD & MONAGHAN (1977) [GM77] was the Gaussian kernel which takes the form

$$W(r, h) = \frac{\omega}{h^d} e^{-(r/h)^2}, \quad r = |\mathbf{x} - \mathbf{y}|,$$

where the normalization constant ω depends on the problem dimension d

$$\omega = \pi^{-\frac{d}{2}}.$$

This kernel is infinitely smooth and hence exhibits good accuracy properties. However, this function does not have the compact support. This disadvantage makes it a poor choice from the computational point of view. In order to reduce drastically the number of interacting particles, it is better to choose a smoothing function with compact support. Such a kernel can be constructed, for example, using spline functions. A very popular kernel nowadays with compact support is given by a cubic spline:

We say that a function has compact support if it is identically equal to zero outside of an interval.

There are obviously other options for the kernel function choice, but we do not provide them here. The reader can find them in the abundant literature on the SPH method.

$$W(\mathbf{r}, h) = \frac{\omega}{h^d} \begin{cases} 1 - \frac{3}{2}\kappa^2 + \frac{3}{4}\kappa^3, & 0 \leq \kappa < 1, \\ \frac{1}{4}(2 - \kappa)^3, & 1 \leq \kappa < 2, \\ 0, & 2 \leq \kappa \end{cases} \quad \kappa := \frac{r}{h}, \quad r = |\mathbf{x} - \mathbf{y}|,$$

where the normalization constant depends again on the dimension d

$$\omega = \begin{cases} \frac{2}{3}, & d = 1, \\ \frac{10}{7\pi}, & d = 2, \\ \frac{1}{\pi}, & d = 3. \end{cases}$$

One can see now that the support of this kernel is compact and it is confined to the domain $|\mathbf{x} - \mathbf{y}| < 2h$. It has an important consequence for the practical computer implementation of the SPH method: we have to count only interactions among the particles which have the supports with *non-zero intersection*. If we have in total N_p particles, there are $C_{N_p}^2 = \frac{N_p(N_p-1)}{2} \propto \mathcal{O}(N_p^2)$ pairs. However, only a small fraction of these pairs contribute to the balance of forces of an active particle due to the compact support property of the kernel $W(\mathbf{r}, h)$. Another hint to a successful SPH implementation is shown on Figure 11.1. Namely, one can use a fixed underlying grid with the spacing equal to the compact support width (*i.e.* $2h$ for the cubic spline kernel). The candidate particles to have a non-zero interaction are located in the same cell with the active particle, but also in adjacent cells. In total, it implies that one has to test particles from only 9 cells in $2D^1$. In this way the algorithm complexity diminishes considerably from N_p^2 to roughly $N_p \log N_p$.

A good smoothing kernel function $W(\mathbf{r}, h)$ should satisfy the following properties:

- It is normalized, *i.e.* $\int_{\mathbb{R}^d} W(\mathbf{r}, h) dV = 1$
- It has a compact support
- It is a positive monotonic function of r . Partially negative or oscillating smoothing kernels can lead to unphysical results
- In the limit $h \rightarrow 0$ it tends to the Dirac δ -function $\lim_{h \rightarrow 0} W(\mathbf{x} - \mathbf{y}, h) = \delta(\mathbf{x} - \mathbf{y})$
- It is an even function of $\mathbf{r} = \mathbf{x} - \mathbf{y}$ (to guarantee at least the 2^{nd} order accuracy of the approximation).

¹ Please, count how many cells one has to visit in 1D and in 3D?

Let us show, for example, the last property. For this purpose we assume the function $g(\mathbf{x})$ to be smooth enough in a neighbourhood of a point \mathbf{x} . By applying the 3rd order Taylor expansion one obtains

$$\begin{aligned} \dot{g}(\mathbf{x}) &= \int_{\mathbb{R}^d} g(\mathbf{y}) W(\mathbf{x} - \mathbf{y}, h) dV_{\mathbf{y}} = \int_{\mathbb{R}^d} \left[g(\mathbf{x}) + (\mathbf{x} - \mathbf{y}) \cdot \nabla_{\mathbf{y}} g(\mathbf{x}) + \right. \\ &\quad \left. \frac{1}{2} ((\mathbf{x} - \mathbf{y}) \cdot \nabla_{\mathbf{x}})^2 g(\mathbf{x}) + \mathcal{O}(|\mathbf{x} - \mathbf{y}|^3) \right] W(\mathbf{x} - \mathbf{y}, h) dV_{\mathbf{y}} = \\ g(\mathbf{x}) &\underbrace{\int_{\mathbb{R}^d} W(\mathbf{x} - \mathbf{y}, h) dV_{\mathbf{y}}}_{=1, \text{ by normalization}} + \nabla_{\mathbf{x}} g(\mathbf{x}) \cdot \underbrace{\int_{\mathbb{R}^d} (\mathbf{x} - \mathbf{y}) W(\mathbf{x} - \mathbf{y}, h) dV_{\mathbf{y}}}_{=0 \text{ by parity}} + \\ &\frac{1}{2} \int_{\mathbb{R}^d} ((\mathbf{x} - \mathbf{y}) \cdot \nabla_{\mathbf{x}})^2 g(\mathbf{x}) W(\mathbf{x} - \mathbf{y}, h) dV_{\mathbf{y}} = g(\mathbf{x}) + \mathcal{O}(h^2). \end{aligned}$$

Consequently, in smooth regions the convolution representation (11.1) is 2nd order accurate.

11.2.1 Particle pairing

Particle pairing refers to a numerical phenomenon where two particles stick together. This issue can appear in SPH simulations almost instantly when the ratio of smoothing length to particle spacing $h/\Delta > 1.5$ (in the standard cubic spline kernel given above). In 3D it corresponds to about 100 neighbours. Particle pairing (or *merging*) occurs almost for sure when $h/\Delta > 1.3$ (i.e. more than 65 neighbours in 3D). The explanation of this phenomenon is simple. The interaction force between two particles is given by the gradients on interaction kernels. Since the kernel function is an even function, its derivative is small in the neighbourhood of the origin $\mathbf{r} = |\mathbf{x} - \mathbf{y}| = 0$. This means, that if two particles are initially close enough, the interaction force is no longer strong enough to repel them. The solution to this problem is simple [Pri12c]. The user has to limit the number of neighbours by adjusting the smoothing length h .

11.3 DISCRETIZATION OF EQUATIONS

First, we consider the conservative case of Euler equations. Dissipative terms will be treated separately below (see Section 11.3.2). In view of the discretization using particles, it is convenient to use the Euler equations in the following semi-Lagrangian form:

This form of equations is usually referred to in the literature as the Lagrangian form. However, it is not fully correct. See Chapter 7 for more details.

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}, \quad (11.4)$$

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{u}, \quad (11.5)$$

$$\frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho} \nabla p, \quad (11.6)$$

The first equation is needed as well, since it describes the kinematics of fluid particles. This set of equations can be eventually completed by the energy equation in the following form

$$T \frac{Ds}{Dt} = 0, \quad T \text{ is the thermodynamic temperature,}$$

which simply means that the entropy is conserved by fluid particles (in the absence of shock waves or other entropy production mechanisms).

The pressure remains unspecified in the system (11.4) – (11.6) above. One possibility would be to assume the flow incompressible and determine the pressure from the pressure Poisson equation. An incompressible SPH projection method was proposed and applied for the first time in [CR99]. The projection scheme [Cho68] is based upon the Helmholtz–Hodge decomposition of a vector field. However, this method requires solving of one Poisson equation in \mathbb{R}^d per time step. This operation is quite CPU-time consuming. Consequently, we suggest to assume the fluid to be (quasi-)compressible. In this case the pressure is computed through an Equation of State (EOS). The most common form of EOS used in SPH simulations is

$$p_i(\rho_i) = \frac{\rho_{0i} c_{si}^2}{\gamma} \left[\left(\frac{\rho_i}{\rho_{0i}} \right)^\gamma - 1 \right],$$

where ρ_{0i} is the reference density of particle i and γ is the polytropic constant. For a liquid phase $\gamma = 7$ and $\gamma = 1.4$ for a gaseous phase (e.g. dry air). Of course, other values can be set for your particular application. The speed of sound in such medium can be easily computed

$$c_{si} \equiv c_s(\rho_i) = \sqrt{\left. \frac{\partial p}{\partial \rho} \right|_{\rho=\rho_i}},$$

where the derivative is taken by keeping the entropy s constant.

Another option consists in using the ideal gas EOS:

$$p(\rho, \epsilon) = (\gamma - 1)\rho\epsilon,$$

where ϵ is the internal energy. However, the usage of this EOS requires the inclusion into our system of an additional energy equation. This complication is not necessarily uninteresting.

11.3.1 Semi-discrete scheme

In order to discretize the Euler equation (11.5), (11.5) in the semi-Lagrangian form, we apply the method of lines. Namely, it consists in discretizing first the equations in space to obtain a semi-discrete system of coupled ODEs and only then this ODE system is discretized in time to provide us with a fully discrete scheme (see Section 11.3.3). Equation (11.4) is already an ODE, so its discretization in space is straightforward

$$\frac{d\mathbf{x}}{dt} = \mathbf{u} \implies \frac{d\mathbf{x}_i}{dt} = \mathbf{u}_i.$$

11.3.1.1 Continuity equation

Let us apply the SPH discretization to continuity equation (11.5). A straightforward differentiation turns out not to be conservative. In order to improve this point we rewrite equation (11.5) in a mathematically equivalent way (for sufficiently smooth functions):

$$\frac{D\rho}{Dt} = \nabla \cdot (\rho \mathbf{u}) - \mathbf{u} \cdot \nabla \rho.$$

Now we can apply the SPH gradient estimation (11.3) to the first and second terms separately:

$$\frac{d\rho_i}{dt} = \sum_{j=1}^{N_p} \frac{m_j}{\rho_j} \rho_j \mathbf{u}_j \cdot \nabla_j W_{ij} - \mathbf{u}_i \sum_{j=1}^{N_p} \frac{m_j}{\rho_j} \rho_j \nabla_j W_{ij},$$

or after some simplifications we finally obtain the requested semi-discrete form:

$$\frac{d\rho_i}{dt} = - \sum_{j=1}^{N_p} m_j (\mathbf{u}_i - \mathbf{u}_j) \nabla_j W_{ij}.$$

11.3.1.2 Momentum equation

As the reader could already intuit, the discretization cannot be applied straightforwardly to equation (11.6). In order to obtain a conservative scheme, we have to apply a similar trick to the momentum conservation equation as we did with the continuity equation above. Namely, we use the following identity:

$$\nabla \left(\frac{p}{\rho} \right) = \frac{1}{\rho} \nabla p - \frac{p}{\rho^2} \nabla \rho.$$

or put another way around

$$-\frac{1}{\rho} \nabla p = -\nabla \left(\frac{p}{\rho} \right) - \frac{p}{\rho^2} \nabla \rho.$$

Thus, equation (11.6) can be equivalently rewritten (again under the assumption that all functions are sufficiently smooth) as

$$\frac{D\mathbf{u}}{Dt} = -\nabla \left(\frac{p}{\rho} \right) - \frac{p}{\rho^2} \nabla \rho.$$

SPH discretization of two terms on the right hand side can be obtained according to (11.3):

$$\begin{aligned} \nabla \rho &= \sum_{j=1}^{N_p} \frac{m_j}{\rho_j} \rho_j \nabla_j W_{ij} = \sum_{j=1}^{N_p} m_j \nabla_j W_{ij}, \\ \nabla \left(\frac{p}{\rho} \right) &= \sum_{j=1}^{N_p} \frac{m_j}{\rho_j} \frac{p_j}{\rho_j} \nabla_j W_{ij} = \sum_{j=1}^{N_p} m_j \frac{p_j}{\rho_j^2} \nabla_j W_{ij}. \end{aligned}$$

Combining all ingredients together we obtained the momentum equation discretization:

$$\frac{d\mathbf{u}_i}{dt} = - \sum_{j=1}^{N_p} m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \nabla_j W_{ij}.$$

11.3.2 Viscous terms

The SPH formulation presented so far has been fully conservative both at the continuous (see equations (11.4) – (11.6)) and at the discrete levels. However, sometimes the viscous effects have to be added, because they are present in Physics of our flow or for some numerical reasons. These two situations will be discussed below.

11.3.2.1 Artificial viscosity

In numerical simulations involving strong shock waves some viscosity is required. First of all, the propagation of a shock wave is necessarily accompanied by the production of entropy. Therefore it is obvious that if we do not include any dissipation, then our solution will fail to reproduce the right physical behaviour. A way to correct this drawback consists in simply including an artificial viscosity of von Neumann–Richtmyer type

(named after J. VON NEUMANN (1903 – 1957) and Robert D. RICHTMYER (1910 – 2003)). The force \mathbf{F}_i exerted on particle i will read now

$$\mathbf{F}_i = - \sum_{j=1}^{N_p} m_i m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} + \Pi_{ij} \right) \nabla_j W_{ij},$$

with the artificial viscosity term Π_{ij} given by

$$\Pi_{ij} = -\alpha h \frac{c_{si} + c_{sj}}{\rho_i + \rho_j} \frac{(\mathbf{u}_i - \mathbf{u}_j) \cdot \mathbf{r}_{ij}}{r_{ij}^2 + \varepsilon h^2}.$$

Here α is a positive constant controlling the dissipation strength, the term with $\varepsilon \propto 10^{-2}$ allows to avoid singularities when particles are too close to each other. This artificial viscosity corresponds to an *effective* kinematic viscosity ν equal to

$$\nu = \frac{1}{8} \alpha h c_s.$$

11.3.2.2 Laminar Navier–Stokes viscosity

A straightforward computation of second order derivatives from the SPH representation (11.2) results in huge numerical errors, since the employed particle interpolation scheme is only 2nd order accurate. Consequently, a smarter approach has to be used [MFZ97]. The main idea is to use the Taylor expansion, assuming that particles i and j are close

$$\mathbf{u}_j = \mathbf{u}_i + \nabla \mathbf{u} \cdot (\mathbf{x}_j - \mathbf{x}_i) + \mathcal{O}(|\mathbf{x}_j - \mathbf{x}_i|^2),$$

or after rearranging the terms

$$\mathbf{u}_i - \mathbf{u}_j = \nabla \mathbf{u} \cdot (\mathbf{x}_j - \mathbf{x}_i) + \mathcal{O}(|\mathbf{x}_j - \mathbf{x}_i|^2).$$

By neglecting the reminder term, the velocity gradient $\nabla \mathbf{u}|_{\mathbf{x}_i}$ can be estimated as

$$\nabla \mathbf{u}|_{\mathbf{x}_i} \approx \frac{(\mathbf{u}_i - \mathbf{u}_j) \otimes \mathbf{r}_{ij}}{r_{ij}^2},$$

where $\mathbf{r}_{ij} = \mathbf{x}_i - \mathbf{x}_j$. The viscous term $\frac{1}{\rho} \nabla \cdot (\mu \nabla \mathbf{u})$ in the Navier–Stokes equations is discretized in SPH method as

$$\left(\frac{1}{\rho} \nabla \cdot (\mu \nabla \mathbf{u}) \right)_i = \sum_{j=1}^{N_p} \frac{m_j (\mu_i + \mu_j) \mathbf{r}_{ij} \cdot \nabla_j W_{ij}}{\rho_i \rho_j (r_{ij}^2 + \varepsilon h^2)} (\mathbf{u}_i - \mathbf{u}_j),$$

where $\mu_i = \rho_i \nu$ is the dynamic viscosity. Finally, the force appearing in the Navier–Stokes momentum equation discretized with SPH reads

$$\mathbf{F}_i = - \sum_{j=1}^{N_p} m_i m_j \left(\frac{\mathbf{p}_i}{\rho_i^2} + \frac{\mathbf{p}_j}{\rho_j^2} \right) \nabla_j W_{ij} + \sum_{j=1}^{N_p} \frac{m_i m_j (\mu_i + \mu_j) \mathbf{r}_{ij} \cdot \nabla_j W_{ij}}{\rho_i \rho_j (r_{ij}^2 + \varepsilon h^2)} (\mathbf{u}_i - \mathbf{u}_j).$$

Here a small $\varepsilon \propto 10^{-2}$ term is added to improve the robustness of the implementation.

Alternatively, one can take a more general form $\frac{1}{\rho} \nabla \cdot \boldsymbol{\tau}$ of the viscous term in the Navier–Stokes equation, which is more suitable for the modeling of non-Newtonian fluids. Its discretization in the SPH framework reads

$$\left(\frac{1}{\rho} \nabla \cdot \boldsymbol{\tau} \right)_i = \sum_{j=1}^{N_p} m_j \left(\frac{\boldsymbol{\tau}_i}{\rho_i^2} + \frac{\boldsymbol{\tau}_j}{\rho_j^2} \right) \cdot \nabla_j W_{ij}.$$

11.3.3 Fully discrete scheme

After applying the particle discretization in space as described above, we obtain a system of ODEs:

$$\begin{aligned} \frac{d\mathbf{u}_i}{dt} &= \mathbf{F}_i, \\ \frac{d\mathbf{x}_i}{dt} &= \mathbf{u}_i, \\ \frac{d\rho_i}{dt} &= D_i, \end{aligned}$$

where \mathbf{F}_i is the sum of forces acting on particle i and D_i is the discretization of $-(\rho \nabla \cdot \mathbf{u})_i$. In order to obtain a fully discrete scheme, we apply the following two-stages Verlet scheme, where the superscripts denote $\mathbf{u}_i^{(n)} = \mathbf{u}_i(t_n) = \mathbf{u}_i(t_0 + n\Delta t)$. Then, the first stage reads

$$\begin{aligned} \mathbf{u}_i^{(n+\frac{1}{2})} &= \mathbf{u}_i^{(n)} + \frac{\Delta t}{2} \mathbf{F}_i^{(n)}, \\ \mathbf{x}_i^{(n+\frac{1}{2})} &= \mathbf{x}_i^{(n)} + \frac{\Delta t}{2} \mathbf{u}_i^{(n)}, \\ \rho_i^{(n+\frac{1}{2})} &= \rho_i^{(n)} + \frac{\Delta t}{2} D_i^{(n)}. \end{aligned}$$

During the first stage all variables are propagated during $\Delta t/2$. Then, the forces can be evaluated at $\mathbf{t} = \mathbf{t}_n + \frac{\Delta t}{2}$ since the velocities $\mathbf{u}_i^{(n+\frac{1}{2})}$ are known. Finally, during the second stage mid-point particle velocities, positions and densities are updated to their values at $\mathbf{t} = \mathbf{t}_{n+1}$:

$$\begin{aligned}\mathbf{u}_i^{(n+1)} &= \mathbf{u}_i^{(n)} + \Delta t \mathbf{F}_i^{(n+\frac{1}{2})}, \\ \mathbf{x}_i^{(n+1)} &= \mathbf{x}_i^{(n+\frac{1}{2})} + \frac{\Delta t}{2} \mathbf{u}_i^{(n+1)}, \\ \rho_i^{(n+1)} &= \rho_i^{(n+\frac{1}{2})} + \frac{\Delta t}{2} D_i^{(n+1)}.\end{aligned}$$

Obviously, the most expensive step in SPH simulations is the computation of forces $\mathbf{F}_i(\mathbf{u}, \mathbf{x})$.

11.3.3.1 Stability

The scheme proposed above is fully explicit. Thus, for the stability of the discrete solution the time step Δt has to satisfy the following Courant–Friedrichs–Lewy (CFL) condition [CFL28]:

$$\Delta t \leq \frac{h}{2c_s},$$

where h is the smoothing length and c_s is the maximal speed of sound in the simulation. For instance, in multi-fluid simulations c_s represents the largest speed of sound. This condition is named after Richard COURANT (1888 – 1972), Kurt Otto FRIEDRICH (1901 – 1982) and Hans LEWY (1904 – 1988).

Remark 11.2 (CFL Limit). *In the presence of viscous laminar terms the CFL condition on the time step Δt has to be modified in this way*

$$\Delta t \leq \frac{h^2}{8\nu},$$

where ν is the lowest kinematic viscosity.

11.4 A BLACK FLY IN YOUR CHARDONNAY

The SPH method was applied successfully to many problems in Hydrodynamics. However, in this particular Section we would like to discuss the drawbacks of this method, since its main advantages were already outlined in Section 11.1 and can be found in abundant SPH literature. For

The same expression in Russian-speaking cultures would be: “A spoon of tar in a barrel of honey.”

instance, we would like to mention a recent extensive numerical study devoted to the SPH method [BS12], which compared it to some other methods based on fixed and moving meshes. They found that the standard SPH formulation (as it is implemented in GADGET-3 code) fails to reproduce correctly turbulence in the subsonic regime (see Figure 11.2 taken from that study and discussion of these results in [Pri12a]). Namely, the large-scale eddies are quickly damped and decay into small-scale velocity noise. The authors argue that the origin of this noise lies in errors committed in estimating the gradients, especially for the comparatively irregular particle distributions. Moreover they think that:

[...] the problems of SPH in resolving subsonic turbulence are fundamental. It is unlikely that they can be solved by just increasing the resolution or the number of smoothing neighbours, the latter is anyway problematic due to the tensile instability.

For more details, please refer to “*Discussion and conclusions*” section in [BS12] and references therein. We could also add that the performance of the SPH method for incompressible flows is relatively poor, since the method does not guarantee the conservation of volume $V = \sum_{i=1}^{N_p} \frac{m_i}{\rho_i}$ (in contrast to the exact conservation of mass). In general it is advantageous to introduce some weak compressible effects into the code through the equation of state $p = p(\rho, s)$ in order to avoid the CPU-time consuming Poisson equation solving (which adjusts the pressure to satisfy the incompressibility constraint). The absence of numerical dissipation was listed above among the advantages. However, the same point can be a disadvantage as well. It means that in all situations where dissipation is required physically, the corresponding terms have to be explicitly added. Several other “popular” critics of the SPH method (such as the tensile instability, particles pairing, *etc.*) were discussed in [Pri12c, Pri12a]. We invite the readers to have a look on these quite interesting references as well.

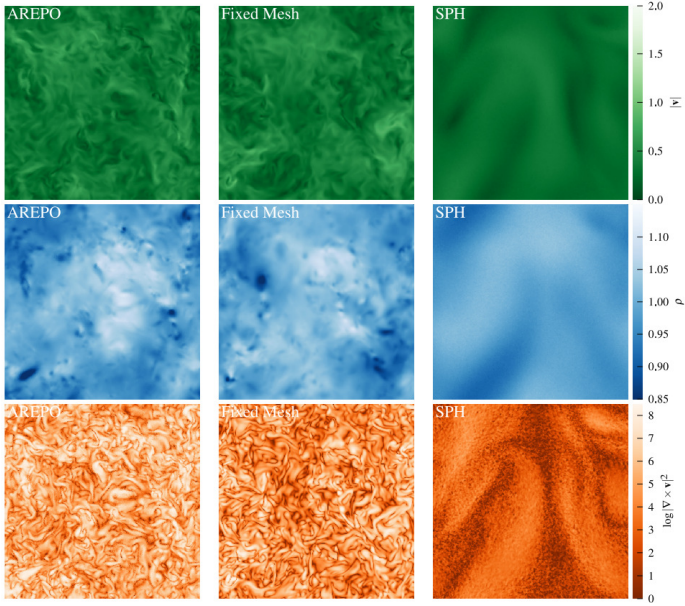


Figure 11.2.: A comparison of a subsonic turbulent fluid simulated in a moving mesh code (left), in fixed-grid mode (center), and the SPH code Gadget-3. Taken from [BS12].

Part IV

APPENDIX

A

MATHEMATICAL TOOLS

*Do not worry about your difficulties in Mathematics.
I can assure you mine are still greater.*

— Albert Einstein

I am acutely aware of the fact that the marriage between mathematics and physics, which was so enormously fruitful in past centuries, has recently ended in divorce.

— Freeman Dyson (*Missed Opportunities*, 1972)

In this auxiliary Chapter we shall briefly introduce some mathematical tools which are used in the main text above. Some of these tools (such as the differential forms, for example) can make some objects more precise (e.g. the physical force, the mechanical work, etc.) and simplify greatly the work with them in the Continuum Mechanics.

A.1 FRÉCHET DERIVATIVE

Named after Maurice FRÉCHET, the Fréchet derivative generalizes the operation of differentiation on Banach spaces. It defines the functional derivative extensively used in the calculus of variations. The Fréchet derivative has numerous applications in physics and nonlinear functional analysis.

Definition A.1. Let \mathcal{U} and \mathcal{V} be Banach spaces. A functional $F : \mathcal{U} \mapsto \mathcal{V}$ is said to be Fréchet differentiable at $\mathbf{u} \in \mathcal{U}$ if there exists a bounded linear operator $dF(\mathbf{u}) : \mathcal{U} \mapsto \mathcal{V}$ such that

$$\lim_{\mathbf{h} \rightarrow 0} \frac{\|F(\mathbf{u} + \mathbf{h}) - F(\mathbf{u}) - dF(\mathbf{u})[\mathbf{h}]\|_{\mathcal{V}}}{\|\mathbf{h}\|_{\mathcal{U}}} = 0.$$

If the limit exists $dF(\mathbf{u})$ is called the Fréchet derivative of the functional F at \mathbf{u} .

A functional $F : \mathcal{U} \mapsto \mathcal{V}$ which has a Fréchet derivative in every point $\mathbf{u} \in \mathcal{U}$ is said to be of class C^1 if the following map is continuous

$$\begin{aligned} dF : \mathcal{U} &\mapsto L(\mathcal{U}, \mathcal{V}), \\ \mathbf{u} &\mapsto dF_{\mathbf{u}}, \end{aligned}$$

where $L(\mathcal{U}, \mathcal{V})$ is a set of linear bounded functionals. Note that this notion is fundamentally different from the continuity of the derivative functional $dF(\mathbf{u})[h]$.

A.1.1 Properties

The Fréchet differentiation operation is linear, *i.e.* if both $F, G : \mathcal{U} \mapsto \mathcal{V}$ are differentiable at \mathbf{u} , then $\alpha F + \beta G$ is also differentiable and

$$d(\alpha F + \beta G)(\mathbf{u}) = \alpha dF(\mathbf{u}) + \beta dG(\mathbf{u}).$$

The usual chain rule is also valid for the Fréchet derivative. Let the functionals $F : \mathcal{U} \mapsto \mathcal{V}$ and $G : \mathcal{V} \mapsto \mathcal{W}$ are such that the following diagram commutes

$$\begin{array}{ccccc} \mathcal{U} & \xrightarrow{F} & \mathcal{V} & \xrightarrow{G} & \mathcal{W} \\ & \searrow & & \nearrow & \\ & & G \circ F & & \end{array}$$

We assume that F is differentiable at \mathbf{u} and the functional G is differentiable at $\mathbf{v} = F(\mathbf{u})$. Then, the chain rule reads

$$d(G \circ F)(\mathbf{u}) = dG(\mathbf{v}) \circ dF(\mathbf{u}).$$

If \mathcal{U} and \mathcal{V} are finite dimensional spaces, the Fréchet derivative reduces to the usual derivation operation. In this case, the linear differentiation operator d can be conveniently represented with the Jacobian matrix J :

$$dF : \mathbb{R}^n \mapsto \mathbb{R}^m, \quad J_{\mathbf{u}} := dF(\mathbf{u}), \quad J_{\mathbf{u}} \in \text{Mat}_{n \times m}(\mathbb{R}).$$

For the Fréchet differentiability in the finite dimensional settings it is sufficient that all partial derivatives of a function F exist and are continuous.

A.1.2 Higher derivatives

The derivative $dF : \mathcal{U} \mapsto L(\mathcal{U}, \mathcal{V})$ of a differentiable functional $F : \mathcal{U} \mapsto \mathcal{V}$ is also a function from \mathcal{U} to another Banach space (of linear bounded operators operators from \mathcal{U} to \mathcal{V}). This function dF may also be

This particular Banach space is called the dual space.

differentiable. In this case, this derivative will be called the *second order derivative*

$$d^2F : \mathcal{U} \mapsto \mathcal{L}(\mathcal{U}, \mathcal{L}(\mathcal{U}, \mathcal{V})) \simeq \mathcal{L}^2(\mathcal{U} \times \mathcal{U}, \mathcal{V}),$$

where the dual space $\mathcal{L}(\mathcal{U}, \mathcal{L}(\mathcal{U}, \mathcal{V}))$ is isomorphic to the space of bounded continuous bilinear operators $\mathcal{L}^2(\mathcal{U} \times \mathcal{U}, \mathcal{V})$. This process can be continued by induction to higher order derivatives if they exist.

A.2 GÂTEAUX DERIVATIVE

The Gâteaux derivative, named after René GÂTEAUX, a young brilliant French mathematician who died during the World War I, is a generalization of the classical directional derivative to Banach spaces. Similarly to Fréchet derivative, the Gâteaux differential is used to formalize the functional derivatives commonly used in physics and calculus of variations.

Banach spaces can be replaced by more general locally convex topological vector spaces.

Definition A.2. Let \mathcal{U} and \mathcal{V} be Banach (or other locally convex topological) spaces and $F : \mathcal{U} \mapsto \mathcal{V}$ is a map. If the following limit exists

$$dF(\mathbf{u})[\mathbf{h}] := \lim_{\varepsilon \rightarrow 0} \frac{F(\mathbf{u} + \varepsilon \mathbf{h}) - F(\mathbf{u})}{\varepsilon} = \left. \frac{d}{d\varepsilon} F(\mathbf{u} + \varepsilon \mathbf{h}) \right|_{\varepsilon=0}, \quad (\text{A.1})$$

it is called the Gâteaux differential $dF(\mathbf{u})[\mathbf{h}]$ at $\mathbf{u} \in \mathcal{U}$ in the direction $\mathbf{h} \in \mathcal{U}$. If the limit (A.1) exists for all $\forall \mathbf{h} \in \mathcal{U}$ then F is said to be Gâteaux differentiable at \mathbf{u} .

A.2.1 Properties

In every point $\mathbf{u} \in \mathcal{U}$ where the map F is differentiable, its Gâteaux differential defines a homogeneous function in the second argument

$$dF(\mathbf{u})[\cdot] : \mathcal{U} \mapsto \mathcal{V} \quad \text{such that} \quad dF(\mathbf{u})[\alpha \mathbf{h}] \equiv \alpha dF(\mathbf{u})[\mathbf{h}].$$

However, this map is not necessarily additive and continuous in \mathbf{h} , as it will be shown below.

The chain rule holds also for the Gâteaux derivative and reads

$$d(G \circ F)(\mathbf{u})[\mathbf{h}] = dG(F(\mathbf{u})) [dF(\mathbf{u})[\mathbf{h}]],$$

where the maps F and G satisfy the same conditions as in the previous section. However, the chain rule is not generally true if the derivatives are discontinuous.

A.2.1.1 Relation with the Fréchet derivative

If a map F is differentiable in the sense of Fréchet, then it is also differentiable in the sense of Gâteaux. The converse is not true since the Fréchet derivative is necessarily linear, while the Gâteaux derivative may be a nonlinear function. So, the Gâteaux differentiability does not necessarily imply the existence of a derivative in the sense of Fréchet.

EXAMPLE IN FINITE DIMENSION. In order to illustrate these different notions, let us consider the following finite-dimensional real-valued function $F : \mathbb{R}^2 \mapsto \mathbb{R}$:

$$F(x, y) = \begin{cases} \frac{y^3}{x^2 + y^2}, & \text{if } (x, y) \neq (0, 0) \\ 0, & \text{if } (x, y) = (0, 0). \end{cases}$$

The Gâteaux derivative of this function can be easily computed:

$$dF(0, 0)[s, t] = \begin{cases} \frac{t^3}{s^2 + t^2}, & \text{if } (s, t) \neq (0, 0) \\ 0, & \text{if } (s, t) = (0, 0). \end{cases}$$

Now it is obvious that the derivative $dF(0, 0)$ is not linear in the directions (s, t) .

A.2.2 Higher derivatives

Higher order Gâteaux derivatives in the direction h are defined as

$$d^n F(u)[h] := \left. \frac{d^n}{d\varepsilon^n} F(u + \varepsilon h) \right|_{\varepsilon=0}, \quad n > 0.$$

Note that function $d^n F(u)[h]$ is not a multilinear function in its second argument h , in contrast to the Fréchet derivative. However, it is still a homogeneous function of order n in the argument h .

Using higher order derivatives, one can write also a Taylor expansion if $F \in C^k$

$$\begin{aligned} F(u + h) = & F(u) + dF(u)[h] + \frac{1}{2!} d^2 F(u)[h] + \dots \\ & \dots + \frac{1}{(k-1)!} d^{k-1} F(u)[h] + R_k(u)[h], \end{aligned}$$

where R_k is the remainder term. If the segment $[u, u + h] \in \mathcal{U}$, then one can write the remainder term R_k in the integral form given by

$$R_k(u)[h] = \frac{1}{(k-1)!} \int_0^1 (1-t)^{k-1} d^k F(u + th)[h] dt.$$

A.2.3 Example in infinite dimensions

Finally, let us show how these tools can be applied to compute the variation of a real-valued *nonlinear* functional $\mathcal{F} : L^2(\Omega) \mapsto \mathbb{R}$, where $L^2(\Omega)$ is the Hilbert space of square integrable functions on a Lebesgue measurable set $\Omega \subseteq \mathbb{R}^n$. This functional \mathcal{F} is given by the following integral

$$\mathcal{F}(u) = \int_{\Omega} F(u(x)) dx, \quad u : \Omega \mapsto \mathbb{R}, \quad F(u) \in L^2(\Omega), \quad (\text{A.2})$$

where the kernel $F(\cdot)$ is assumed to be a differentiable function. Let us compute the Gâteaux derivative of (A.2) by following the Definition A.2:

$$\begin{aligned} \frac{\mathcal{F}(u + \varepsilon h) - \mathcal{F}(u)}{\varepsilon} &= \frac{1}{\varepsilon} \left[\int_{\Omega} F(u + \varepsilon h) dx - \int_{\Omega} F(u) dx \right] = \\ &= \frac{1}{\varepsilon} \int_{\Omega} \int_0^1 \frac{d}{d\tau} F(u + \varepsilon \tau h) d\tau dx = \int_{\Omega} \int_0^1 F'(u + \varepsilon \tau h) h d\tau dx. \end{aligned}$$

After taking the limit $\varepsilon \rightarrow 0$ we obtain the required Gâteaux derivative

$$d\mathcal{F}(u)[h] = \int_{\Omega} F'(u(x)) h(x) dx.$$

The latter integral is nothing else but the inner scalar product $\langle F', h \rangle$ in the Hilbert space $L^2(\Omega)$.

A.3 EXTERIOR CALCULUS

*To Thales the primary question was not what do we know,
but how do we know it.*

— Aristotle

In this Section we shall introduce informally some notions of the exterior algebra and exterior differential calculus. Moreover, we shall illustrate their usage on several examples from the Calculus and Mechanics.

The vectorial calculus turns out to be very useful in the three-dimensional space \mathbb{R}^3 due to its very special mathematical structure. For instance, the

Without entering into details for the moment, we shall say that $n = 3$ turns out to be the only solution to the equation $C_2^n = n$, where C_k^n is a binomial coefficient. See below for the explanations.

usual vectorial product $\mathbf{a} \times \mathbf{b}$ of two vectors \mathbf{a} and \mathbf{b} is, in fact, a mathematical trick which works only in \mathbb{R}^3 . A mathematically sound generalization of the Vectorial Calculus to higher dimensional (and eventually non-flat) spaces is given by the Exterior Calculus, whose flavour we shall give below. The exposition will be conducted for simplicity in \mathbb{R}^d , $d = 2, 3$. However, the generalization to any other Euclidean space \mathbb{R}^n , $n > 3$ is straightforward.

The basics of the exterior calculus stem from the pioneering works of H. POINCARÉ and É. CARTAN in the beginning of the XXth century.

A.3.1 0-forms

By convention, any function $\omega = f(x, y, z)$ will be called a 0-form.

A.3.2 1-forms

The application of a 1-form on a vector is simply a real number. A basis in \mathbb{R}^3 is given by three independent (and orthonormal) vectors \mathbf{e}_1 , \mathbf{e}_2 and \mathbf{e}_3 , a 1-form can be defined simply by its action on the basis elements, since any other vector $\mathbf{u} \in \mathbb{R}^3$ can be decomposed into a linear combination

$$\mathbf{u} = u_1 \mathbf{e}_1 + u_2 \mathbf{e}_2 + u_3 \mathbf{e}_3.$$

In a similar way we can introduce a basis in the space of 1-forms. For example, there exists a unique 1-form, that we will denote as dx , such as

$$dx(\mathbf{e}_1) = 1, \quad dx(\mathbf{e}_2) = 0, \quad dx(\mathbf{e}_3) = 0.$$

We would like to underline that dx is *not related to any infinitesimal quantity*. It is just a generally adopted notation to denote one particular differential form. In a similar way one can define 1-forms dy and dz . Now it is easy to compute the action of dx , dy , dz on the vector \mathbf{u} :

$$dx(\mathbf{u}) = u_1, \quad dy(\mathbf{e}_2) = u_2, \quad dz(\mathbf{e}_3) = u_3.$$

In the Classical Mechanics the forces correspond to 1-forms. The *mechanical work*, for example, is given by the application of this differential form on the displacement vector (it is assumed implicitly that the displacement is done under the action of this force).

We note also that the integral calculus of 1-differential forms can be developed as well. It results in a generalization of the usual curvilinear integral from the Calculus.

A.3.3 2-forms

The elementary 1-forms introduced in the previous Section serve as *atoms* to construct more complex objects. For this person we shall need an

additional algebraic operation — the so-called *exterior* or *wedge* product¹, which allows to construct 2-forms from the “atoms”, e.g. $\omega = dx \wedge dy$. The formal definition can be found in any textbook on the exterior algebra. Here we shall recall only the main properties of this operation:

We can also recommend a very comprehensive book by M. SPIVAK [Spi71].

ASSOCIATIVITY: $(de_1 \wedge de_2) \wedge de_3 = de_1 \wedge (de_2 \wedge de_3)$

ANTI-COMMUTATIVITY: (valid only for the forms of degree one)

$$de_1 \wedge de_2 = -de_2 \wedge de_1$$

DISTRIBUTIVITY ON THE LEFT:

$$de_1 \wedge (\alpha de_2 + \beta de_3) = \alpha de_1 \wedge de_2 + \beta de_1 \wedge de_3$$

DISTRIBUTIVITY ON THE RIGHT:

$$(\alpha de_1 + \beta de_2) \wedge de_3 = \alpha de_1 \wedge de_3 + \beta de_2 \wedge de_3$$

NILPOTENCY: (it is a direct corollary of the anti-commutativity) $de \wedge de = 0$ (valid only for the forms of degree one)

In the Euclidean space \mathbb{R}^n the basis of 2-forms consists of all the elements $de_i \wedge de_j$, where $\{e_i\}$, $i = 1, \dots, n$ is an orthonormal basis in \mathbb{R}^n . The dimension of this space is equal to $C_2^n = \frac{n(n-1)}{2}$. It can be noticed that for $n = 3$ (and *only* for $n = 3$!) the dimension of this space is equal to n as well. As a consequence, it is custom to associate in \mathbb{R}^3 the wedge product $de_i \wedge de_j$ with the vector product and represent it with the vector normal to the plane spanned by e_i and e_j . However, we would like to bring the reader's attention to the fact that this representation is *impossible* in any other dimension $n \neq 3$.

¹ The proper definition of the wedge product of two polylinear forms $p(e_1, \dots, e_m)$ and $q(e_1, \dots, e_n)$ involves the alternator operation

$$p \wedge q := \frac{(m+n)!}{m!n!} \text{Alt}[p \otimes q],$$

where the alternator $\text{Alt}(\omega)$, $\deg \omega = n$, is defined as

$$\text{Alt}[\omega](e_1, e_2, \dots, e_n) := \frac{1}{n!} \sum_{\sigma \in S_n} \text{sign } \sigma \cdot \omega(e_{\sigma(1)}, e_{\sigma(2)}, \dots, e_{\sigma(n)}).$$

In this definition the summation is taken over all the elements of the symmetric group S_n (i.e. the permutations). Notice the similarities with the definition of the determinant in the Linear Algebra.

A.3.4 k-forms

In a similar way, the 1-forms (or “atoms”) can be combined together using the wedge product to produce k-forms, e.g. $\omega = de_{i_1} \wedge \dots \wedge de_{i_k}$. The number k is also called the degree of a form ω and it is noted as $k = \deg \omega$. It is easy to see that the dimension of the space of all k-forms is equal to $C_k^n = \frac{n!}{k!(n-k)!}$. The wedge product for k-forms is not commutative in general, as a direct consequence of this formula:

$$p \wedge q = (-1)^{\deg p \cdot \deg q} q \wedge p.$$

As it was noticed earlier, the nilpotency property $\omega \wedge \omega = 0$ holds for the differential forms of degree one. However, the nilpotency does not hold in general, as it follows from the example below. Consider a 2-differential form $\omega = dt \wedge dx + dy \wedge dz$. Direct computations show that

$$\omega \wedge \omega = 2dt \wedge dx \wedge dy \wedge dz.$$

A.3.5 n-forms

The n-forms in \mathbb{R}^n have a special geometrical meaning. Namely, it is the right type of product to compute an element of the volume

$$dV = de_1 \wedge de_2 \wedge \dots \wedge de_n.$$

This form can be directly used to compute the signed volume of parallelepipeds and through the integration the volumes of more general domains.

Remark A.1. *For the sake of completeness we shall mention that the volume V of a domain $\Omega \subset \mathbb{R}^3$ bounded by a closed surface $S = \partial\Omega$ can be computed using the following surface integral:*

$$V = \frac{1}{3} \iint_S x \, dy \wedge dz + y \, dz \wedge dx + z \, dx \wedge dy.$$

A.3.6 External derivation

The external derivative operation transforms a k-form into a $(k+1)$ -form. Again, instead of giving formal definitions we shall provide the reader with several important examples. The general principle can be understood from them:

- Let $\omega = f(x, y, z)$ be a 0-form. Then, trivially one can obtain

$$d\omega = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz$$

We can see that $d\omega$ represents the gradient of the function $f(x, y, z)$. From this example one can see that the gradient is not a vector, but a 1-form.

- Now let us take a 1-form $\omega = p(x, y, z) dx + q(x, y, z) dy + r(x, y, z) dz$. Its derivation can be performed in three steps. The first step will be given explicitly here:

$$\begin{aligned} d(p(x, y, z)dx) &= \left(\frac{\partial p}{\partial x} dx + \frac{\partial p}{\partial y} dy + \frac{\partial p}{\partial z} dz \right) \wedge dx = \\ &= -\frac{\partial p}{\partial y} dx \wedge dy - \frac{\partial p}{\partial z} dx \wedge dz \end{aligned}$$

After performing similar manipulations with other terms and gathering all the results, one obtains

$$\begin{aligned} d\omega &= \left(-\frac{\partial p}{\partial y} + \frac{\partial q}{\partial x} \right) dx \wedge dy + \left(-\frac{\partial q}{\partial z} + \frac{\partial r}{\partial y} \right) dy \wedge dz + \\ &\quad + \left(-\frac{\partial p}{\partial z} + \frac{\partial r}{\partial x} \right) dx \wedge dz \quad (\text{A.3}) \end{aligned}$$

This time $d\omega$ coincides with the rotational operator of a vector field.

- As a final example, let us take a 2-form $\omega = r(x, y, z) dx \wedge dy + p(x, y, z) dy \wedge dz + q(x, y, z) dz \wedge dx$. Its derivative can be readily computed to give

$$d\omega = \left(\frac{\partial p}{\partial x} + \frac{\partial q}{\partial y} + \frac{\partial r}{\partial z} \right) dx \wedge dy \wedge dz$$

As a result, one can recognize the divergence operator of a vector field.

From these examples one can see that all common operators of the vectorial calculus in 3D can be obtained as exterior derivatives of some differential forms. The main advantage of the language of differential forms is twofold:

- It is independent of the dimension,
- It is independent of the chosen coordinate system.

The general algorithm to compute the exterior derivative is the following. One takes an elementary differential form $\omega = f(x_1, \dots, x_n) d\mathbf{e}_{i_1} \wedge \dots \wedge d\mathbf{e}_{i_k}$ and computes the usual differential of the coefficient $df = \frac{\partial f}{\partial x_1} d\mathbf{e}_1 + \dots + \frac{\partial f}{\partial x_n} d\mathbf{e}_n$. Then, every obtained term in the direction $d\mathbf{e}_i$ has to be multiplied externally by $d\mathbf{e}_{i_1} \wedge \dots \wedge d\mathbf{e}_{i_k}$ to produce a

The rotation $\nabla \times \mathbf{F}$ and divergence $\nabla \cdot \mathbf{F}$ operators were both introduced by J. C. MAXWELL. However, he considered the quantity $-\nabla \cdot \mathbf{F}$ that he referred to as the convergence.

$(k+1)$ -form $d\mathbf{e}_i \wedge d\mathbf{e}_{i_1} \wedge \dots \wedge d\mathbf{e}_{i_k}$. Finally, the resulting expression $d\omega = \sum_{i=1}^n \frac{\partial f}{\partial x_i} d\mathbf{e}_i \wedge d\mathbf{e}_{i_1} \wedge \dots \wedge d\mathbf{e}_{i_k}$ has to be simplified using the properties of the wedge product.

The following result describes all higher order exterior derivatives:

Lemma A.1 (H. POINCARÉ).

$$d^2\omega = d(d\omega) = 0.$$

This Lemma shows that the structure of the exterior derivation is very simple and all higher order derivatives are equal precisely to zero. Instead of making the complete proof, we will just provide here an explicit calculation for a particular 0-form $\omega = f(x, y)$, which illustrates the main idea of the proof:

$$d\omega = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy,$$

$$d^2\omega = d(d\omega) = \left(-\frac{\partial^2 f}{\partial y \partial x} + \frac{\partial^2 f}{\partial x \partial y}\right) dx \wedge dy \equiv 0.$$

A.3.6.1 Derivative of the product

The following result generalizes the usual formula for the derivative of the product of two functions to the exterior product of two differential forms:

$$d(\omega_1 \wedge \omega_2) = d\omega_1 \wedge \omega_2 + (-1)^{\deg \omega_1} \omega_1 \wedge d\omega_2. \quad (\text{A.4})$$

In some cases it can facilitate the derivation of differential forms, which can be decomposed into the products of simpler ones. The integration by parts of differential forms is based on this result as well (see Section A.3.7.1 for more details).

A.3.6.2 Application to conservation laws

The conservation laws are omnipresent in Physics in general and, in particular, in Continuum Mechanics. Let $u(x, t)$ denote a conservative quantity (e.g. the density, momentum, energy, etc.) and $F(u)$ be its flux. Then, the conservation equation takes the following form:

$$\frac{\partial u}{\partial t} + \nabla \cdot F(u) = 0. \quad (\text{A.5})$$

In the language of differential forms this equation has a simple geometric interpretation. For simplicity, we consider the case with one spatial

dimension first. Consider an arbitrary element in space-time with dimensions dx and dt along with the differential form $\omega = u dx - F dt$. Then, the conservation law (A.5) has the following elegant form $d\omega = 0$. In the space of higher dimensions this elegant writing remains invariant. However, one has to redefine the differential form ω . In three spatial dimensions one has to consider the following differential form:

The differential forms having the property $d\omega = 0$ are called closed.

$$\omega = u dx \wedge dy \wedge dz - (F_1 dy \wedge dz + F_2 dz \wedge dx + F_3 dx \wedge dy) \wedge dt.$$

The sign $-$ in front of the second term comes from the convention to consider the outgoing normal, which implies that the incoming flux is, thus, negative.

A.3.7 Integration of differential forms

The integration theory for differential forms on manifolds can be also developed [Spi71]. Here we provide only the central result of this theory:

Theorem A.1. *Let S be a compact oriented k -dimensional manifold with a border ∂S , which has an implied orientation. Let ω be a $(k-1)$ -form on S . Then the following equality holds*

$$\int_S d\omega = \int_{\partial S} \omega,$$

Below we will consider the most important corollaries of this fundamental theorem of the calculus on manifolds.

A.3.7.1 Integration by parts

We assume that all assumptions of the Stokes theorem A.1 hold. Using the Stokes theorem along with a product derivation formula (A.4), one readily obtains the following rule to integrate the differential forms by parts:

$$\int_S d\omega_1 \wedge \omega_2 = \int_{\partial S} \omega_1 \wedge \omega_2 - (-1)^{\deg \omega_1} \int_S \omega_1 \wedge d\omega_2.$$

A.3.7.2 Green theorem

Theorem A.2. *Let $S \subset \mathbb{R}^2$ be a compact two-dimensional manifold with a border. Additionally we assume that S has a standard orientation and ∂S has an*

implied orientation (also known as the counter-clockwise direction). Let $p, q : S \rightarrow \mathbb{R}$ are two differentiable functions. Then, the following equality holds:

$$\int_{\partial S} p \, dx + q \, dy = \iint_S \left(\frac{\partial q}{\partial x} - \frac{\partial p}{\partial y} \right) dx \wedge dy$$

Proof. It is sufficient to consider the differential form $\omega = p \, dx + q \, dy$ and to notice that $d\omega = \left(\frac{\partial q}{\partial x} - \frac{\partial p}{\partial y} \right) dx \wedge dy$. \square

A.3.7.3 Gauß–Ostrogradsky theorem

Theorem A.3. Let $S \subset \mathbb{R}^3$ be a compact three-dimensional manifold with a border, $\mathbf{n} = (n_1, n_2, n_3)$ be the unitary normal to ∂S pointing in the outward direction and $\mathbf{F} = (F^1, F^2, F^3)$ be a differentiable vector field on S . Then the following equality holds

This theorem is also known in the literature as the divergence theorem.

$$\int_S \nabla \cdot \mathbf{F} \, dV = \int_{\partial S} \mathbf{F} \cdot \mathbf{n} \, d\sigma,$$

where $dV, d\sigma$ are volume and surface elements correspondingly.

Proof. In order to prove this Theorem it is enough to consider the 2-differential form $\omega = F^1 \, dy \wedge dz + F^2 \, dz \wedge dx + F^3 \, dx \wedge dy$. Then, it is straightforward to show that $d\omega = \nabla \cdot \mathbf{F} \, dV$. Finally, by noticing that

$$\begin{aligned} n_1 \, d\sigma &= dy \wedge dz, \\ n_2 \, d\sigma &= dz \wedge dx, \\ n_3 \, d\sigma &= dx \wedge dy, \end{aligned}$$

then on ∂S we have

$$\mathbf{F} \cdot \mathbf{n} \, d\sigma = F^1 n_1 \, d\sigma + F^2 n_2 \, d\sigma + F^3 n_3 \, d\sigma = \omega.$$

\square

A.3.7.4 Stokes theorem

Theorem A.4. Let $S \subset \mathbb{R}^3$ be a compact oriented manifold with a border, ∂S is supplied with the induced orientation and $\mathbf{n} = (n_1, n_2, n_3)$ be the unitary normal to ∂S pointing in the outward direction. Let $\mathbf{F} = (F^1, F^2, F^3)$ be a differentiable vector field on an open set containing the manifold S . Then the following equality holds

$$\int_S (\nabla \times \mathbf{F}) \cdot \mathbf{n} \, d\sigma = \int_{\partial S} \mathbf{F} \, ds, \quad (\text{A.6})$$

where $d\sigma, ds$ are surface and length elements correspondingly.

Remark A.2. Equality (A.6) can be written also as

$$\int_{\partial S} F^1 dx + F^2 dy + F^3 dz = \iint_S \left[n_1 \left(\frac{\partial F^3}{\partial y} - \frac{\partial F^2}{\partial z} \right) + n_2 \left(\frac{\partial F^1}{\partial z} - \frac{\partial F^3}{\partial x} \right) + n_3 \left(\frac{\partial F^2}{\partial x} - \frac{\partial F^1}{\partial y} \right) \right] d\sigma.$$

Proof. The proof of this theorem can be done by considering the 1-form $\omega = F^1 dx + F^2 dy + F^3 dz$ and by noticing that $d\omega = (\nabla \times \mathbf{F}) \cdot \mathbf{n} d\sigma$ (see formula (A.3) and the proof of the previous Theorem for the details). \square

A.3.8 The Hodge operator

In mathematical physics the Laplace operator plays the fundamental rôle. However, from the Poincaré lemma we saw that a straightforward application of two successive differential operators annihilates any differential k -form. In other words, any differential form is a “harmonic function”. Consequently, something else has to be done to define a meaningful analogue of the Laplace operator.

In the flat space \mathbb{R}^n there is a particular differential form which corresponds to the volume element $\omega = d\mathbf{e}_1 \wedge \dots \wedge d\mathbf{e}_n \equiv dV$. Once it is fixed, we can define the Hodge operator \star which associates to a k -form ω the unique $(n - k)$ -form $\star\omega$ such that

$$\omega \wedge (\star\omega) \equiv dV.$$

This operator has already been used above without giving it a name. For instance, in \mathbb{R}^3 we have the following examples:

$$\star dx = dydz,$$

$$\star dy = dzdx,$$

$$\star dz = dxdy.$$

This Section can be omitted for the first reading.

A.3.8.1 Laplace operator

Now we can proceed to the meaningful definition of the Laplace operator. Let us take a 0-form $\omega = u(x, y, z)$. The following equalities can be readily obtained:

$$\begin{aligned} d\omega &= \frac{\partial u}{\partial x} dx + \frac{\partial u}{\partial y} dy + \frac{\partial u}{\partial z} dz, \\ \star d\omega &= \frac{\partial u}{\partial x} dy \wedge dz + \frac{\partial u}{\partial y} dz \wedge dx + \frac{\partial u}{\partial z} dx \wedge dy, \\ d(\star d\omega) &= \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) dx \wedge dy \wedge dz. \end{aligned}$$

The last 3-form provides us with the usual Laplace operator. It is a good sign since we worked in a flat Euclidean space \mathbb{R}^3 . However, the expression $d(\star d\omega)$ remains valid in any coordinate system.

A.3.8.2 d'Alembert operator

In the Minkowsky space-time \mathbb{M}^3 an element of the volume is given by the differential form $\omega = -dt \wedge dx \wedge dy$. As we proceeded above for the Laplace operator, we will define the differential 0-form $\omega = u(t, x, y)$. Then, we compute

$$\begin{aligned} d\omega &= -\frac{\partial u}{\partial t} dt + \frac{\partial u}{\partial x} dx + \frac{\partial u}{\partial y} dy, \\ \star d\omega &= \frac{\partial u}{\partial t} dx \wedge dy + \frac{\partial u}{\partial x} dt \wedge dy + \frac{\partial u}{\partial y} dt \wedge dx, \\ d(\star d\omega) &= \left(-\frac{\partial^2 u}{\partial t^2} + \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) dt \wedge dx \wedge dy. \end{aligned}$$

The last operator is a 3-form representing the celebrated d'Alembert operator which appears in all kinds of wave equations arising in the mathematical physics.

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