A BRIEF INTRODUCTION INTO HYDRODYNAMICS

Variational point of view

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Denys Dutykh: *A brief Introduction into Hydrodynamics. Variational point of view* © April 2015



ABSTRACT

In this manuscript we present some basic notions of Hydrodynamics in view of free surface flows modelling. 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

The author is grateful to Prof. Dauren Zhakebaev for the kind invitation to deliver a series of lectures at al-Farabi Kazakh National University in Almaty during December 2014. It was the first step towards making this book possible. Then, there was another invitation of Prof. Elena Akhmatskaya to deliver a short course on Hydrodynamics in Bilbao in April 2015. In this way the Chapter on the Smoothed Particles Hydrodynamics appeared. The material of these lectures constitutes the basis of this manuscript. Most probably, these notes will serve the author several times in the future.

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 whome I learnt a lot.

CONTENTS

i CLASSICAL MECHANICS	7
1 LAGRANGIAN MECHANICS	9
1.1 Least Action Principle	9
1.2 Euler–Lagrange equations	10
1.3 Form of the Lagrangian	10
1.3.1 Maupertuis's action	10
2 HAMILTONIAN MECHANICS	11
2.1 A geometrical parenthesis	11
ii CONTINUUM MECHANICS: EULERIAN DESCRIPTION	10
	12
3 FLUID DYNAMICS EQUATIONS	14
3.1 Derivation of the governing equations	
3.1.1 Choice of the coordinate system	
3.1.2 Mass conservation	15
3.1.3 Momentum conservation	16
3.1.4 Energy conservation	16
4 WATER WAVE PROBLEM	17
5 LAGRANGIAN VARIATIONAL PRINCIPLE	19
6 HAMILTONIAN FORMULATION	20
iii CONT. MECHANICS: LAGRANGIAN DESCRIPTION	21
7 LAGRANGIAN FLUID DYNAMICS	23
7.1 On the notion of a fluid particle	23
8 VARIATIONAL STRUCTURE	24
9 LONG WAVES	2 ₅
10 SOME EXACT SOLUTIONS	26
11 SMOOTHED PARTICLE HYDRODYNAMICS	27
11.1 Why particle methods?	
11.2 Particle interpolation	
11.3 A black fly in your Chardonnay	
iv APPENDIX	30
A MATHEMATICAL TOOLS	31
A.1 Fréchet derivative	31
A.1.1 Properties	32
A.1.2 Higher derivatives	32
A.2 Gâteaux derivative	32
A.2.1 Properties	33
A.2.2 Higher derivatives	34
A.2.3 Example in infinite dimensions	34
A Differential forms	0.5

A.3.1	o-forms	35
A.3.2	1-forms	35
A.3.3	2-forms	36
A.3.4	k-forms	37
A.3.5	n-forms	37
A.3.6	External derivation	37
A.3.7	Integration of differential forms	40
A.3.8	The Hodge operator	42
BIBLIO	GRAPHY	43
INDEX		46

PRFFACE

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 [Jayo3], 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; XX th 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 nonrigorous 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 dimostrzioni mathematiche, intorno a due nove scienze alla meccanica ed i movimenti locali". This period was finished in 1687 when Isaac Newton published his book "PhilosophiæNaturalis Principia Mathematica".

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

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 entroversy, 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 popularizator 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 tretise "*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 XVIII th 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 with consequences which can be found today in general relativity, gauge theory of fundamental interactions and many other fields.

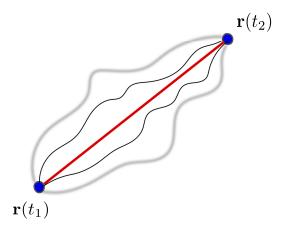


Figure 0.1.: Optimal trajectory (in red) joining two points in space-time $\mathbf{r}(t_1)$ and $\mathbf{r}(\mathsf{t}_2)$.

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 precursos 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 [Baso7] 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.

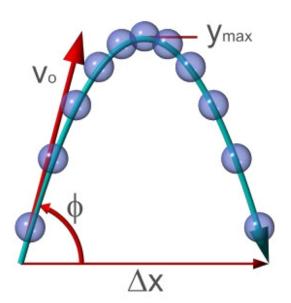
EXERCISES

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). Nondissipative 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 $\dot{x}(t) \coloneqq \frac{d\,x}{dt}$. 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* $\mathscr L$ as the following integral

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

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

1.3 FORM OF THE LAGRANGIAN

1.3.1 Maupertuis's action

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

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

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 socalled 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

$$\{F,G\} = \sum_{i=1}^{n} \left(\frac{\partial F}{\partial q_{i}} \frac{\partial G}{\partial p_{i}} - \frac{\partial F}{\partial p_{i}} \frac{\partial G}{\partial q_{i}} \right) + \sum_{i,k=1}^{l} \pi_{jk}(y) \frac{\partial F}{\partial y_{j}} \frac{\partial G}{\partial y_{k}},$$

where $\pi_{jk}(y) = -\pi_{kj}(y)$ are certain functions of the (y_1, \ldots, 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.

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

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 whics 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

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

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

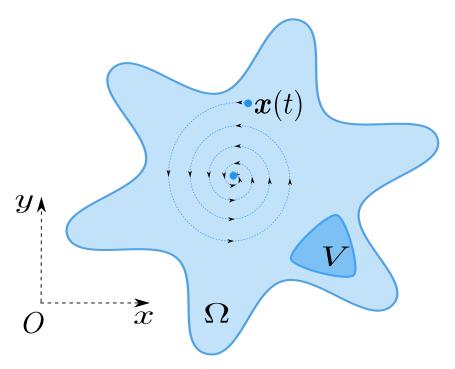


Figure 3.1.: *Sketch of the flow domain* Ω *along with a possible particle trajectory and a control volume* dV.

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 $\mathfrak{m}_V(t)$ of the fluid contained in V is then given by

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

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

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

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 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.

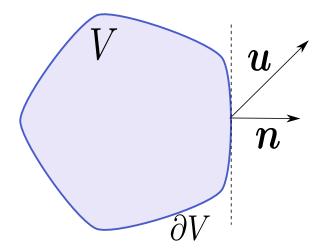


Figure 3.2.: An elementary volume V with an outward normal \mathbf{n} and fluid particle velocity \mathbf{u} at this point on the boundary. The mass flux is positive since $\mathbf{u} \cdot \mathbf{n} > 0$.

boundary ∂V by the velocity field $\mathfrak{u}(x,t)$ (see Figure 3.2 for the illustration). Since the mass is neither being generated nor destroyed, both rates of change have to be equal

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{V} \rho(\mathbf{x}, t) \, \mathrm{d}V = -\int_{\partial V} \rho \mathbf{u} \cdot \mathbf{n} \, \mathrm{d}\sigma, \tag{3.1}$$

where $d\sigma$ is the element of surface. The sign – comes from the convention that the positive normal 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:

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

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 $\rho(x,t)$ or u(x,t) has discontinuities (*i.e.* shock waves), the integral form (3.1) has to be used.

3.1.3 Momentum conservation

3.1.4 Energy conservation

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 $\rho \mathbf{u} \cdot \mathbf{n}$.

4 | WATER WAVE PROBLEM



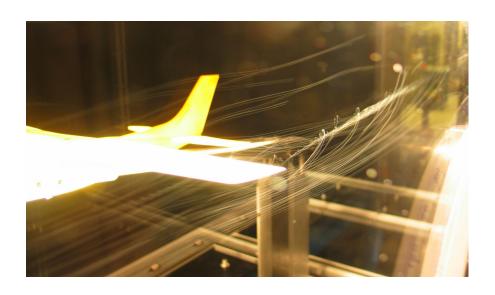
5 LAGRANGIAN VARIATIONAL PRINCIPLE

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 names Eulerian/Lagrangian are completely conventional since both descriptions were proposed by Leonhard EULER.



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

Z LAGRANGIAN FLUID DYNAMICS

7.1 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 H₂O or air O₂ 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 contstraint 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 10⁷ molecules. It is considered to be enough to have stable statistical averages over this ensemble. Of course, for rarefied gases all these estimations have to be readjusted.

8 | VARIATIONAL STRUCTURE

9 LONG WAVES

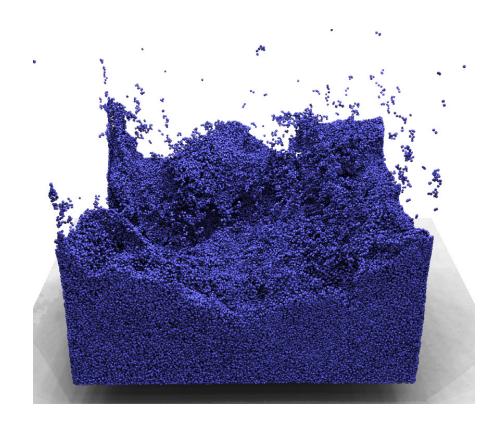
10 | SOME EXACT SOLUTIONS

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 [Mono5]. An extension to MHD is explained in [Pri12]. 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.



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
- 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 11.3.

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 7.1.

11.2 PARTICLE INTERPOLATION

The smoothing kernels appeared already in works of Russian/Soviet mathematicians Vladimir A. Steklov and Sergei L. Sobolev.

11.3 A BLACK FLY IN YOUR CHARDONNAY

The same expression in Russian-speaking cultures would read: "A spoon of tar in a barrel of honey."

Part IV APPENDIX

A MATHEMATICAL TOOLS

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

— Albert Einstein

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

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

If the limit exists dF(u) is called the Fréchet derivative of the functional F

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

$$\begin{array}{ccc} dF: U & \mapsto & L(U,V), \\ & u & \mapsto & dF_u, \end{array}$$

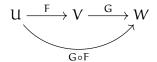
where L(U,V) is a set of linear bounded functionals. Note that this notion is fundamentally different from the continuity of the derivative functional dF(u)[h].

A.1.1 Properties

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

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

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



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

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

If U and 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:

$$dF\colon\thinspace\mathbb{R}^n\mapsto\mathbb{R}^m,\qquad J_\mathfrak{u}\ \coloneqq\ dF(\mathfrak{u}),\qquad J_\mathfrak{u}\in Mat_{n\times m}(\mathbb{R}).$$

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 $dF: U \mapsto L(U, V)$ of a differentiable functional $F: U \mapsto V$ is also a function from U to another Banach space (of linear bounded operators operators from U to V). This function dF may also be differentiable. In this case, this derivative will be called the *second* order derivative

This particular
Banach space is
called the dual space.

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

where the dual space L(U, L(U, V)) is isomorphic to the space of bounded continuous bilinear operators $L^2(U \times U, V)$. 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 U and V be Banach (or other locally convex topological) spaces and $F: U \mapsto V$ is a map. If the following limit exists

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

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

A.2.1 Properties

In every point $u \in U$ where the map F is differentiable, its Gâteaux differential defnes a homogeneous function in the second argument

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

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

The chain rule holds also for the Gâteaux derivative and reads

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

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

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

Note that function $d^nF(u)[h]$ 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 $F \in C^k$

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

where R_k is the remainder term. If the segment $[u, u + h] \in U$, 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

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

$$\frac{\mathcal{F}(u+\varepsilon h) - \mathcal{F}(u)}{\varepsilon} = \frac{1}{\varepsilon} \left[\int_{\Omega} F(u+\varepsilon h) dx - \int_{\Omega} F(u) dx \right] =$$

$$= \frac{1}{\varepsilon} \int_{\Omega} \int_{0}^{1} \frac{d}{d\tau} F(u+\varepsilon \tau h) ds dx = \int_{\Omega} \int_{0}^{1} F'(u+\varepsilon \tau h) h ds dx.$$

After taking the limit $\varepsilon \to 0$ 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 DIFFERENTIAL FORMS

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 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.

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 e_1 , e_2 and 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

$$u = u_1 e_1 + u_2 e_2 + u_3 e_3.$$

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

$$dx(e_1) = 1$$
, $dx(e_2) = 0$, $dx(e_3) = 0$.

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

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.

The basics of the exterior calculus stem from the pioneering works of H. Poincaré and É. Cartan in the beginning of the XX th century.

dz. Now it is easy to compute the action of dx, dy, dz on the vector \mathbf{u} :

$$dx(u) = u_1, dy(e_2) = u_2, dz(e_3) = u_3.$$

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

ANTICOMMUTATIVITY: (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 anticommutativity) $de \wedge de = 0$ (valid only for the forms of degree one)

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

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

$$\mathrm{Alt}[\omega](e_1,e_2,\ldots,e_n)\coloneqq \frac{1}{n!}\sum_{\sigma\in S_n}\mathrm{sign}\,\sigma\cdot\omega(e_{\sigma(1)},e_{\sigma(2)},\ldots,e_{\sigma(n)}).$$

In this definition the summation is taken ovel 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.

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

In the Euclidean space \mathbb{R}^n the basis of 2-forms consists of all the elements $de_i \wedge de_j$, where $\{e_i\}$, $i=1,\ldots,n$ 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 $n \neq 3$.

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. $\omega = de_{i_1} \wedge ... \wedge de_{i_k}$. 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

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

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:

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

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:

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

$$= -\frac{\partial p}{\partial y} dx \wedge dy - \frac{\partial p}{\partial z} dx \wedge dz$$

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

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

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 derivatived 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 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.

The general algorithm to compute the exterior derivative is the following. One takes an elementary differential form $\omega = f(x_1, \dots x_n) de_{i_1} \wedge \dots \wedge de_{i_k}$ and computes the usual differential of the coefficient $df = \frac{\partial f}{\partial x_1} de_1 + \dots + \frac{\partial f}{\partial x_n} de_n$. Then, every obtained term in the direction de_i has to be multiplied externally by $de_{i_1} \wedge \dots \wedge de_{i_k}$ to produce a (k+1)-form $de_i \wedge de_{i_1} \wedge \dots \wedge de_{i_k}$. Finally, the resulting expression $d\omega = \sum_{i=1}^n \frac{\partial f}{\partial x_i} de_i \wedge de_{i_1} \wedge \dots \wedge de_{i_k}$ 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:

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

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 $\mathfrak{u}(x,\mathfrak{t})$ denote a conservative quantity (e.g. the density, momentum, energy, etc.) and $F(\mathfrak{u})$ be its flux. Then, the conservation equation takes the following form:

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

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 ω = udx – Fdt. Then, the conservation law (A.5) has the following elegant form d ω = 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

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

Below we will consider the most important corrolaries 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:

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

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 $p, q : S \mapsto \mathbb{R}$ 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 $d\omega = \left(\frac{\partial \, q}{\partial x} - \frac{\partial \, p}{\partial y}\right) \, dx \wedge dy$.

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 $\mathbf{F} = (\mathsf{F}^1, \mathsf{F}^2, \mathsf{F}^3)$ be a differentiable vector field on S. Then the following equality holds

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

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

where dV, do 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 $\omega = \nabla \cdot F$ dV. Finally, by noticing that

$$n_1 d\sigma = dy \wedge dz$$
,
 $n_2 d\sigma = dz \wedge dx$,
 $n_3 d\sigma = dx \wedge dy$,

then on ∂S we have

$$\mathbf{F} \cdot \mathbf{n} \, d\sigma = \mathbf{F}^1 \mathbf{n}_1 \, d\sigma + \mathbf{F}^2 \mathbf{n}_2 \, d\sigma + \mathcal{F}^3 \mathbf{n}_3 \, d\sigma = \omega.$$

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

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

where do, 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 $d\omega = (\nabla \times F) \cdot \mathbf{n} d\sigma$ (see formula (A.3) and the proof of the previous Theorem for the details).

This Section can be omitted for the first reading.

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 meaningul analogue of the Laplace operator.

In the flat space \mathbb{R}^n there is a particular differential form which corresponds to the volume element $\omega = de_1 \wedge ... \wedge de_n \equiv dV$. 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:

$$*dx = dydz,$$
 $*dy = dzdx,$
 $*dz = dxdy.$

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:

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

$$\star d\omega = \frac{\partial u}{\partial x} dy \wedge dz + \frac{\partial u}{\partial y} dz \wedge dx + \frac{\partial u}{\partial z} dx \wedge dy,$$

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

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

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

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.

BIBLIOGRAPHY

- [ATo7] A. V. Aliev and G. A. Tarnavsky. The hierarchical SPH-method for mathematical simulation in gravitational gas dynamics. *Sib. Electr. Math. Rep.*, 4:376–434, 2007.
- [Baso7] J.-L. Basdevant. *Variational Principles in Physics*. Springer-Verlag, New York, 2007.
- [BWSo5] J. C. Baez, D. K. Wise, and B. Smith. Lectures on Classical Mechanics. Technical report, University of California, Riverside, 2005.
- [CM93] A. Chorin and J. Marsden. *A Mathematical Introduction to Fluid Mechanics*. Springer, 3rd edition, 1993.
- [Fero6] R. L. Fernandes. Poisson vs. Symplectic Geometry. *CIM Bulletin*, 20:15–19, 2006.
- [GM77] R. A. Gingold and J. J. Monaghan. Smoothed particle hydrodynamics: theory and application to non-spherical stars. *Mon. Not. R. Astron. Soc.*, 181:375–389, 1977.
- [Jayo3] E. T. Jaynes. *Probability Theory*. Cambridge University Press, Cambridge, 2003.
- [LL76] L.D. Landau and E.M. Lifshitz. *Mechanics*. Elsevier Butterworth-Heinemann, Amsterdam, 1976.
- [LL86] L.D. Landau and E.M. Lifshitz. *Theory of Elasticity*. Elsevier Sciences, Oxforf, 1986.
- [Luc77] L. B. Lucy. A numerical approach to the testing of the fission hypothesis. *Astron. J.*, 82:1013–1024, 1977.
- [MH94] J. E. Marsden and T. J. R. Hughes. *Mathematical Foundations of Elasticity*. Dover Publications, Englewood Cliffs, 1994.
- [Mon94] J. J. Monaghan. Simulating free surface flows with SPH. *Phys. D*, 110:399–406, 1994.
- [Mono5] J. J. Monaghan. Smoothed particle hydrodynamics. *Rep. Prog. Phys.*, 68:1703–1759, 2005.
- [MS98] D. McDuff and D. Salamon. *Introduction to symplectic topology*. Oxford University Press, New York, 2nd edition, 1998.
- [Pri12] D. J. Price. Smoothed particle hydrodynamics and magneto-hydrodynamics. *J. Comp. Phys.*, 231(3):759–794, 2012.

- [Sal88] R. Salmon. Hamiltonian fluid mechanics. *Ann. Rev. Fluid Mech.*, 20:225–256, 1988.
- [Sou97] J.-M. Souriau. Structure of Dynamical Systems: a Symplectic View of Physics. Springer, New York, 1997.
- [Spi71] M. Spivak. Calculus on Manifolds: A Modern Approach to Classical Theorems of Advanced Calculus. Westview Press, Princeton, 1971.
- [Wei83] A. Weinstein. The local structure of Poisson manifolds. *J. Diff. Geom.*, 18:523–557, 1983.

INDEX

0-forms, 35 1-forms, 35 Élie Cartan, 35	Hamiltonian, 20 Henri Poincaré, 35, 39 Hilbert space, 34, 35 Hodge operator, 42
Action, 10 Alternator, 36 Antoine Lavoisier, 15	Integration by parts, 40 Isaac Newton, 4
Banach space, 31, 33	Jacobian matrix, 32
Calculus of variations, 31 Chain rule, 32, 33	James Clerk Maxwell, 38 Joseph-Louis Lagrange, 4
Conservation laws, 39	Lagrangian functional, 9
Continuity, 31	Laplace operator, 42
Continuum assumption, 14	Least time principle, 4
Continuum mechanics, 12	Leibniz identity, 11
Copernicus, 4	Leonhard Euler, 4, 21
	Lie bracket, 11
d'Alembert operator, 42	Linear operation, 32
Darboux's theorem, 11	M(' A 1 ('
Density, 14	Mécanique Analytique, 5
Derivative of the product, 39	Mass conservation, 15
Differential forms, 35	Maurice Fréchet, 31
Divergence operator, 38	Mechanical work, 36 Mesh, 29
Energy conservation, 16	Meshless methods, 29
Exterior calculus, 35	Michael Spivak, 36
Exterior product, 36	Mikhail Lomonosov, 15
	Momentum conservation, 16
Felix Klein, 5	Wientertrain conservation, 10
Fluid parcel, 23	Parallelepipeds, 37
Fluid particle, 23	Pierre de Fermat, 4
Fréchet derivative, 31	Pierre-Louis Moreau de
Functional, 34	Maupertuis, 4
	Poincaré lemma, 39
Gâteaux derivative, 32	Poisson bracket, 11
Galileo Galilei, 4	Poisson geometry, 11
Gauß-Ostrogradsky theorem,	Poisson manifold, 11
41	David David
Geometrical optics, 4	René Descartes, 4
Gradient, 38	René Gâteaux, 32
Green theorem, 40	Rotational operator, 38

Scalar product, 35

Second order derivative, 32

Stokes theorem, 40, 41

Symplectic geometry, 11

Symplectic manifold, 11

Wedge product, 36

Topological changes, 29

Vector product, 37

Vectorial calculus, 35

Velocity, 14

Volume, 16, 37

Wedge product, 36

William R. Hamilton, 4



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