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Lecture Notes

Selected Topics in Fluid Dynamics

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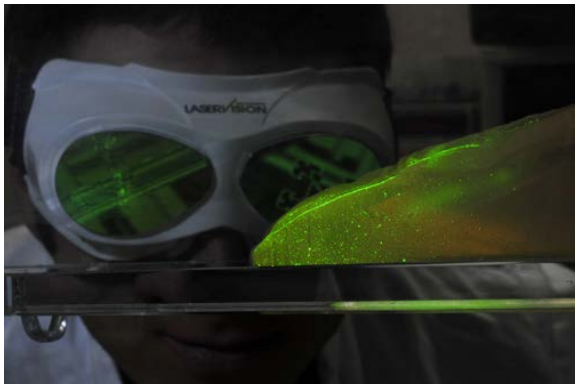

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Selected Topics in Fluid Dynamics / C. Ancey

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« Le physicien ne peut demander à l'analyste de lui révéler une vérité nouvelle ; tout au plus celui-ci pourrait-il l'aider à la pressentir. Il y a longtemps que personne ne songe plus à devancer l'expérience, ou à construire le monde de toutes pièces sur quelques hypothèses hâtives. De toutes ces constructions où l'on se complaisait encore naïvement il y a un siècle, il ne reste aujourd'hui plus que des ruines. Toutes les lois sont donc tirées de l'expérience, mais pour les énoncer, il faut une langue spéciale ; le langage ordinaire est trop pauvre, elle est d'ailleurs trop vague, pour exprimer des rapports si délicats, si riches et si précis. Voilà donc une première raison pour laquelle le physicien ne peut se passer des mathématiques ; elles lui fournissent la seule langue qu'il puisse parler. »

Henri Poincaré, in *La valeur de la science*

The physician cannot ask the analyst to reveal a new truth; at best the analyst could help him to have a feel of it. It has been a long time that nobody has not anticipated the experience or built the world from scratch on a few hasty assumptions. All these constructions where people still naively delighted a century ago, are today in ruins. All laws are drawn from experience, but expressing them requires a special language; usual language is too poor, it is also too vague to express relations that are so delicate, so rich and precise. That is the main reason why physicists cannot live without mathematics; it provides them the only language they can speak.

Henri Poincaré, in *The Value of Science*

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Notations, formulas, & Conventions

The following notations and rules are used:

- Vectors, matrices, and tensors are in bold characters.
- For mathematical variables, I use slanted fonts.
- Functions, operators, and dimensionless numbers are typed using a Roman font.
- The symbol O (capital O) indicates that there is a one-sided bound, e.g., $u = O(v)$ means that the limit of u/v exists and is finite (neither zero nor infinity). On many occasions, it means "is of the order of", but not always (so be careful).
- The symbol o is a shorthand notation to for 'much smaller than', e.g. $u = o(v)$ means that $u \ll v$.
- I do not use the notation D/Dt to refer to the material derivative (also called convective or Lagrangian derivative), but $\mathrm{d}/\mathrm{d}t$ (that must not be confused with ordinary time derivative). I believe that the context is mostly sufficient to determine the meaning of the differential operator.
- The symbol $\propto$ means "proportional to".
- The symbol $\sim$ or $\approx$ means "nearly equal to".
- I use units of the international system (IS): meter [m] for length, second [s] for time, and kilogram [kg] for mass. Units are specified by using square brackets.
- For the computations with complex numbers, I use $\Re$ to refer to the real part of a complex and $\imath$ is the imaginary number.
- The superscript † after a vector/tensor means the transpose of this vector/tensor.
- We use $\mathbf{1}$ to refer to the unit tensor (identity tensor/matrix).

- Einstein's convention means that when summing variables, we omit the symbol $\sum$ and we repeat the indice. For instance we have $\mathbf{a} \cdot \mathbf{b} = a_i b_i$.
- The gradient operator is denoted by the *nabla* symbol ∇. The divergence of any scalar or tensorial quantity f is denoted by $\nabla \cdot f$. For the Laplacian operator, I indifferently use ∇^2 or $\triangle$. The curl of any vector $\mathbf{v}$ is denoted by $\nabla \times \mathbf{v}$. We can use the following rule to check the consistency of an operator

Operation name	*Operator symbol*	*Order of result*
gradient	∇	$\Sigma + 1$
divergence or outer product	$\nabla\cdot$	$\Sigma - 1$
curl	$\nabla\times$	Σ
Laplacian	∇^2	Σ

- The scalar product of two vectors $\mathbf{a}$ and $\mathbf{b}$ is denoted by $\mathbf{a}\cdot\mathbf{b}$. The dyadic or tensor product of $\mathbf{a}$ and $\mathbf{b}$ is denoted by $\mathbf{ab}$. The product between a tensor $\mathbf{A}$ and a vector $\mathbf{a}$ is denoted by $\mathbf{A} \cdot \mathbf{a}$. The cross product of two vectors $\mathbf{a}$ and $\mathbf{b}$ is denoted by $\mathbf{a} \times \mathbf{b}$. The inner product of two tensors is denoted by the double dot ":" (keep in mind that for second-order tensors $\mathbf{a}$ and $\mathbf{b}$ we have $\mathbf{a} : \mathbf{b} = \mathrm{tr}\mathbf{ab}$). We can use the following rule to check the consistency of a multiplication

Operation name	*Multiplication sign*	*Order of result*
dyadic or tensorial product	none	Σ
cross or outer product	$\times$	$\Sigma - 1$
scalar or inner product	$\cdot$	$\Sigma - 2$
double product	:	$\Sigma - 4$

  Recall that the order of a scalar is 0, a vector is of order 1, and a tensor is of order at least 2. For instance, if $\mathbf{a}$ and $\mathbf{b}$ denotes vectors and $\mathbf{T}$ is a tensor, $\mathbf{T} \cdot \mathbf{a}$ is order $2 + 1 - 2 = 1$.

- The gradient of a vector $\mathbf{a}$ is a tensor $\nabla\mathbf{a}$, whose components in a Cartesian frame x_i are
$$\frac{\partial a_j}{\partial x_i}.$$
  The divergence of a second-order tensor M_{ij} is a vector $\nabla \cdot \mathbf{M}$, whose jth component in a Cartesian frame is
$$\frac{\partial M_{ij}}{\partial x_i}.$$
- The tensorial product of two vectors $\mathbf{a}$ and $\mathbf{b}$ provides a tensor $\mathbf{ab}$ such that for any vector $\mathbf{c}$, we have $(\mathbf{ab})\mathbf{c} = (\mathbf{b} \cdot \mathbf{c})\mathbf{a}$.

- A vector field such that $\nabla \cdot \mathbf{v} = \mathbf{0}$ is said to be *solenoidal*. A function f satisfying the Laplace equation $\nabla^2 f = 0$ is said to be *harmonic*. A function f such that $\nabla^4 f = 0$ is said to be *biharmonic*. A vectorial field $\mathbf{v}$ such $\nabla \times \mathbf{v} = 0$ is said to be *irrotational*.

- An extensive use is made of the *Green-Ostrogradski* theorem (also called the *divergence* theorem):

$$\int_{\mathcal{V}} \nabla \cdot \ \mathbf{u} \, \mathrm{d}\mathcal{V} = \int_{\mathcal{S}} \mathbf{u} \cdot \mathbf{n} \, \mathrm{d}\mathcal{S},$$

  where $\mathcal{S}$ is the surface bounding the volume $\mathcal{V}$ and $\mathbf{n}$ is the unit normal to the infinitesimal surface $\mathrm{d}\mathcal{S}$. A closely related theorem for scalar quantities f is

$$\int_{\mathcal{V}} \nabla f \, \mathrm{d}\mathcal{V} = \int_{\mathcal{S}} f \mathbf{n} \, \mathrm{d}\mathcal{S}.$$

- For some algebraic computations, we need to use

  - Cartesian coordinates (x, y, z); or
  - spherical coordinates $(x = r\cos\varphi\sin\theta)$, $y = r\sin\theta\sin\varphi$, $z = r\cos\theta)$ with $0 \leq \theta \leq \pi$ and $-\pi \leq \varphi \leq \pi$, $\mathrm{d}S = r^2 \sin\theta \mathrm{d}\theta\mathrm{d}\varphi$ on a sphere of radius r, $\mathrm{d}V = r^2 \sin\theta \mathrm{d}r\mathrm{d}\theta\mathrm{d}\varphi$.

- Some useful formulas on vector and tensor products

$$\mathbf{N} : \mathbf{M} = \mathbf{M} : \mathbf{N},$$

$$\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = (\mathbf{a} \cdot \mathbf{c})\mathbf{b} - (\mathbf{a} \cdot \mathbf{b})\mathbf{c},$$

$$(\mathbf{M} \cdot \mathbf{a}) \cdot \mathbf{b} = \mathbf{M} : (\mathbf{ab}) \ \text{ and } \ \mathbf{a} \cdot (\mathbf{b} \cdot \mathbf{M}) = \mathbf{M} : (\mathbf{ab}),$$

$$\mathbf{ab} : \mathbf{cd} = \mathbf{a} \cdot (\mathbf{b} \cdot \mathbf{cd}) = \mathbf{a} \cdot ((\mathbf{b} \cdot \mathbf{c})\mathbf{d}) = (\mathbf{a} \cdot \mathbf{b})(\mathbf{c} \cdot \mathbf{d}) = \mathbf{ac} : \mathbf{bd}$$

$$\nabla(fg) = g\nabla f + f\nabla g,$$

$$\nabla \cdot (f\mathbf{a}) = \mathbf{a} \cdot \nabla f + f\nabla \cdot \mathbf{a},$$

$$\nabla \cdot (\mathbf{a} \times \mathbf{b}) = \mathbf{b}(\nabla \times \mathbf{a}) - \mathbf{a}(\nabla \times \mathbf{b}),$$

$$\nabla \cdot \nabla\mathbf{a} = \frac{1}{2}\nabla(\mathbf{a} \cdot \mathbf{a}) - \mathbf{a} \times (\nabla \times \mathbf{a}),$$

$$\nabla \cdot \mathbf{ab} = \mathbf{a}\nabla\mathbf{b} + \mathbf{b}\nabla \cdot \mathbf{a}$$

$$\mathbf{1} : \nabla\mathbf{a} = \nabla \cdot \mathbf{a},$$

$$\nabla \cdot (f\mathbf{1}) = \nabla f,$$

- and on derivatives

$$(\mathbf{a}\cdot\nabla)\mathbf{b} = \mathbf{a}\cdot(\nabla\mathbf{b})^T,$$
$$\frac{\partial f(x)}{\partial \mathbf{x}} = \frac{\mathbf{x}}{x}\frac{\partial f(x)}{\partial x},$$
$$\mathbf{ab} : (\nabla\mathbf{c}) = \mathbf{a}\cdot(\mathbf{b}\nabla)\,\mathbf{c},$$

  with $x = |\mathbf{x}|$.

- For some computations, we need the use the *Dirac function* $\int_{\mathbb{R}^3}\delta(\mathbf{x})\mathrm{d}\mathbf{x} = 1$, $\int_{\mathbb{R}^3}\delta(\mathbf{x}-\mathbf{x}_0)g(\mathbf{x})\mathrm{d}\mathbf{x} = g(\mathbf{x}_0)$, and $\delta(\mathbf{x}) = -\nabla^2(4\pi x)^{-1} = -\nabla^4 x(8\pi)^{-1}$, where $x = |\mathbf{x}|$. The last two expressions are derived by applying the Green formula to the function $1/x$ (see any textbook on distributions).

- The *Fourier transform* in an n-dimensional space is defined as

$$\hat{f}(\boldsymbol{\xi}) = \int_{\mathbb{R}^n} f(\mathbf{x})e^{-\imath\boldsymbol{\xi}\cdot\mathbf{x}}\mathrm{d}\mathbf{x},$$

  for any continuous function. Conversely, the inverse Fourier transform is defined as

$$f(\mathbf{x}) = \int_{\mathbb{R}^n} \hat{f}(\mathbf{x})e^{\imath\boldsymbol{\xi}\cdot\mathbf{x}}\mathrm{d}\boldsymbol{\xi}.$$

Further reading

These lecture notes gives an overview of tools and concepts in fluid dynamics through a series of different problems of particular relevance to free-surface flows. For each topic considered here, we will outline the key elements and point the student toward the most helpful references and authoritative works.

Continuum Mechanics, rheology

- P. Chadwick, *Continuum Mechanics, Concise Theory and Problems*, (Dover, New York) 187 p.
- K. Hutter and K. Jöhnk, *Continuum Methods of Physical Modeling* (Springer, Berlin, 2004) 635 p.
- H.A. Barnes, J.F. Hutton and K. Walters, *An introduction to rheology* (Elsevier, Amsterdam, 1997).
- H.A. Barnes, *A Handbook of Elementary Rheology* (University of Wales, Aberystwyth, 2000).
- K. Walters, *Rheometry* (Chapman and Hall, London, 1975).
- D.V. Boger and K. Walters, *Rheological Phenomena in Focus* (Elsevier, Amsterdam, 1993) 156 p.
- B.D. Coleman, H. Markowitz and W. Noll, *Viscometric flows of non-Newtonian fluids* (Springer-Verlag, Berlin, 1966) 130 p.
- C. Truesdell, *Rational Thermodynamics* (Springer Verlag, New York, 1984).
- C. Truesdell, The meaning of viscometry in fluid dynamics, *Annual Review of Fluid Mechanics*, **6** (1974) 111–147.

Mathematical skills

- Zwillinger, D., Handbook of differential equations, 775 pp., Academic Press, Boston, 1992.

- King, A.C., J. Billingham, and S.R. Otto, *Differential Equations: Linear, Nonlinear, Ordinary, Partial*, 541 pp., Cambridge University Press, Cambridge, 2003.
- Zauderer, E., *Partial Differential Equations of Applied Mathematics*, 779 pp., John Wiley & Sons, New York, 1983.
- Mei, C.C., *Mathematical Analysis in Engineering*, 461 pp., Cambridge University Press, Cambridge, 1995.
- Bender, C.M., and S.A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers*, 593 pp., Springer, New York, 1999.

Fluid mechanics

- S.B. Pope, *Turbulent Flows* (Cambridge University Press, Cambridge, 2000) 771 p.
- W. Zdunkowski and A. Bott, *Dynamics of the Atmosphere* (Cambridge University Press, Cambridge, 2003) 719 p.
- C. Pozrikidis, *Boundary Integral and Singularity Methods for Linearized Viscous Flows* (Cambridge University Press, Cambridge, 1992) 259 p.
- G.K. Batchelor, *An introduction to fluid dynamics* (Cambridge University Press, 1967) 614 p.
- H. Lamb, *Hydrodynamics* (Cambridge University Press, Cambridge, 1932).

1 Conservation laws

Within the framework of continuum mechanics, the details of the material microstructure are forgotten and we only examine the bulk behavior, e.g. how does a material deform when it experiences a given state of stress? Mathematically, we introduce the *constitutive equation*, which relates deformations and/or rates of deformation to stresses. Essentially continuum mechanics provides tools and rules that make it possible to:

- express constitutive equations in a proper form, i.e., in a tensorial form that satisfies the rules of physics;
- obtain equations that govern the bulk motion.

Most phenomenological laws we can infer from experiments are in a scalar form. For instance, in rheometry, the only information we obtain in most cases is the flow curve, i.e., the relation $\tau = f(\dot{\gamma})$, whereas we need more information to model the three-dimensional behavior of fluids. The question is how to express a three-dimensional constitutive equations. We shall see that the reply is not as easy as can be thought at first glance. We start with the Newtonian case, the simplest case that we can imagine. We then continue by reviewing the basic equations used in continuum mechanics (conservation of mass, momentum, and energy). Emphasis is then given to providing a few examples of application.

1.1 Why is continuum mechanics useful? An historical perspective

Newton's and Trouton's experiments were run on very viscous materials, but their interpretation, if cursorily made, leads to different values of viscosity.

1.1.1 Paradoxical experimental results?

In 1687, Isaac Newton stated that "the resistance which arises from the lack of slipperiness of the parts of the liquid, other things being equal, is proportional to the velocity with which the parts of the liquid are separated from one another". This forms the basic statement that underpins Newtonian fluid theory. Translated into modern scientific terms, this sentence means that the resistance to flow (per unit area) τ is proportional to the velocity gradient U/h:

$$\tau = \mu \frac{U}{h}, \tag{1.1}$$

where U is the relative velocity with which the upper plate moves and h is the thickness of fluid separating the two plates (see Fig. 1.1). μ is a coefficient intrinsic to the material, which is termed *dynamic viscosity*. This relationship is of great practical importance for many reasons:

- it is the simplest way of expressing the constitutive equation for a fluid (linear behavior);
- it provides a convenient experimental method for measuring the constitutive parameter μ by measuring the shear stress exerted by the fluid on the upper plate moving with a velocity U (or conversely by measuring the velocity when a given tangential force is applied to the upper plate).

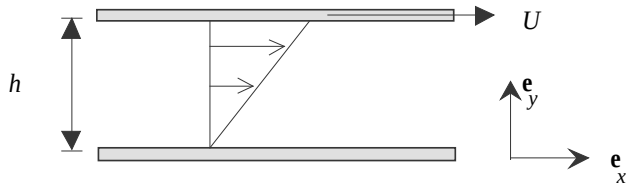

Figure 1.1: *Illustration of a fluid sheared by a moving upper plate.*

In 1904, Trouton did experiments on mineral pitch, which involved elongational stretching of the fluid at very low rate. Figure 1.2 depicts the principle of this experiment. The fluid undergoes a uniaxial elongation achieved with a constant

elongation rate $\dot{\alpha}$, defined as the relative deformation rate: $\dot{\alpha} = \dot{l}/l$, where l is the fluid sample length. For his experiments, Trouton found a linear relationship between the applied force per unit area $\boldsymbol{\sigma}$ and the elongation rate:

$$\boldsymbol{\sigma} = \mu_e \alpha = \mu_e \frac{1}{l} \frac{\mathrm{d}l}{\mathrm{d}t}. \tag{1.2}$$

This relationship was structurally very similar to the one proposed by Newton but it introduced a new material parameter, which is now called *Trouton viscosity*. This constitutive parameter was found to be three times greater than the Newtonian viscosity inferred from steady simple-shear experiments: $\mu_e = 3\mu$. At first glance, this result is both comforting since behavior is still linear (the resulting stress varies linearly with the applied strain rate) and disturbing since the value of the linearity coefficient depends on the type of experiment.

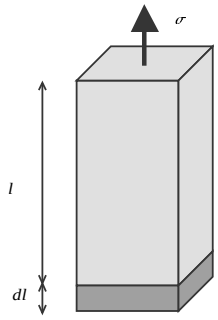

Figure 1.2: *Typical deformation of a material experiencing elongation under the effect of a traction σ applied to the top of the sample.*

1.1.2 How to remove the paradox?

In fact, Trouton's result does not lead to a paradox if we are careful to express the constitutive parameter in a tensorial form rather than a purely scalar form. This was achieved by Navier and Stokes, who independently developed a consistent three-dimensional theory for Newtonian viscous fluids. For a simple fluid, the stress tensor σ can be cast in the following form:

$$\sigma = -p\mathbf{1} + \mathbf{s}, \tag{1.3}$$

where p is called the *fluid pressure* and $\mathbf{s}$ is the extra-stress tensor representing the stresses resulting from a relative motion within the fluid. It is also called the *deviatoric stress tensor* since it represents the departure from equilibrium. The pressure term used in Eq. (1.3) is defined as (minus) the average of the three normal stresses $p = -\mathrm{tr}\,\boldsymbol{\sigma}/3$. This also implies that $(\mathrm{tr}\,\mathbf{s} = 0)$. The pressure used

in Eq. (1.3) is analogous to the hydrostatic fluid pressure in the sense that it is a measure of the local intensity of the squeezing of the fluid. The connection between this purely mechanical definition and the term pressure used in thermodynamics is not simple. For a Newtonian viscous fluid, the Navier-Stokes equation postulates that the extra-stress tensor is linearly linked to the strain-rate tensor $\mathbf{d} = (\nabla\mathbf{u} + \nabla\mathbf{u}^\dagger)/2$:

$$\mathbf{s} = 2\eta\mathbf{d}, \tag{1.4}$$

where $\mathbf{u}$ is the local fluid velocity and η is called the *Newtonian viscosity*. It is worth noticing that the constitutive equation is expressed as a relation between the extra-stress tensor and the local properties of the fluid, which are assumed to depend only on the instantaneous distribution of velocity (more precisely, on the departure from uniformity of that distribution). There are many arguments from continuum mechanics and analysis of molecular transport of momentum in fluids, which show that the local velocity gradient $\nabla\mathbf{u}$ is the parameter of the flow field with most relevance to the deviatoric stress. On the contrary, the pressure is not a constitutive parameter of the moving fluid. When the fluid is compressible, the pressure p can be inferred from the free energy, but it is indeterminate for incompressible Newtonian fluids. If we return to the previous experiments, we infer from the momentum equation that the velocity field is linear : $\mathbf{u} = U\mathbf{e}_x y/h$. We easily infer that the shear rate is: $\dot{\gamma} = \partial u/\partial y = U/h$ and then comparing (1.4) to (1.1) leads to: $\eta = \mu$.

Thus, the Newtonian viscosity corresponds to the *dynamic viscosity*, measured in a simple-shear flow. In the case of a uniaxial elongation and when inertia can be neglected, the components of the strain-rate tensor are:

$$\mathbf{d} = \begin{bmatrix} \dot{\alpha} & 0 & 0 \\ 0 & -\dot{\alpha}/2 & 0 \\ 0 & 0 & -\dot{\alpha}/2 \end{bmatrix}. \tag{1.5}$$

At the same time, the stress tensor can be written as:

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{1.6}$$

Comparing (1.3), (1.5), and (1.6) leads to: $p = -\eta\dot{\alpha}$ and $\sigma = 3\eta\dot{\alpha}$, that is: $\mu_e = 3\eta$, confirming that the Trouton elongational viscosity is three times greater than the Newtonian viscosity. It turns out that Trouton's and Newton's experiments reflect the same constitutive behavior. This example shows the importance of an appropriate tensorial form for expressing the stress tensor. In the present case, the tensorial form (1.4) may be seen as a simple generalization of the simple shear expression (1.1).

1.2 Fundamentals of Continuum Mechanics

1.2.1 Kinematics

It is customary to start a continuum mechanics course with the notion of Lagrangian and Eulerian descriptions:

- in an Eulerian description of the matter, attention is focused on what happens in a given volume control regardless of the history of particles contained in this volume;
- in a Lagrangian description, we follow up the motion of a particle that was at a given position at $t = 0$.

This duality in the description of matter disappears very quickly from students' memory. Fluid mechanicians make use of Eulerian tools almost exclusively since for Newtonian fluids, the physics is governed by the recent history, whereas solid mechanicians give preference to the Lagrangian description because for small deformations, there are no much differences between the descriptions.

However, in an advanced course on rheology and continuum mechanics, emphasis is given to the dual nature of materials which can exhibit both solid-like and fluid-like properties. Much attention has been brought to providing a unified vision of continuum mechanics that is sufficiently general to be applied to a wide range of rheological behaviors. This unified view extends the classic mechanics in several ways:

- large deformations to cope with viscoplasticity and viscoelasticity;
- thermodynamics to take irreversible processes into account.

Here we will focus our attention to a classic description of material deformation and the reader is referred to specialized books that expound more sophisticated theories of deformation (Bird *et al.*, 1987; Tanner, 1988; Morrison, 2001).

In the following, we shall following focus on Eulerian form of the equations of motion, but keep in mind that, especially in advanced fluid mechanics, Lagrangian representations of the equations are very useful (e.g., see Pope, 2000; Minier & Peirano, 2001; Zdunkowski & Bott, 2003, in the field of turbulence or atmospheric flows).

The gradient tensor

In order to characterize the deformation of a body, it is usually helpful to determine how neighboring points behave, i.e. how the increment $\mathrm{d}\mathbf{X}$ in an initial frame is

transformed (see Fig. 1.3), including:

- stretching/contraction of length,
- rotation of elements due to solid rotation and shearing.

We take three neighboring points in the initial frame of reference $\mathcal{C}_0$, called A, B, and C, forming a right angle (see Fig. 1.3). Because of deformation, there may be

- stretching in a direction $\mathbf{e}_1$ or $\mathbf{e}_2$,
- solid rotation around a given axis with an angle α,
- pure shear, i.e. the angle $\theta_0 = \pi/2$ between $\mathbf{X}_1 = \mathbf{AB}$ and $\mathbf{X}_2 = \mathbf{BC}$ has been altered.

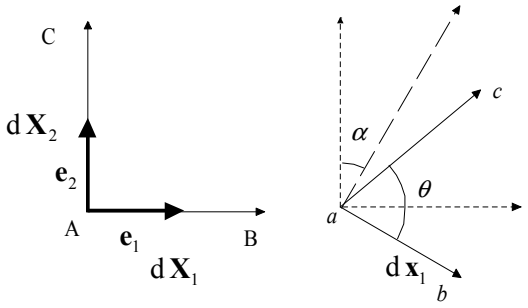

Figure 1.3: *Deformation of a right angle.*

For this purpose, we introduce the transformation

$$\mathrm{d}\mathbf{X} \to \mathrm{d}\mathbf{x},$$

where $\mathbf{x}(\mathbf{X},\ t)$ is the position occupied at time t by a particle that was earlier at $t = 0$ at the position $\mathbf{X}$ in the initial frame of reference $\mathcal{C}_0$. Positioning $\mathbf{x}$ can be achieved in the same frame of reference $\mathcal{C}_0$ or in another frame $\mathcal{C}(t)$. Differentiating the relation $\mathbf{x} = \mathbf{x}(\mathbf{X},\ t)$ leads to

$$\mathrm{d}\mathbf{x} = \mathbf{F} \cdot \mathrm{d}\mathbf{X},$$

where $\mathbf{F}$ is called the *gradient tensor*. When we use the same frame to refer to the current and initial configurations, we can introduce the displacement vector $\mathbf{u}$ such that

$$\mathbf{x} = \mathbf{u} + \mathbf{X},$$

from which we infer (after differentiation)

$$F_{ij} = \delta_{ij} + \frac{\partial u_i}{\partial X_j}.$$

The deformation of the angle (AB, AC) can be determined by using the scalar product

$$\mathrm{d}\mathbf{x}_1 \cdot \mathrm{d}\mathbf{x}_2 = (\mathbf{F} \cdot \mathrm{d}\mathbf{X}_1) \cdot (\mathbf{F} \cdot \mathrm{d}\mathbf{X}_2),$$

which can be transformed into

$$\mathrm{d}\mathbf{x}_1 \cdot \mathrm{d}\mathbf{x}_2 = \mathrm{d}\mathbf{X}_1 \cdot (\mathbf{C} \cdot \mathrm{d}\mathbf{X}_2),$$

where $\mathbf{C} = \mathbf{F}^\dagger \cdot \mathbf{F}$ is a symmetric tensor called the *stretch tensor* or *Cauchy-Green tensor*. The relative variation of the scalar product is then

$$\mathrm{d}\mathbf{x}_1 \cdot \mathrm{d}\mathbf{x}_2 - \mathrm{d}\mathbf{X}_1 \cdot \mathrm{d}\mathbf{X}_2 = 2\mathrm{d}\mathbf{X}_1 \cdot (\mathbf{E} \cdot \mathrm{d}\mathbf{X}_2),$$

where

$$\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{1}) = \frac{1}{2}(\mathbf{F}^\dagger \cdot \mathbf{F} - \mathbf{1}),$$

is the *strain tensor of Green-Lagrange*.

Let us now express the stretching of a length increment $\mathrm{d}s = \sqrt{\mathrm{d}\mathbf{x}_1 \cdot \mathrm{d}\mathbf{x}_1}$

$$\mathrm{d}s_1 = (\mathbf{e}_1 \cdot \mathbf{C} \cdot \mathbf{e}_1)^{1/2}\mathrm{d}S,$$

where $\mathrm{d}S_1 = \sqrt{\mathrm{d}\mathbf{X}_1 \cdot \mathrm{d}\mathbf{X}_1}$. We deduce the relative stretching, i.e. the strain in direction $\mathbf{e}_1$

$$\epsilon_1 = \frac{\mathrm{d}s_1 - \mathrm{d}S_1}{\mathrm{d}S_1} = (\mathbf{e}_1\mathbf{C}\mathbf{e}_1)^{1/2} - 1 = \sqrt{1 + 2E_{11}} - 1.$$

We can also characterize the angle θ

$$\cos\theta = \frac{\mathrm{d}\mathbf{x}_1 \cdot \mathrm{d}\mathbf{x}_2}{\mathrm{d}s_1 \mathrm{d}s_2} = \frac{2E_{12}}{\sqrt{1 + 2E_{11}}\sqrt{1 + 2E_{22}}},$$

which shows that

- the diagonal components of $\mathbf{E}$ give information on strains in the axis directions;
- the off-diagonal terms of $\mathbf{E}$ specify how a angle of an initially right wedge is deformed.

In order to get rid of the solid rotation that is not related to deformation, we make use of a theorem, called the *polar decomposition* theorem, that says that any tensor can be broken down in a unique way into an orthogonal[1] tensor $\mathbf{R}$ (representing block rotation) and symmetric (pure deformation) tensor [length-increment variation + angle variation]. Applied to the gradient tensor, this theorem allows us to write:

$$\mathbf{F} = \mathbf{R} \cdot \mathbf{U} = \mathbf{V} \cdot \mathbf{R},$$

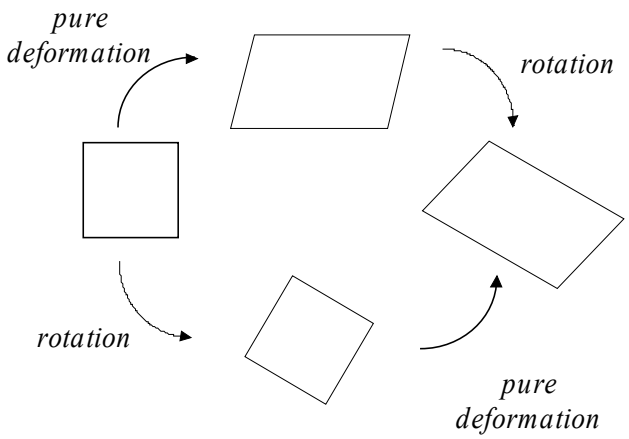

Figure 1.4: *Polar decomposition of the gradient tensor.*

where $\mathbf{U}$ (resp. $\mathbf{V}$) is the right (resp. left) pure strain tensor.

This theorem can also be applied to other tensors such as $\mathbf{C}$ and $\mathbf{E}$, but in that case we can take benefit from the symmetry[2] of these tensors together with the symmetry in $\mathbf{U}$ (or $\mathbf{V}$). In the eigenvector basis, deformation corresponds to length variations with no angle variation.

In addition to the length, we can also characterize the deformation of surfaces and volumes. The transformation of an infinitesimal volume $\mathrm{d}V$ in the initial frame is given by the Jacobian J of the transformation $\mathrm{d}\mathbf{X} \to \mathrm{d}\mathbf{x}$

$$\mathrm{d}v = J\mathrm{d}V \text{ with } J = |\det \mathbf{F}|.$$

Similarly, an oriented infinitesimal element of surface $\mathrm{d}\mathbf{A}$ can be expressed as $\mathrm{d}\mathbf{A} = \mathrm{d}\mathbf{X}_1 \times \mathrm{d}\mathbf{X}_2$, which is transformed into

$$\mathrm{d}\mathbf{a} = \mathrm{d}\mathbf{x}_1 \times \mathrm{d}\mathbf{x}_2 = J(\mathbf{F}^{-1})^\dagger \cdot \mathrm{d}\mathbf{A}.$$

♣ **Example.** – For instance, let us consider a shear strain in the form

$$x_1 = X_1 + \gamma(t)X_2,\ x_2 = X_2, \text{ and } x_3 = X_3,$$

where $\gamma(t)$ is called the shear amplitude and $(x_1,\ x_2,\ x_3)$ is the coordinates in a Cartesian frame. We find that this transformation keeps the volumes constant $(J = 1)$ and

$$\mathbf{F} = \begin{bmatrix} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},\ \mathbf{C} = \begin{bmatrix} 1 & \gamma & 0 \\ \gamma & 1+\gamma^2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \text{ and } \mathbf{E} = \begin{bmatrix} 0 & \gamma/2 & 0 \\ \gamma/2 & \gamma^2/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

[1]Recall that if a tensor is orthogonal, then $\mathbf{R}^\dagger \cdot \mathbf{R} = \mathbf{R} \cdot \mathbf{R}^\dagger = \mathbf{1}$ and $\det \mathbf{R} = 1$.

[2]Recall that a real-valued symmetric tensor can be diagonalized and its eigenvector basis is orthogonal.

□

Small deformations

When deformations are small, we can linearize the tensors to get rid of nonlinear terms. Essentially this means that the displacement $\mathbf{u} = \mathbf{x} - \mathbf{X}$ between the current and initial positions is very small. We can deduce that

- there is no much differences between the frame $\mathcal{C}_0$ and $\mathcal{C}(t)$, which can then be assumed to be the same;
- we can write $\mathbf{F} = \mathbf{1} + \mathbf{H}$ with $\mathbf{H} = \nabla_X \mathbf{x}$ with "small" entries.

We deduce that the Cauchy-Green tensor can be linearized in the following way

$$\mathbf{C} = \mathbf{F}^\dagger \cdot \mathbf{F} = \mathbf{1} + \mathbf{H} + \mathbf{H}^\dagger = 1 + 2\boldsymbol{\epsilon},$$

where $\boldsymbol{\epsilon}$ is called the (linearized) strain tensor and is defined as the symmetric part of $\mathbf{H}$

$$\boldsymbol{\epsilon} = \frac{1}{2}(\mathbf{H} + \mathbf{H}^\dagger) = \frac{1}{2}\left(\nabla_X \mathbf{x} + \nabla_X \mathbf{x}^\dagger\right) = \mathbf{E}.$$

Rate of strain

In order to characterize the velocity, we introduce the time derivative of $\mathbf{x}(\mathbf{X},\ t)$. In a Lagrangian system, $\mathbf{X}$ corresponds to the initial condition at $t = 0$, whereas in an Eulerian system, $\mathbf{X}$ is the position previously occupied by a particle and is a function of time.

The time derivative of an infinitesimal length increment is

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}\mathbf{x} = \dot{\mathbf{F}} \cdot \mathrm{d}\mathbf{X} = \dot{\mathbf{F}} \cdot \mathbf{F}^{-1} \cdot \mathrm{d}\mathbf{x} = \mathbf{L} \cdot \mathrm{d}\mathbf{x},$$

where $\mathbf{L} = \dot{\mathbf{F}} \cdot \mathbf{F}^{-1} = \nabla_x \mathbf{v}$ is called the *velocity gradient tensor*. It is customary to break down into a symmetric and antisymmetric contribution

$$\mathbf{d} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^\dagger) \text{ and } \mathbf{w} = \frac{1}{2}(\mathbf{L} - \mathbf{L}^\dagger).$$

The symmetric part $\mathbf{d}$ describes the strain rate and hence is called the *strain-rate tensor* (sometimes the stretching tensor), whereas the antisymmetric part $\mathbf{w}$ called the *vorticity tensor* (sometimes the spin tensor) corresponds to the rotational of the velocity field.

Recall that when a tensor $\mathbf{w}$ is antisymmetric, this implies the existence of a vector $\boldsymbol{\omega}$ such that for any vector $\mathbf{n}$, we have $\mathbf{w} \cdot \mathbf{n} = \boldsymbol{\omega} \times \mathbf{n}$. Let us expand the velocity $\mathbf{v}(\mathbf{x} + \mathrm{d}\mathbf{x})$

$$\mathbf{v}(\mathbf{x} + \mathrm{d}\mathbf{x}) = \mathbf{v}(\mathbf{x}) + \nabla_x \mathbf{v} \cdot \mathrm{d}\mathbf{x} + \cdots = \mathbf{v}(\mathbf{x}) + \mathbf{d}(\mathbf{x}) \cdot \mathrm{d}\mathbf{x} + \mathbf{w}(\mathbf{x}) \cdot \mathrm{d}\mathbf{x} + \cdots,$$

which means that to first order, we have

$$\mathbf{v}(\mathbf{x} + \mathrm{d}\mathbf{x}) = \mathbf{v}(\mathbf{x}) + \mathbf{d} \cdot \mathrm{d}\mathbf{x} + \boldsymbol{\omega} \times \mathrm{d}\mathbf{x}.$$

This means that the local variation in the velocity field can be broken down into a strain-rate contribution and another contribution corresponding to solid rotation

Refined kinematical description

Here we have deliberately ignored the issues related to the frames in which the tensor components are written. We have just introduced the configurations $\mathcal{C}_0$ and $\mathcal{C}(t)$ and any quantity can be defined in either configuration. Another approach is to introduce a curvilinear coordinate system that is linked to the material deformations: when the body deforms, the initial axes of $\mathcal{C}_0$ deform in the same way and define a system of material coordinates that is embedded in the material and deform with it, as shown in Figure 1.5.

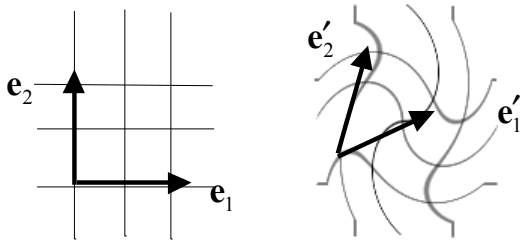

Figure 1.5: *Polar decomposition of the gradient tensor.*

The idea of a convected coordinate system embedded in a flowing film and deforming with it was developed by Oldroyd (1950) in the 1950s. This idea was motivated by the desire to formulate constitutive equations that are (i) independent of any frame of reference, (ii) independent of the position, and translational and rotational motion, of the element as a whole in space, and (iii) independent of the states of neighboring material elements.

1.2.2 Stress tensor

Definition of the stress tensor

We are going to introduce a new tensor called the *stress tensor*, which is used to compute the stresses exerted on an infinitesimal surface δS oriented by the outward unit vector $\mathbf{n}$. The stress $\boldsymbol{\tau}$ exerted on δS is defined as the ratio of the forces $\mathbf{f}$ per unit surface when δS becomes smaller and smaller:

$$\boldsymbol{\tau} = \lim_{\delta S \to 0} \frac{\mathbf{f}}{\delta S}.$$

Using Cauchy's lemma (force balance on a tetrahedron), it can be shown that there exists a tensor $\boldsymbol{\sigma}$, the *stress tensor*, such that

$$\boldsymbol{\tau} = \boldsymbol{\sigma} \cdot \mathbf{n}, \tag{1.7}$$

which means that the stress linearly varies with the normal $\mathbf{n}$. In a Cartesian frame, this tensor is represented by a symmetric matrix.

It is worth reminding that this construction is based on a postulate (force balance with no torque), which implies that other constructions are possible (e.g., micropolar or Cosserat medium) (Germain, 1973*a*,*b*). More generally, it is possible to use the virtual power principle to derive all the fundamental equations used in continuum mechanics and in that case, the stress tensor can formally be derived from the inner energy dissipation rate Φ

$$\sigma_{ij} = \frac{\partial \Phi}{\partial d_{ij}}. \tag{1.8}$$

This approach to continuum mechanics turns out to be fruitful for a number of problems in elasticity (membrum and shell theory) and in fluid mechanics. Indeed, on some occasions, it is easier to compute the energy dissipated in a system and, in that case, to compute the stress tensor using (1.8); for instance, a number of approximate computations of the bulk viscosity of a dilute particle suspension were done in this way (Einstein, 1911; Frankel & Acrivos, 1967).

Pressure and extra-stress

For a simple fluid at rest, the stress tensor reduces to

$$\boldsymbol{\sigma} = -p\mathbf{1},$$

where p is called the *pressure*. From the thermodynamic viewpoint, the pressure is a function of the density ρ and temperature T: $p = p(\rho,\ T)$. Making use of the (Helmholtz) free energy $F = E - TS$, with S entropy, E internal energy, then we can show

$$p = \rho^2 \frac{\partial F}{\partial \rho}.$$

When the density is constant (incompressible material) or the flow is isochoric, the thermodynamic definition of pressures is no longer valid and the *thermodynamic pressure* must be replaced by the *hydrodynamic pressure*. The latter is an undetermined function that can be specified on solving the governing equations with specific boundary conditions.

When an incompressible simple fluid at rest is slightly disturbed, we can imagine that the stress can be expressed as

$$\boldsymbol{\sigma} = -p\mathbf{1} + \mathbf{s},$$

where $\mathbf{s}$ is called the extra-stress tensor and represents the departure from the static equilibrium. We shall see that for a wide class of fluids, this extra-stress is a function of the strain-rate tensor alone $\mathbf{d}$, which leads to posing: $\boldsymbol{\sigma} = -p\mathbf{1} + \mathbf{s}(\mathbf{d})$. The simplest dependence of $\mathbf{s}$ on $\mathbf{d}$ that we can imagine is the linear relation: $\mathbf{s} = 2\mu\mathbf{d}$, i.e., the Newtonian constitutive equation. There is another motivation for writing the stress tensor as the sum of a pressure term and an additional contribution $\mathbf{s}$. Indeed, for an incompressible fluid, the mass balance imposes some constraints on the motion; there are internal stresses $\boldsymbol{\sigma}'$ that make the fluid incompressible. If these stresses are assumed to induce no energy dissipation, then for any deformation, we must have $\Phi = \mathrm{tr}(\boldsymbol{\sigma}\mathbf{d}) = 0$ or, in other words, $\boldsymbol{\sigma}' = -p\mathbf{1}$ since $\mathrm{tr}\mathbf{d} = 0$ (incompressible fluid). In the sequel, we shall see that there are some rules that must be satisfied in specifying a particular form of constitutive equation.

This way of expressing the stress tensor can be generalized to any type of material. It is customary in rheology to break down the stress tensor into two parts:

$$\boldsymbol{\sigma} = -p\mathbf{1} + \mathbf{s},$$

where p is now called the *mean pressure*

$$p = -\frac{1}{3}\mathrm{tr}\boldsymbol{\sigma},$$

and $\mathbf{s}$ is called the *deviatoric stress tensor* since it represents the departure from an equivalent equilibrium state.

Describing the rheological behavior of a material involves determining the relation between the stress tensor $\boldsymbol{\sigma}$ and the gradient tensor $\mathbf{F}$. The relation $\boldsymbol{\sigma} = \mathcal{F}(\mathbf{F})$, where $\mathcal{F}$ is a functional is called the *constitutive equation*. When the material is incompressible, the constitutive equation is usually defined with the extra-stress tensor since the stress tensor is defined to within an arbitrary function (pressure): $\mathbf{s} = \mathcal{F}(\mathbf{F})$.

Keep in mind that pressure may have a meaning that differs depending on the context: thermodynamic pressure, hydrodynamic pressure, mean pressure.

1.2.3 Admissibility of a constitutive equations

There are a number of rules that must be used to produce constitutive equations that are admissible from the rational and physical standpoints. The establishment of these rules have been the subject of long debates and has been approached in a number of ways, the interrelation of which are by no means easy to understand (Oldroyd, 1950; Truesdell, 1966, 1974). Here we will deal with general principles without expounding all the details.

Objectivity or material indifference

A constant behavior in physics is to express laws that do not depend on a particular system of reference. Let us try now to apply this fundamental principle to the formulation of constitutive equation. We assume that a constitutive equation is a mathematical relation between the stress and the deformation, using a short-hand notation, we express

$$\boldsymbol{\sigma} = \mathcal{F}(\mathbf{F})$$

where $\mathcal{F}$ is a functional depending on the gradient tensor $\mathbf{F}$. We have seen earlier that $\mathbf{F}$ can include solid rotation. Solid rotation as wells as translation of a reference or a change of clock frame must not modify the physics, which implies that we must get rid of solid rotation and translation when expressing a constitutive equation.

Principle 1: *A constitutive equations is invariant under any change of reference frame.*

In practice this means that we make a change of variable

$$\mathbf{x}' = \mathbf{R} \cdot \mathbf{x} + \mathbf{b} \text{ and } t' = t + a,$$

which means that the image $\mathbf{x}'$ experiences a rotation (the tensor $\mathbf{R}$ can be time-dependent) and a translation ($\mathbf{b}$ is a constant vector) with respect to the original point $\mathbf{x}$; in addition there is change in the time reference (a being a constant). Then, for a quantity to be objective we must check that:

- a scalar field remains the same: $s'(\mathbf{x}',\ t') = s(\mathbf{x},\ t)$,
- a vector must satisfy $\mathbf{x}'(\mathbf{x}',\ t') = \mathbf{R} \cdot \mathbf{x}(\mathbf{x},\ t)$
- a tensor $\mathbf{T}$ is objective if it transforms objective vectors into objective vectors, i.e., $\mathbf{T}' \cdot \mathbf{x}' = \mathbf{R} \cdot \mathbf{T} \cdot \mathbf{x}$ or equivalently

$$\mathbf{T}'(\mathbf{x}',\ t') = \mathbf{R} \cdot \mathbf{T}(\mathbf{x},\ t) \cdot \mathbf{R}^{\dagger}.$$

The issue lies in the dependence of $\mathbf{F}$ on a particular frame. For instance, we introduce a rotation of the reference frame, the gradient tensor in the new frame is

$$F'_{ij} = \frac{\partial x'_i}{\partial X_j} = \frac{\partial x'_i}{\partial x_k}\frac{\partial x_k}{\partial X_j},$$

with $R_{ik} = \partial x'_i / \partial x_k$ an orthogonal tensor that corresponds to a frame rotation: $\mathbf{x}' = \mathbf{R} \cdot \mathbf{x}$ (see Figure 1.6). We deduce that $\mathbf{F}' = \mathbf{R} \cdot \mathbf{F}$, which is not admissible.

Now, if we make use of the Cauchy tensor

$$\mathbf{C}' = \mathbf{F}'^{\dagger} \cdot \mathbf{F}' = \mathbf{F}^{\dagger} \cdot \mathbf{R}^{\dagger} \cdot \mathbf{R} \cdot \mathbf{F} = \mathbf{F}^{\dagger} \cdot \mathbf{F} = \mathbf{C},$$

which shows that $\mathbf{C}$ is not an objective tensor since it does depend on the frame. Similarly, it can be shown that the strain tensor $\mathbf{E}$ and the strain-rate tensor $\mathbf{d}$ are objective.

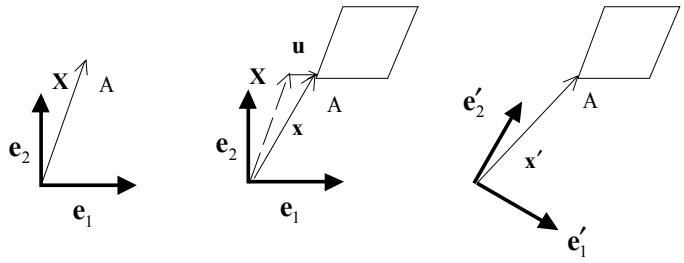

Figure 1.6: *Change of reference.*

Determinism

Principle 2: *The history of the thermo-kinetic process experienced by the material fully determines the current rheological and thermodynamic state of the material.* This principle must be relaxed slightly when the material is incompressible because the stress state is determined to within the hydrostatic pressure (which depends on the boundary conditions and the problem geometry).

Local action

Principle 3: *The thermodynamic process of a material at a given point is completely determined by the history of the thermo-kinetic process to which the neighborhood of the point was submitted.* In other words, the stress tensor at a given point does not depend on movements occurring at finite distance from this point.

1.2.4 Specific properties of material

A material is said to be

- *homogeneous* when the constitutive equation does not depend on the point considered;
- *isotropic* when the material response is invariant under rotation, i.e., when we consider a direction or another, we measure the same response;
- characterized by a *fading memory* when the material response depends on the very recent history.

The reader can refer to the book by Hutter & Jöhnk (2004) for further developments on *symmetry* in materials and their consequences in the constitutive equations.

1.2.5 Representation theorems

Cayley-Hamilton theorem

In linear algebra, the *Cayley-Hamilton theorem* says that from a second order tensor $\mathbf{M}$, we can build a third-order polynomial

$$P_M(\lambda) = \det(\mathbf{M} - \lambda\mathbf{1}) = -\lambda^3 + M_I\lambda^2 - M_{II}\lambda + M_{III},$$

where M_I, M_{II}, and M_{III} are called the fundamental invariants of $\mathbf{M}$, with

$$M_I = \mathrm{tr}\mathbf{M},\ M_{II} = \frac{1}{2}\left((\mathrm{tr}\mathbf{M})^2 - \mathrm{tr}\mathbf{M}^2\right), \text{ and } M_{III} = \det\mathbf{M}.$$

The zeros of this polynomial are the eigenvalues of $\mathbf{M}$ and, moreover, we have the relation

$$P_M(\mathbf{M}) = 0.$$

The remarkable result is that it is possible to define three independent scalar quantities that are objective, i.e., they do not depend on the frame in which we can express $\mathbf{M}$ since they are scalar. From this viewpoint, it is equivalent to write $f = f(\mathbf{M})$ or $f = f(M_I, M_{II}, M_{III})$. The benefit is twofold

- it is mostly easier to handle scalar quantities than tensors;
- we can reduce the number of variables needed for describing the behavior. For instance, instead of a second-order symmetric tensor (with 6 independent variables), we can use the three invariants without loss of information.

We will now show that it is possible to interpret the invariants physically.

Physical interpretation

Any combination of invariants is invariant. Using this principle, we can build invariants that are physically meaningful. For the stress tensor $\boldsymbol{\sigma}$ and the strain tensor $\boldsymbol{\epsilon}$, we introduce

- the first invariants of the stress tensor and the strain tensor are defined as

$$I_{1,\sigma} = \mathrm{tr}\boldsymbol{\sigma} = 3\sigma_m \text{ and } I_{1,\epsilon} = \mathrm{tr}\boldsymbol{\epsilon} = \frac{\Delta V}{V},$$

  showing that the first invariant of the stress tensor gives an idea of the mean pressure at a given point, while the first invariant of the strain tensor specifies the relative volume variation.

- the second invariant is usually defined as

$$I_{2,\sigma} = \mathrm{tr}\mathbf{s}^2 \text{ and } I_{2,\epsilon} = \mathrm{tr}\mathbf{e}^2,$$

where $\mathbf{s} = \boldsymbol{\sigma} - \sigma_m \mathbf{1}$ is the deviatoric stress tensor and $\mathbf{e} = \boldsymbol{\epsilon} - I_{1,\epsilon}\mathbf{1}/3$ is the deviatoric strain tensor. The second invariant indicated how large the departure from the mean state is.

- the third invariant is mostly defined as

$$I_{3,\sigma} = \mathrm{tr}\mathbf{s}^3 \text{ and } I_{3,\epsilon} = \mathrm{tr}\mathbf{e}^3.$$

We can show that the third invariant makes it possible to define a phase angle in the deviatoric plane[3].

$$\cos\phi = -\frac{\sqrt{6}I_3}{I_2^{3/2}}.$$

To illustrate these notions, let us assume that we know the stress tensor at a given point M. The stress tensor being symmetric, we know that there there is an orthogonal basis made up of the eigenvectors of $\boldsymbol{\sigma}$. In the stress space, where the coordinates are given by the eigenvalues of $\boldsymbol{\sigma}$ (hereafter referred to as σ_i with $1 \leq i \leq 3$), the stress state at M is represented by a point.

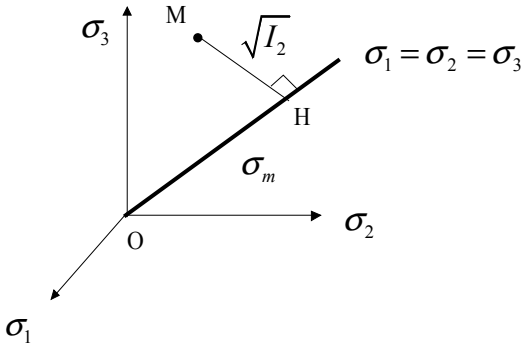

Figure 1.7: *Stress space.*

The position of this stress point can be given in terms of the Cartesian coordinates or in terms of invariants. Indeed, let us call H the projection of M onto the first trissectrice (straight line $\sigma_1 = \sigma_2 = \sigma_3$). To locate M, we need to know the distances OH and HM together with an angle ϕ with respect to an arbitrary direction in the deviatoric plane. It is straightforward to show that

- OH represents the mean stress at M;
- HM represents the departure from an isotropic state and $|HM|^2 = I_{2,\sigma} = s_1^2 + s_2^2 + s_3^2$ where s_i are the eigenvalues of the deviatoric stress tensor.

[3]plane passing through H and the normal of which is the first trissectrice

Representation theorems

Representation theorems are an ensemble of rules that specify how to transform a tensor-valued expression into an expression involving invariants (Boehler, 1987; Zheng, 1994).

For instance, let us assume that we have to compute the strain energy function W of an elastic body. We can write that $W = W(\mathbf{E})$, where $\mathbf{E}$ is the strain tensor, or we can write $W = W(E_i)$ with E_i with $1 \leq i \leq 6$ the six independent components of $\mathbf{E}$. Using invariants, we can also write

$$W = W(I_{1,\epsilon},\ I_{2,\epsilon},\ I_{3,\epsilon}).$$

In doing so, we reduce the number of variables from 6 to 3. If we assume that there is a preferred direction of deformation $\mathbf{n}$, then we can write $W = W(\mathbf{E},\ \mathbf{n})$ (i.e., 9 variables) or

$$W = W(I_{1,\epsilon},\ I_{2,\epsilon},\ I_{3,\epsilon},\ \mathbf{n}\cdot\mathbf{E}\cdot\mathbf{n},\ \mathbf{n}\cdot\mathbf{E}^2\cdot\mathbf{n}),$$

reducing the number of variables from 9 to 5.

Representation of tensor-valued functions in complete irreducible forms has been proved to be very helpful in formulating nonlinear constitutive equations for isotropic or anisotropic materials.

1.2.6 Balance equations

Transport theorem

In any course on functional analysis, one can find the Leibnitz formula that shows how to derive an integral real-valued function, the boundaries of which may vary with time

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{a(t)}^{b(t)} f(x,\ t)\mathrm{d}t = \int_{a(t)}^{b(t)} \frac{\partial f(x,\ t)}{\partial t}\mathrm{d}x + f(b(t))\frac{\mathrm{d}b}{\mathrm{d}t} - f(a(t))\frac{\mathrm{d}a}{\mathrm{d}t}. \tag{1.9}$$

Leibnitz relation can be generalized to multiple integrals, i.e. integration is made on volumes instead of intervals. One obtains the following relation called *transport theorem*

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\int_V f\mathrm{d}V = \int_V \frac{\partial f}{\partial t}\mathrm{d}V + \int_S f\mathbf{u}\cdot\mathbf{n}\mathrm{d}S,} \tag{1.10}$$

where V is the control volume containing a given mass of fluid, S is the surface bounding this volume, and $\mathbf{n}$ is the vector normal to the surface S ; $\mathbf{n}$ is unitary ($|\mathbf{n}| = 1$) and outwardly oriented. This relation written here for a scalar function f holds for any vectorial function $\mathbf{f}$.

Equation (1.10) is fundamental since it makes it possible to derive all the equations needed in continuum mechanics. It can be interpreted as follows. Any variation in f over time within the control volume V results from

- local change in f with time;
- flux of f through S (flux = inflow – outflow through V).

An helpful variant of the transport theorem is obtained by using the Green-Ostrogradski theorem :

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\int_V f\mathrm{d}V = \int_V \left(\frac{\partial f}{\partial t} + \nabla\cdot(f\mathbf{u})\right)\mathrm{d}V}.$$

This expression shall be used to derive local governing equations in the following.

A control volume is most often a material volume, i.e., it is made up of a collection of particles that are followed up in their motion; its borders are fluid and move with the fluid, which means that the boundary velocity corresponds to the local velocity at the boundary. On some occasions, we can also define an arbitrary control volume, the velocity of which $\mathbf{u}$ at the border surface S does not correspond to that of the fluid.

Another important variant of the transport theorem is the *Reynolds theorem* that applies to integrands that take the form ρf, with ρ the fluid density. This theorem reads:

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho f\mathrm{d}V = \int_V \rho\frac{\mathrm{d}}{\mathrm{d}t}f\mathrm{d}V.} \tag{1.11}$$

Conservation of mass

Let us apply the transport theorem (1.10) to $f = \rho$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho\mathrm{d}V = \int_V \frac{\partial\rho(\mathbf{x},\ t)}{\partial t}\mathrm{d}V + \int_S \rho\mathbf{u}\cdot\mathbf{n}\mathrm{d}S.$$

Making use of the divergence theorem (Green-Ostrogradski), we find

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho\mathrm{d}V = \int_V \left(\frac{\partial\rho(\mathbf{x},\ t)}{\partial t} + \nabla\cdot(\rho\mathbf{u})\right)\mathrm{d}V = 0.$$

Note that the total mass is constant because we follow up a finite number of particles and there is no production or loss of particles.

When ρ is continuous, then we can pass from a control-volume formulation to a local equation

$$\boxed{\frac{\partial\rho(\mathbf{x},\ t)}{\partial t} + \nabla\cdot\rho\mathbf{u} = 0.} \tag{1.12}$$

This equation is often called *continuity equation*. It can also be cast in the following form:

$$\frac{1}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho\nabla\cdot\mathbf{u}.$$

Recall that passing from global to local equations is permitted only if the field is continuous. This is not always the case, e.g. when there is a *shock* inside the control volume. Specific equation must be used (see below).

Here are other helpful definitions

- a flow is said *isochoric* when $\frac{1}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t} = 0$ (e.g., when the Mach number is less than unity, air flow is isochoric);
- a material is said *incompressible* when ρ is constant at any point and any time (water can be considered as incompressible under normal flow conditions).

Conservation of momentum

One applies the transport theorem (1.10) tho the momentum $f = \rho\mathbf{u}$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho\mathbf{u}\mathrm{d}V = \int_V \frac{\partial\rho\mathbf{u}}{\partial t}\mathrm{d}V + \int_S \rho\mathbf{u}(\mathbf{u}\cdot\mathbf{n})\mathrm{d}S.$$

There are many variants of this equation, based either on different ways of expressing the material derivative of $\rho\mathbf{u}$ or on different ways of expressing the velocity (e.g., streamline function, vorticity). On applying the divergence theorem, one gets :

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho\mathbf{u}\mathrm{d}V = \int_V \left(\frac{\partial\rho\mathbf{u}}{\partial t} + \nabla\cdot\rho\mathbf{u}\mathbf{u}\right)\mathrm{d}V,$$

or equivalently

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho\mathbf{u}\mathrm{d}V = \int_V \rho\left(\frac{\partial\mathbf{u}}{\partial t} + \nabla\cdot\mathbf{u}\mathbf{u}\right)\mathrm{d}V.$$

The fundamental principle of Mechanics is that any time variation in momentum results from applying body or surface force(s) on the control volume

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho\mathbf{u}\mathrm{d}V = \text{forces applied on } V.$$

Once again, we can obtain a local expression of the momentum balance equation if the fields are continuous:

$$\frac{\partial\rho\mathbf{u}}{\partial t} + \nabla\cdot\rho\mathbf{u}\mathbf{u} = \rho\mathbf{g} + \nabla\cdot\boldsymbol{\sigma},$$

or

$$\boxed{\rho\frac{\partial\mathbf{u}}{\partial t} + \rho\mathbf{u}\cdot\nabla\mathbf{u} = \rho\mathbf{g} + \nabla\cdot\boldsymbol{\sigma} = \rho\mathbf{g} - \nabla p + \nabla\cdot\mathbf{s}} \tag{1.13}$$

Be aware that $\mathbf{u}\cdot\nabla\mathbf{u}$ does not mean the product between $\mathbf{u}$ and the tensor $\nabla\mathbf{u}$. Rigorously speaking, it would be better to write $(\mathbf{u}\cdot\nabla)\mathbf{u}$, the parentheses are used to say that $\mathbf{u}\cdot\nabla$ is a differential operator applied to $\mathbf{u}$.

1.2.7 Conservation of energy

Kinetic energy

The transport theorem (1.10) is now applied to the kinetic energy $f = E_c = \frac{1}{2}\rho|\mathbf{u}|^2$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \frac{1}{2}\rho|\mathbf{u}|^2\mathrm{d}V = \int_V \frac{\partial E_c}{\partial t}\mathrm{d}V + \int_S \frac{1}{2}\rho|\mathbf{u}|^2(\mathbf{u}\cdot\mathbf{n})\mathrm{d}S.$$

As earlier for the momentum equation, there are variants of this equation depending on how the material derivative of E_c is expressed. Making use of the divergence theorem leads to

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V E_c\mathrm{d}V = \int_V \left(\frac{\partial E_c}{\partial t} + \nabla\cdot\left(\frac{1}{2}\rho|\mathbf{u}|^2\mathbf{u}\right)\right)\mathrm{d}V,$$

Note that the equation can be inferred from (1.13) by multiplying it by $\mathbf{u}$, then replacing terms such as $\mathbf{u}\partial\mathbf{u}$ with $\partial|\mathbf{u}|^2/2$, and then integrating over the control volume V. We then deduce the bulk expression of the *kinetic energy theorem*

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V E_c\mathrm{d}V = \text{power supplied to the volume } V - \text{power dissipated in } V,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V E_c\mathrm{d}V = \int_V \rho\mathbf{u}\cdot\mathbf{g}\mathrm{d}V + \int_V \mathbf{u}\cdot(\nabla\cdot\boldsymbol{\sigma})\mathrm{d}V.$$

When the fields are continuous and making use of

$$\mathbf{u}\cdot(\nabla\cdot\boldsymbol{\sigma}) = \nabla\cdot(\mathbf{u}\cdot\boldsymbol{\sigma}) - \boldsymbol{\sigma} : \nabla\mathbf{u},$$

we can derive the local equation

$$\boxed{\frac{\partial E_c}{\partial t} + \nabla\cdot(E_c\mathbf{u}) = \rho\mathbf{u}\cdot\mathbf{g} + \nabla\cdot(\mathbf{u}\cdot\boldsymbol{\sigma}) - \boldsymbol{\sigma} : \nabla\mathbf{u}.} \tag{1.14}$$

We refer to $\Phi = \boldsymbol{\sigma} : \nabla\mathbf{u}$ as the *energy dissipation rate*. Using the decomposition of the strain rate tensor into its symmetric and antisymmetric parts, we also obtain

$$\Phi = \boldsymbol{\sigma} : \mathbf{d} = \mathrm{tr}(\boldsymbol{\sigma}\cdot\mathbf{d}).$$

Recall that the energy balance theorem contains nothing more that the momentum balance equation does. For a regular problem, we can select either theorem;

the choice is a matter of personal convenience or strategy (for alleviating computation). On some occasions, only one of these equations can be used in practice. For instance, when studying shock formation, it is usually better to use momentum balance equations because shocks induce energy dissipation that is not easy to compute.

$\Rrightarrow$ In many practical applications (incompressible fluid in a steady regime), the energy balance equation can be transformed into the Bernoulli equation

$$\boxed{\frac{\partial E_c}{\partial t} + \nabla \cdot \left(\mathbf{u} \frac{\rho |\mathbf{u}|^2 + 2p_*}{2} \right) = \nabla \cdot (\mathbf{u} \cdot \mathbf{s}) - \mathbf{s} : \mathbf{d},}$$

where $p_* = p + \psi$ is the *generalized pressure*, with $\psi = \rho g z$ the gravity potential ($\rho \mathbf{g} = -\nabla \psi$). The *Bernoulli theorem* is obtained by assuming that

- the flow is steady, i.e. $\partial E_c / \partial t = 0$;
- the Reynolds number is high (the fluid is inviscid).

We then obtain

$$\nabla \cdot \left(\mathbf{u} \frac{\rho |\mathbf{u}|^2 + 2p_*}{2} \right) = \mathbf{u} \cdot \nabla \left(\frac{\rho |\mathbf{u}|^2}{2} + p_* \right) = 0,$$

which means that

$$\boxed{\Psi = \frac{1}{2} \rho |\mathbf{u}|^2 + p_* = \frac{1}{2} \rho |\mathbf{u}|^2 + p + \rho g z} \tag{1.15}$$

is constant along a streamline.

First axiom of thermodynamics

The first law of thermodynamics applied to a control volume V is the following statement

$$\begin{aligned} \text{rate of change of total energy} = \ & \text{rate of change of work of the forces applied to } V \\ & + \text{rate of heat addition.} \end{aligned} \tag{1.16}$$

We define the following quantities

- The *total energy* is the sum of the internal energy $E = \rho e$ (e internal energy per unit mass) and the kinetic energy $\rho u^2/2$.
- The rate of work is the power of the forces applied to the boundary and the body forces (e.g., gravity).

- The heat supplied to the control volume results from heat generated at points within V and from heat transmitted through the boundaries. The heat supply density is denoted by r and the heat flux is written $q = \mathbf{q} \cdot \mathbf{n}$, with $\mathbf{q}$ the heat flux vector (Stokes relation). When the Fourier law holds, the heat flux vector is related to the gradient temperature $\mathbf{q} = -\kappa \nabla T$, where κ is the *heat conductivity*.

Translated into mathematical terms, this statement becomes

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho\left(e + \frac{1}{2}u^2\right)\mathrm{d}V = \int_V \rho\mathbf{u}\cdot\mathbf{g}\mathrm{d}V + \int_A \mathbf{u}\cdot(\boldsymbol{\sigma}\cdot\mathbf{n})\mathrm{d}A + \int_V \rho r\mathrm{d}V - \int_A \mathbf{q}\cdot\mathbf{n}\mathrm{d}A,}$$

where A is the surface bounding V. The local form is

$$\rho\frac{\mathrm{d}}{\mathrm{d}t}\left(e + \frac{1}{2}u^2\right) = \rho\mathbf{u}\cdot\mathbf{g} + \nabla\cdot(\boldsymbol{\sigma}\mathbf{u}) - \nabla\mathbf{q} + \rho r.$$

Making use of the kinetic energy theorem leads to the following relation

$$\boxed{\rho\frac{\mathrm{d}e}{\mathrm{d}t} = \Phi - \nabla\mathbf{q} + \rho r,}$$

where $\Phi = \boldsymbol{\sigma} : \mathbf{d}$ is the dissipation rate (also called stress power). Variations in the internal energy are caused by (viscous) dissipation, the flux of heat, and/or a source/sink of heat.

Second axiom of thermodynamics

We end our discussion on energy conservation by recalling the second principle used in thermodynamics, which reflects the irreversibility of time processes associated with energy dissipation. The second law states that

$$\rho\dot{f} - \Phi + \rho\dot{T}s + \frac{1}{T}\mathbf{q}\cdot\nabla T \leq 0$$

with $f = e - Ts$ the free energy per unit mass, s the entropy per unit mass, Φ the energy dissipation rate, $\mathbf{q}$ the heat flux vector, and T the temperature.

1.2.8 Jump conditions

In practice, there are a number of situations for which there are rapid changes in the flow features over relatively short distances. For instance, a high-speed airplane or spatial capsule creates a shock wave as it breaks the sound barrier, as is shown in Figures 1.8 and 1.9

In theory, it is usually appropriate to consider the shock as a discontinuity surface, i.e. a surface through which some of the flow variables (density, velocity,

Figure 1.8: *A U.S. Navy airplane creates a shock wave as it breaks the sound barrier. The shock wave is visible as a large cloud of condensation formed by the cooling of the air. A smaller shock wave can be seen forming on top of the canopy.(U.S. Navy photo by John Gay).*

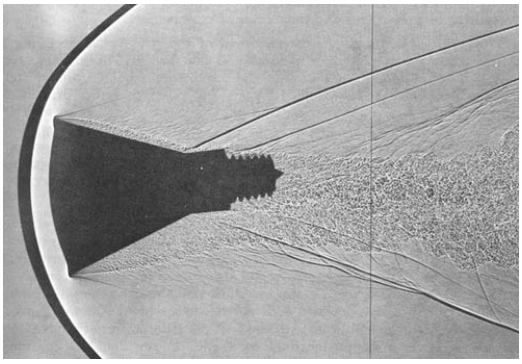

Figure 1.9: *A shadowgraph of the Project Mercury reentry capsule, showing the bow-shock wave in front of it and the flow fields behind the capsule. Photograph from NASA).*

etc.) may be become discontinuous. The local balance equations are valid on either side of the jump, but not at the shock surface. This implies that we have to specify the jump conditions on the flow variables induced by a shock. Note that a discontinuity surface may be an existing boundary (e.g. a free surface) or it may be created under some flow conditions. Spontaneous creation or disappearance of a shock surface is typical for hyperbolic partial differential equations (Courant & Friedrich, 1948). We will focus here on the latter case (see also § 3.2.2).

Let us first consider the scalar case. We have to solve a hyperbolic problem in the form:

$$\frac{\partial f(x,\ t)}{\partial t} + \frac{\partial G[f(x,\ t)]}{\partial x} = a(x,\ t),$$

where G is a function and a another function called the source term. Note that the equations looks like the balance equations we have seen earlier. Usually such an equation originates from the conservation of a quantity in a given control volume, i.e. an equation in the following integral form

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V f(x,\ t)\mathrm{d}x = G[f(x_2,\ t)] - G[f(x_1,\ t)] + \int_V a(x,\ t)\mathrm{d}x,$$

where the control volume corresponds to the range $[x_1,\ x_2]$ in the scalar case. When f is continuous over V, the two equations are equivalent. Let us assume that there is a moving point $x = s(t)$ within $[x_1,\ x_2]$ at which f admits a discontinuity. Making use of the Leibnitz rule, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{x_1}^{x_2} f(x,\ t)\mathrm{d}x = \int_{x_1}^{s(t)} \frac{\partial f(x,\ t)}{\partial t}\mathrm{d}x + \int_{s(t)}^{x_2} \frac{\partial f(x,\ t)}{\partial t}\mathrm{d}x - \dot{s}[\![f]\!],$$

where we have broken down $[x_1,\ x_2] = [x_1,\ s(t)] + [s,\ x_2(t)]$ and where $[\![f]\!]$ is the jump experienced by f:

$$[\![f]\!] = \lim_{x\to s,\ x>0} f(x) - \lim_{x\to s,\ x<0} f(x).$$

Then taking the limits $x_1 \to s$ and $x_2 \to s$, leads to

$$[\![G[f(x,\ t)] - \dot{s}f(x,\ t)]\!] = 0.$$

The quantity is $G[f] - f\dot{s}$ is conserved through the shock. We can also deduce the shock velocity

$$\dot{s} = \frac{[\![G[f(x,\ t)]]\!]}{[\![f(x,\ t)]\!]}.$$

For instance, we can retrieve the *Rankine-Hugoniot shock conditions* used in gas dynamics if we take

- $f = \rho u$ (u being a velocity and ρ a density), $G[f] = \frac{1}{2}\rho u^2 + p$, and $a = 0$ (with p the pressure), we have the (scalar) momentum equation along an axis. The shock condition is then $[\![p + \frac{1}{2}\rho u^2]\!] = \dot{s}[\![\rho u]\!]$ at $x = s(t)$.
- $f = \rho$, $G[f] = \rho u$, and $a = 0$, we have the (scalar) mass equation along an axis. The shock condition is then $[\![\rho u]\!] = \dot{s}[\![\rho]\!]$ at $x = s(t)$. If we introduce the relative velocity $u' = u - \dot{s}$, we have also $[\![\rho u']\!] = 0$, which means that in the frame relative to the shock, the mass flux is conserved.

This equation can be generalized to higher dimensions without any problem.

When dealing with shocks, it is very important to use the original conservation equations (in an integral form) from which the local equation has been derived. Typically, when the field are continuous, the equations

$$\frac{\partial \rho u}{\partial t} + u\frac{\partial \rho u}{\partial x} = 0,$$

and

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0,$$

are equivalent because of the continuity equation. However, the former equation comes directly from the conservation of momentum (hence it is called the *conservative* form and ρu a conservative variable), whereas the latter is a simplification (called *non-conservative* form). It we reintegrate these equations to obtain the shock conditions, we will not find the same shock velocity. For this reason, care must be taken in computing shock conditions related to a hyperbolic partial differential equation.

1.3 Phenomenological constitutive equations

In many cases, most of the available information on the rheological behavior of a material is inferred from simple shear experiments. But, contrary to the Newtonian (linear) case, the tensorial form cannot be merely and easily generalized from the scalar expression fitted to experimental data. Earlier in this chapter, we have seen that:

- First, building a three-dimensional expression of the stress tensor involves respecting a certain number of formulation principles. These principles simply express the idea that the material properties of a fluid should be independent of the observer or frame of reference (principle of material objectivity) and the behavior of a material element depends only on the previous history of that element and not on the state of neighboring elements (Bird *et al.*, 1987).
- Then it is often necessary to provide extra information or rules to build a convenient expression for the constitutive equation.

We shall illustrate this with several examples.

1.3.1 Newtonian behavior

We start with an application of the representation theorem and the virtual power principle. We have an isotropic, incompressible, homogenous material assumed to be viscous. When it deforms, the energy dissipation rate Φ is fonction of the state of deformation, or more specifically of the strain rate $\mathbf{d}$, hence we write

$$\Phi = \Phi(\mathbf{d}),$$

but, making use of the representation, we can directly deduce the equivalent but more reduced form

$$\Phi = \Phi(d_I,\ d_{II},\ d_{III}),$$

where d_i represents the ith invariant of the strain-rate tensor. Since the material is isotropic, Φ does not depend on d_{III}; since it is incompressible, we have $d_I = 0$. Now we assume that we have a linear behavior, i.e., the energy rate dissipation must be a quadratic function of the invariants since dissipation = stress $\times$ strain rate $\propto$ strain rate^2. So we get

$$\Phi = \Phi(d_I,\ d_{II},\ d_{III}) = -\alpha d_{II},$$

with $\alpha > 0$ a constant and $d_{II} = -\frac{1}{2}\mathrm{tr}\mathbf{d}^2 = -\frac{1}{2}d_{kl}d_{kl}$ (Einstein's convention used). Using (1.8), we show that the extra-stress tensor is defined as

$$s_{ij} = \frac{\partial \Phi}{\partial d_{ij}} = \alpha \frac{1}{2}\frac{\partial d_{kl}d_{kl}}{\partial d_{ij}} = \alpha d_{kl}\delta_{ik}\delta jl = \alpha d_{ij},$$

from which we retrieve the Newtonian constitutive equation by posing $\alpha = 2\mu$.

1.3.2 Viscoplastic behavior

When a fluid exhibits viscoplastic properties, we usually fit experimental data with a Bingham equation as a first approximation (Bird *et al.*, 1983):

$$\dot{\gamma} > 0 \Rightarrow \tau = \tau_c + K\dot{\gamma} \tag{1.17}$$

Equation (1.17) means that

- for shear stresses in excess of a critical value, called the yield stress, the shear stress is a linear function of the shear rate;
- conversely when $\tau \leq \tau_c$ there is no shear within the fluid ($\dot{\gamma} = 0$).

The question arises as to how the scalar expression can be transformed into a tensorial form. The usual way (but not the only one) is to consider a process, called *plastic rule*, as the key process of yielding.

A plastic rule includes two ingredients.

- First, it postulates the existence of a surface in the stress space $(\sigma_1, \sigma_2, \sigma_3)$ delimiting two possible mechanical states of a material element (σ_i denotes a principal stress, that is an eigenvalue of the stress tensor), as depicted in Fig. 1.10. The surface is referred to as the *yield surface* and is usually represented by an equation in the form $f(\sigma_1, \sigma_2, \sigma_3) = 0$. When $f < 0$, behavior is generally assumed to be elastic or rigid. When $f = 0$, the material yields.
- Second it is assumed that, after yielding, the strain-rate is directly proportional to the surplus of stress, that is, the distance between the point the representing the stress state and the yield surface. Translated into mathematical terms, this leads to write: $\dot{\gamma} = \lambda \nabla f$ with λ a proportionality coefficient (Lagrangian multiplier).

How must the yield function f be built to satisfy the principle of material objectivity? For f to be independent of the frame, it must be expressed not as a function of the components of the stress tensor, but as a function of its invariants:

- the first invariant $I_1 = \operatorname{tr} \boldsymbol{\sigma} = \sigma_1 + \sigma_2 + \sigma_3$ represents the *mean stress* multiplied by 3 ($|\mathbf{OP}| = I_1/3$ in Fig. 1.11);
- the second invariant $I_2 = (\operatorname{tr}^2\boldsymbol{\sigma} - \operatorname{tr}\boldsymbol{\sigma}^2)/2 = -\operatorname{tr}(\mathbf{s}^2)/2$ can be interpreted as the deviation of a stress state from the mean stress state ($|\mathbf{PM}|^2 = -2I_2$ in Fig. 1.11) and is accordingly called the *stress deviator*;
- the third invariant $I_3 = -\operatorname{tr}\mathbf{s}^3/6$ reflects the angle in the deviatoric plane made by the direction **PM** with respect to the projection of -axis and is sometimes called the *phase* ($\cos^2 3\varphi = I_3^2/I_2^3$ in Fig. 1.11).

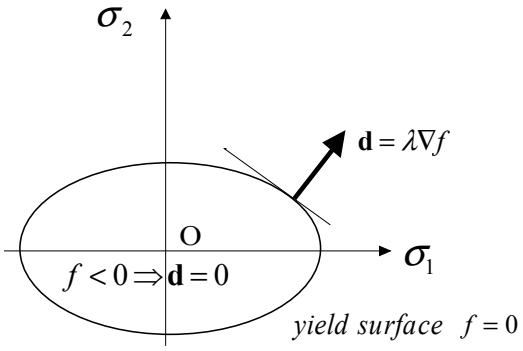

Figure 1.10: *Yield surface delimiting two domains.*

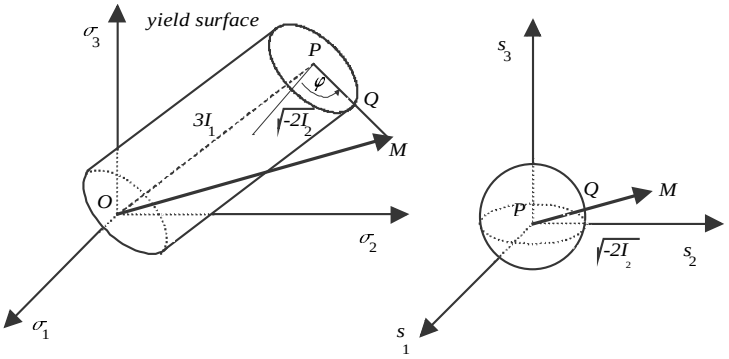

Figure 1.11: *On the left, the yield surface in the stress space when the von Mises criterion is selected as yield function. A stress state is characterized by its three principal stresses and thus can be reported in the stress space. The three invariants of the stress tensor can be interpreted in terms of coordinates.*

If the material is isotropic and homogenous, the yield function f is expected to be independent of the mean pressure and the third invariant. Thus we have $f(\sigma_1, \sigma_2, \sigma_3) = f(I_2)$. In plasticity, the simplest yield criterion is the *von Mises criterion*, asserting that yield occurs whenever the deviator exceeds a critical value (whose root gives the yield stress): $f(I_2) = \sqrt{-I_2} - \tau_c$. As depicted in Fig. 1.11, the yield surface is a cylinder of radius τ_c centered around an axis $\sigma_1 = \sigma_2 = \sigma_3$. If we draw the yield surface in the extra-stress space, we obtain a sphere of radius $\sqrt{2}\tau_c$.

Once the stress state is outside the cylinder defined by the yield surface, a flow occurs within the material. In a linear theory it is further assumed that the strain rate is proportional to the increment in stress (distance from the point representing the stress state M to the yield surface) and collinear to the normal $\partial f / \partial \mathbf{s}$. This

leads to the expression:

$$\mathbf{d} = \lambda \left(\sqrt{I_2} - \tau_c \right) \frac{\mathbf{s}}{\sqrt{I_2}} \tag{1.18}$$

For convenience, we define the proportionality coefficient as: $\lambda^{-1} = 2\eta$. It is generally more usual to express the constitutive equation in the converse form. First, the second invariant of the strain rate tensor J_2 can be expressed as $J_2 = -\mathrm{tr}(\mathbf{d}^2)/2 = \left(\lambda \left(\sqrt{-I_2} - \tau_c\right)\right)^2$. Then we deduce the usual form of the Bingham constitutive equation:

$$\mathbf{d} = 0 \Leftrightarrow \sqrt{-I_2} \leq \tau_c \tag{1.19}$$

$$\mathbf{d} \neq 0 \Leftrightarrow \boldsymbol{\sigma} = -p\mathbf{1} + \left(2\eta + \frac{\tau_c}{\sqrt{-J_2}} \right) \mathbf{d} \tag{1.20}$$

It is worth noting that contrary to the Newtonian case, the general tensorial expression (1.19) cannot not easily be extrapolated from the steady simple-shear equation (1.17).

1.3.3 Viscoelasticity

When studying the linear 1D Maxwell model in § **??**, we obtained an equation in the form

$$\frac{\mathrm{d}\gamma}{\mathrm{d}t} = \frac{1}{G}\frac{\mathrm{d}\tau}{\mathrm{d}t} + \frac{\tau}{\mu},$$

where G is the elastic modulus and μ denotes viscosity. We would like to transform this empirical equation into a 3D tensorial expression and naively we write

$$2\mu\mathbf{d} = \frac{\mu}{G}\frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}t} + \boldsymbol{\sigma},$$

but it is not difficult to see that this expression does not satisfy the objectivity principle. According to this principle, the stress tensor does not depend on the frame in which we use it (or its components) or, in other words, it must be invariant under any rotation. Let us consider the stress tensor when the frame of reference is rotated. We have

$$\boldsymbol{\sigma}' = \mathbf{R} \cdot \boldsymbol{\sigma} \cdot \mathbf{R}^\dagger$$

the image of $\boldsymbol{\sigma}$, where $\mathbf{R}$ is an orthogonal tensor. Taking the time derivative leads to

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\sigma}' = \frac{\mathrm{d}\mathbf{R}}{\mathrm{d}t} \cdot \boldsymbol{\sigma} \cdot \mathbf{R}^\dagger + \mathbf{R} \cdot \frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}t} \cdot \mathbf{R}^\dagger + \mathbf{R} \cdot \boldsymbol{\sigma} \cdot \frac{\mathrm{d}\mathbf{R}^\dagger}{\mathrm{d}t} \neq \mathbf{R} \cdot \frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}t} \cdot \mathbf{R}^\dagger,$$

which shows that $\dot{\boldsymbol{\sigma}}$ is not objective. To overcome this issue, we have to define a kind of time derivative that satisfies the objectivity principle. For this purpose, note that if we replace $\boldsymbol{\sigma}$ with $\mathbf{R}^\dagger \cdot \boldsymbol{\sigma}' \cdot \mathbf{R}$ and introduce $\boldsymbol{\Omega} = \dot{\mathbf{R}} \cdot \mathbf{R}^\dagger$, we have $\dot{\boldsymbol{\sigma}}' = \mathbf{R} \cdot \boldsymbol{\sigma} \cdot \mathbf{R} + \boldsymbol{\Omega} \cdot \boldsymbol{\sigma}' + \boldsymbol{\sigma}' \cdot \boldsymbol{\Omega}^\dagger$, which can be transformed by making use of the antisymmetry of $\boldsymbol{\Omega}$: $\dot{\boldsymbol{\sigma}}' = \mathbf{R} \cdot \dot{\boldsymbol{\sigma}} \cdot \mathbf{R}^\dagger + \boldsymbol{\Omega} \cdot \boldsymbol{\sigma}' - \boldsymbol{\sigma}' \cdot \boldsymbol{\Omega}$. If we want to transform this derivative into an objective derivative, we have to get rid of the last

two contributing terms. There are different possibilities. Oldroyd introduced the Oldroyd (or convective contravariant) derivative as follows:

$$\overset{\triangle}{\boldsymbol{\sigma}} = \dot{\boldsymbol{\sigma}} - \mathbf{L} \cdot \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot \mathbf{L}^{\dagger},$$

where $\mathbf{L}$ is the velocity gradient tensor. In this way, it is possible to

- provide a proper tensorial formulation of the constitutive equation;
- make an empirical law (primarily valid for small deformations) consistent with large deformations.

The stress tensor is then solution to

$$2\mu\mathbf{d} = \frac{\mu}{G} \overset{\triangle}{\mathbf{s}} + \mathbf{s}.$$

Note that in this particular case, we do not have necessarily tr$\mathbf{s}$, which is a typical example of a fluid for which the extra-stress tensor differs from the deviatoric the stress tensor.

Exercises

Exercice 1.1 Let $\mathbf{S}$ and $\mathbf{A}$ symmetric and antisymmetric tensors. Show that

$$\mathrm{tr}(\mathbf{S} \cdot \mathbf{A}) = 0.$$

Exercice 1.2 Give the definition of a streamline. Show that an equation in a Cartesian frame is

$$\frac{\mathrm{d}x}{u} = \frac{\mathrm{d}y}{v} = \frac{\mathrm{d}z}{w},$$

where $(u,\ v,\ w)$ are the components of the velocity field.

Exercice 1.3 We consider a velocity field of the following form:

$$\mathbf{u} = \mathbf{\Gamma} \cdot \mathbf{x},$$

with

$$\mathbf{\Gamma} = \frac{1}{2}\dot{\gamma} \begin{bmatrix} 1+\alpha & 1-\alpha & 0 \\ -1+\alpha & -1-\alpha & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

$\dot{\gamma}$ denotes the shear rate, and α is a constant satisfying $0 \leq \alpha \leq 1$. Characterize the velocity field depending on α. Hint: compute $\nabla\mathbf{u}$, $\mathbf{D}$ and $\mathbf{W}$. Is flow isochoric?

Exercice 1.4 Let us consider the following velocity field in the upper plane $y > 0$:

$$u = kx \text{ and } v = -ky,$$

with $k > 0$ and where $(u,\ v)$ are the velocity components. Flow is steady. The lower plane $y \leq 0$ is a solid body; the interface at $y = 0$ is then solid.

- compute the tensor "velocity gradient" associated with this velocity field;
- deduce the "rate of strain" tensor;
- compute the stress state for point A (0, 1) ;
- compute the streamlines;
- are the usual boundary conditions satisfied? Are these those of a Newtonian fluid?

Exercice 1.5 Let us consider a steady uniform flow down an infinite plane, which is inclined at θ to the horizontal. The fluid is incompressible with density ϱ. Show that independently of the constitutive equation, the shear stress τ is

$$\tau(y) = \varrho g(h - y),$$

where h is the flow depth, y is the coordinate normal to the plane, and g is gravity acceleration.

We now consider the flow of a Newtonian fluid with viscosity μ. Compute the velocity profile for a steady uniform flow. What are the principal directions of the stress and strain-rate tensors?

2 Equations of mechanics

In this chapter we will take a look at different families of differential equations that we can meet when studying mechanical processes. Bearing in mind the different types of equations and physical phenomena involved will be important later in this course to understand the strategies used for solving practical problems.

2.1 Equation classification

2.1.1 Scalar equation

An equation is said to be *scalar* if it involves only scalar quantities, without differential term. In mechanics, most problems are differential and meeting with purely scalar equations is seldom. A notable exception is the Bernoulli equation which states that the quantity

$$\psi = \varrho\frac{u^2}{2} + \varrho g z + p$$

is constant under some flow conditions, with u fluid velocity, ϱ fluid density, p its pressure, g gravity acceleration, and z elevation with respect to a reference level.

2.1.2 Ordinary differential equation

An *ordinary differential equation* (ODE) is a differential equation where the function is differentiated with respect to a single variable (the independent variable). The ordinary differential equations are quite common:

- either because the problem is basically a one-dimensional problem;
- or because with the help of transformations, we can reduce a problem of partial differential equations (PDEs) to an ordinary differential problem, which is much easier to solve analytically or numerically.

♣ **Example.** – The Pascal equation in fluid statics is an ordinary differential equation

$$\frac{\mathrm{d}p}{\mathrm{d}z} + \varrho g = 0,$$

where ϱ denotes fluid density, p its pressure, g gravity acceleration, and z elevation with respect to a reference level.

The order of an ordinary differential equation is defined as the order of the highest derivative. The order determines the number of initial conditions that are needed to solve the differential equation.

♣ **Example.** – A differential equation of order 2 such that $y'' + ay' + by = c$ requires to specify two boundary conditions. These can be given at a point (for example, we may pose $y(0) = 0$ and $y'(0) = 1$) or at different points (for example, we may ask $y(0) = 0$ and $y'(1) = 1$). In the first case, it is called *initial-value problem*, whereas in the latter case, we refer to is as a *boundary-value problem*[1]. □

An ordinary differential equation is called *linear* if it involves only linear combinations of derivatives of the function and the function itself. For example, $x^3y'' + y' = 0$ is linear (in y), but $y'y'' + x^3 = 0$ is not linear. An equation is called *quasi-linear* if it consists of a linear combination of derivatives, but not necessarily of the function. For example, $yy' + x^2y = 1$ is not linear but quasi-linear.

An ordinary differential equation quasi-linear first order can be cast in the form

$$\frac{\mathrm{d}u}{\mathrm{d}x} = \frac{f(u,\ x)}{g(u,\ x)},$$

with f and g two functions of u and x. This is form is particularly helpful since it allows to obtaining graphical representation of the solution (phase portrait) and analysis of singular points. This equation can also be put in the following differential form

$$g(u,\ x)\mathrm{d}u - f(u,\ x)\mathrm{d}x = 0.$$

The latter form is used to find exact differentials, i.e., functions ψ such that $\mathrm{d}\psi = g(u,\ x)\mathrm{d}u - f(u,\ x)\mathrm{d}x$. If we are successful, we can obtain an implicit solution to the differential equation in the form $\psi(u,\ x) = const$.

2.1.3 Partial differential equations

Most fundamental equations of mechanics such as the Navier-Stokes equations are partial differential equations, i.e. they describe how the process varies—depending

[1] We distinguish two types of conditions because from a numerical point of view, we have to use different techniques depending on the conditions. When conditions are given at different points, we must employ methods such as "shooting methods" to solve the equations numerically.

on time and location—by relating temporal and spatial derivatives. There is a wide variety of problems for PDEs we will uncover in what follows.

There are several ways to write a partial differential equation. For example, the diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

can be written with the short-hand notation $u_t = u_{xx}$ or $\partial_t u = \partial_{xx} u$.

Terminology

The *order* of a partial differential equation is the order of the higher differential term. For example, the equation $u_t = u_{xx}$ is order 2. The dependent variable is the function that we differentiate with respect to the independent variables; in the example above, u is the dependent variable, while x and t are the independent variables. The number of independent variables are the *dimension* of the partial differential equation. As for an ordinary differential equation, a partial differential equation is linear if it is linear in the dependent variable, the equation $u_t = u_{xx}$ is a linear equation because it depends linearly on u or its derivatives.

Classification of linear du second-order partial differential equations

The only general classification of partial differential equations concerns linear equations of second order. These equations are of the following form

$$au_{xx} + 2bu_{xy} + cu_{yy} + du_x + eu_y + fu = g, \tag{2.1}$$

where a, b, c, d, e, f, and g are real-valued functions x and y. When $g = 0$, the equation is said to be *homogeneous*. Linear equations are classified depending on the sign of $\Delta = b^2 - ac > 0$:

- if $\Delta = b^2 - ac > 0$, Equation (2.1) is *hyperbolic*. The wave equation (2.22) is an example. In fluid mechanics, transport equations are often hyperbolic. The *canonical* form is

  $$u_{xx} - u_{yy} + \cdots = 0 \text{ or, equivalently, } u_{xy} + \cdots = 0,$$

  where dots represent terms related to u or its first-order derivatives;

- if $\Delta = b^2 - ac < 0$, Equation (2.1) is *elliptic*. The Laplace equation (2.24) is an example. Equations describing equilibrium of a process are often elliptic. The canonical form is

  $$u_{xx} + u_{yy} + \cdots = 0$$

- if $\Delta = b^2 - ac = 0$, Equation (2.1) is *parabolic*. The heat equation (2.7) is an example. Diffusion equations are often parabolic. The canonical form is

$$u_{yy} + \cdots = 0.$$

There is a strong link between the name given to differential equations and the name of conics. Indeed, if we assume that the coefficients of equation (2.1) are constant and we substitute into Equation(2.1) u_{xx} with x^2, u_x with x, u_{yy} with y^2, u_y with y, and u_{xy} with xy, we obtain the general equation of a conic, which depending on the sign $\Delta = b^2 - ac$ gives a parabola ($\Delta = 0$), an ellipse ($\Delta < 0$), or a hyperbola ($\Delta > 0$), as shown in Figure 2.1. This figure shows that the differential terms are linked and vary according to the constraints intrinsic to each type of curve. We note for example that for hyperbolic equations, there are two branches and part of the $x - y$ plane is not crossed by the curve, which allows discontinuous jumps from one branch to another; such jumps exist in differential equations and are called *shocks*: a hyperbolic equation is able to generate solutions that become discontinuous, i.e. undergo a shock even if initially they were continuous.

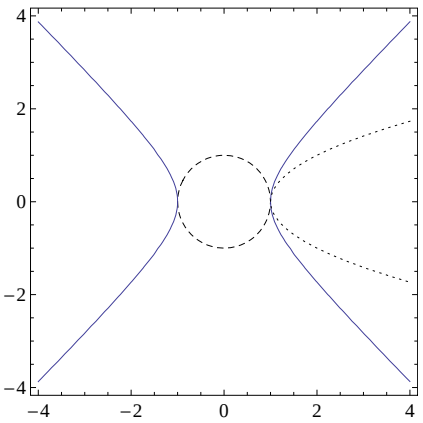

Figure 2.1: *conics of equation $ax^2 + cy^2 + dx = 1$. The solid-line curve is the hyperbola $x^2 - y^2 = 1$ ($a = 1$, $c = -1$, and $d = 0$). The dashed-line curve is the ellipse (circle here) $x^2 + y^2 = 1$ ($a = 1$, $c = 1$, and $d = 0$). The dotted-line curve is the parabole $x - y^2 = 1$ ($a = 0$, $c = -1$, and $d = 1$).*

Characteristic form of first-order equations

Quasi-linear first-order partial differential equations equations are linear in the differential terms and can cast put in the form:

$$P(x,\ y,\ u)\partial_x u + Q(x,\ y,\ u)\partial_y u = R(x,\ y,\ u). \tag{2.2}$$

The implicit solution can be written as $\psi(x,\ y,\ u(x,\ y)) = c$ (with c a constant). ψ is a first integral of the vector field $(P,\ Q,\ R)$. We have:

$$\partial_x \psi(x,\ y,\ u(x,\ y)) = 0 = \psi_x + \psi_u u_x,$$
$$\partial_y \psi(x,\ y,\ u(x,\ y)) = 0 = \psi_y + \psi_u u_y.$$

We can also write: $u_x = -\psi_x/\psi_u$ et $u_y = -\psi_y/\psi_u$. We can get a more symmetric relation:

$$P\psi_x + Q\psi_y + R\psi_u = 0,$$

which can be cast into a vector form, which is easier to interpret:

$$(P,\ Q,\ R) \cdot \nabla\psi = 0. \tag{2.3}$$

This means that at point M, the normal vector to the integral curve should be normal to the vector field $(P,\ Q,\ R)$. If the point O: $(x,\ y,\ u)$ and the neighboring point O': $(x + \mathrm{d}x,\ y + \mathrm{d}y,\ u + \mathrm{d}u)$ belong to the integral curve, then the vector $\mathbf{OO'}$: $(\mathrm{d}x,\ \mathrm{d}y,\ \mathrm{d}u)$ must be normal to $(P,\ Q,\ R)$: $\psi_x dx + \psi_y dy + \psi_u du = 0$. Since this must be true for any increment $\mathrm{d}x$, $\mathrm{d}y$, and $\mathrm{d}u$, we obtain the *characteristic equations*

$$\boxed{\frac{\mathrm{d}x}{P(x,\ y,\ u)} = \frac{\mathrm{d}y}{Q(x,\ y,\ u)} = \frac{\mathrm{d}u}{R(x,\ y,\ u)}} \tag{2.4}$$

Each pair of equations defines a curve in the space $(x,\ y,\ u)$. These curves define a two-parameter family (there are 3 equations, so 3 invariants but only 2 are independent): for example, if p is a *first integral* of the first pair of equations, an integral surface of the first pair is given by an equation of the form $p(x,\ y,\ u) = a$, with a a constant. Similarly for the second pair: $q(x,\ y,\ u) = b$. The functional relation $F(a,\ b) = 0$ defines the integral curve.

Note that all solutions do not necessarily take the form $F(a,\ b) = 0$. This case is encountered, in particular, with *singular* solutions of differential equations.

Using characteristic equations can often help solve quasi-linear first order equations.

♣ **Example.** – We would like to find a solution to:

$$x\frac{\partial u}{\partial x} - y\frac{\partial u}{\partial y} = u^2.$$

Identifying P, Q, and R, we find: $P = x$, $Q = -y$, et $R = u^2$. The characteristic equation is

$$\frac{\mathrm{d}x}{x} = -\frac{\mathrm{d}y}{y} = \frac{\mathrm{d}u}{u^2}.$$

A first integral of the first pair is

$$\frac{\mathrm{d}x}{x} = -\frac{\mathrm{d}y}{y} \Rightarrow \ln x = -\ln y + \ln a,$$

with a a constant of integration. We then have $a = xy$. A first integral of the second pair is

$$-\frac{\mathrm{d}y}{y} = \frac{\mathrm{d}u}{u^2} \Rightarrow \ln y = \frac{1}{u} + b,$$

with b another constante of integration. We then get $b = \ln y - 1/u$. General solutions are of the form

$$F(a,\, b) = 0 \Rightarrow F\left(xy, \ln y - \frac{1}{u}\right) = 0.$$

This is the implicit solution to the equation. An explicit form is obtained by assuming that there is a function G such that $\ln y - 1/u = G(xy)$, that is,

$$u = \frac{1}{\ln y - G(xy)}.$$

Function G must be determined from the boundary conditions. □

Boundary conditions

In mechanics, we solve equations with space and time variables. In general, in order to work out a particular solution u to a partial differential equation, we need

- boundary conditions that specify how u varies along the domain boundaries at any time;
- the initial conditions that specify how varies u at the initial instant for any point in the domain.

We must solve what is called a boundary-value problem with initial conditions or, said differently, *initial boundary-value problem*. In some cases, we do not need as much information. For example, for certain hyperbolic equations, one needs only the initial conditions while the elliptic problems require only boundary conditions (they generally reflect stationary processes).

We distinguish:

- *Dirichlet boundary conditions*: the boundary condition specifies the value u_0 that the function takes at a point or a curve

  $$u(\mathbf{x}\ ;\ t) = u_0(t)$$

  along a curve Γ.
- *Neuman boundary conditions*: the boundary conditions specify the derivative that the function takes at a point or a series of points. Physically, this reflects a flux condition through the domain boundary:

  $$\frac{\partial u}{\partial \mathbf{n}}(\mathbf{n}\ ;\ t) = \boldsymbol{\phi}(t)$$

  along a curve Γ, with $\mathbf{n}$ the normale to Γ and $\boldsymbol{\phi}(t)$ a flux function.

2.1.4 Variational equation

There is a mechanical principle known as the *variational principle* stating that if a process $J[u]$ (with J a functional and u a function) is steady and stable, then it should remain insensitive to small variations of u. This is written $\Delta J = 0$. A functional is a generalized function that involves both u and its derivatives (or integrals). For one-dimensional problems, a generic form of J is for example the form

$$J[u] = \int L(t,\ u,\ \dot{u}, \cdots)\mathrm{d}t, \tag{2.5}$$

with L a function of $u(t)$, t, and its derivatives.

For example, the Hamilton principle states that a particle moves so that the action integral which represents the difference between kinetic and potential energies is minimized

$$J = \int_{t_1}^{t_2} (\text{kinetic energy} - \text{potential energy})\mathrm{d}t.$$

A variational problem of the form $\delta J = 0$ with J given by equation (2.5) can be reduced to a purely differential equation. One can indeed show that $u(t)$ is solution to the following differential equation called the *Euler-Lagrange equation*

$$\frac{\partial L}{\partial u} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{u}}\right) + \frac{\mathrm{d}^2}{\mathrm{d}t^2}\left(\frac{\partial L}{\partial \ddot{u}}\right) + \cdots = 0.$$

♣ **Example.** – For instance, if y denotes the position of a point mass m linked to a spring of strength k, then $y(t)$ is determined by solving $\delta J = 0$, with

$$J = \frac{1}{2}\int_{t_1}^{t_2} (m\dot{y}^2 - ky^2)\mathrm{d}t.$$

After identifying the terms, we find $L(y,\ \dot{y}) = (m\dot{y}^2 - ky^2)/2$. We then deduce $L_y = -ky$ and $L_{\dot{y}} = m\dot{y}$. The resulting Euler-Lagrange equation is

$$-ky - \frac{\mathrm{d}}{\mathrm{d}t}m\dot{y} = 0 \Rightarrow \ddot{y} = -\frac{k}{m}y,$$

which is nothing but the Newton equation for an oscillatory mass. □

2.2 Equations in mechanics

We are going to see the main types of partial differential equations encountered in mechanics.

2.2.1 Convection equation

Convection is a mode of transfer of an element or a quantity that is advected by the fluid. For example, if a pollutant is released into a river, it is transported at the same speed as water. This is what we call *convection* or *advection* (convection is most often employed to describe thermal heat transfer).

The simplest convection equation is the following one

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = 0, \tag{2.6}$$

where $f(x, t)$ is a quantity advected by a stream at constant velocity u. This is a first-order linear partial differential equation. The characteristic equation associated to the partial differential equation (2.6) is

$$\frac{\mathrm{d}x}{\mathrm{d}t} = u \text{ or equivqlently } \frac{\mathrm{d}x}{u} = \frac{\mathrm{d}t}{1} = \frac{\mathrm{d}f}{0}.$$

As u is assumed to be constant, this means that the solution of the characteristic equation is $x - ut = const$ any function $F(x - ut)$ whose argument is $x - ut$ is a solution of equation (2.6). A feature of this solution is that the original form $F(x)$ (at $t = 0$) is conserved in the course of movement: it is simply translated by ut as shown in Fig. 2.2.

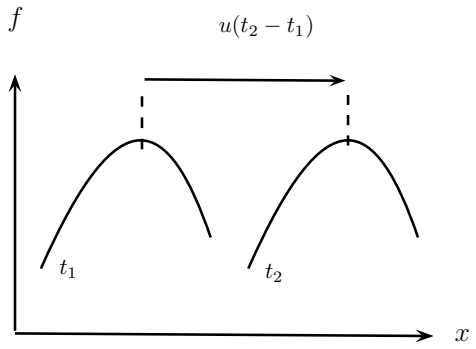

Figure 2.2: *advection of f.*

2.2.2 Diffusion equation (heat equation)

Diffusion is matter transport under the effect of thermal agitation (Brownian motion) or turbulence. In a stream, in addition to mean motion, there are also velocity fluctuations which disperse matter within the fluid volume.

One example is the classic diffusion equation of heat diffusion. The temperature $T(x,\ y\ ,\ t)$ varies over time within a material (dimension 2) according to the equation

$$\frac{\partial T}{\partial t} = \alpha \Delta T = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right), \tag{2.7}$$

with $\alpha = k/(\varrho C)$ thermal diffusivity, ϱ density, k thermal conductivity, C specific heat.

A similar process occurs with matter. The one-dimensional diffusion equation is

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2}, \tag{2.8}$$

with D diffusion coefficient and where $f(x,\, t)$ is a function such as the pollutant concentration in a river. This is a second-order linear partial differential equation.

We talked so far about linear equations. In many problems of practical interest, the diffusion coefficient is not constant but depends on the function f. The diffusion equation is then nonlinear. For example, when a $D(f) = \kappa f^k$, the diffusion equation is

$$\frac{\partial f}{\partial t} = \kappa \frac{\partial}{\partial x} \left(f^k \frac{\partial f}{\partial x} \right), \tag{2.9}$$

with κ a constant and k an integer. For gas diffusion in a porous medium and groundwater flow, we have $k = 1$ (f represents the concentration); for the spreading of Newtonian fluid on a horizontal substrate, we have $k = 3$ (f is the height of fluid); for heat diffusion during the early stages of a nuclear explosion, we have $k = 5$.

Self-similar solution to the Green problem

For some initial conditions, Equation (2.8) admits analytical solutions in the form of self-similar solution $t^m F(\xi)$ with $\xi = x/t^n$. When we substitute f by this form into (2.8), we find that $n = \frac{1}{2}$. We note that m is not determined by the differential equation, but it is given the boundary conditions. Generally, in physical problems, we impose that the quantity of material released is constant

$$\int_{-\infty}^{\infty} f(x) \mathrm{d}x = V,$$

with V total volume (assumed to be constant with time). The change of variable gives $\int f(x) \mathrm{d}x = \int t^{m+1/2} F(\xi) \mathrm{d}\xi = V$. We then pose $m = -\frac{1}{2}$ since V does not depend on t.

The advantage of this change of variable is that it transforms the partial differential equation into a second-order ordinary linear differential equation, which is much easier to solve. Let us take a closer look at this transformation by considering a practical case: in a lake (water at rest), we release a volume V of pollutant, originally contained at point $x = 0$; the initial condition is therefore $f(x, 0) = \delta(x)$ where δ is the Dirac function ($\delta(x) = 1$ if $x = 0$ and $\delta(x) = 0$ if $x \neq 0$). This problem where the initial condition is an impulse, i.e. a quantity localized at a point, is called *Green's problem*. Substituting the form $f = t^{-1/2}F(\xi)$ into Eq. (2.8), we obtain an ordinary differential equation for F and by doing so, we transform a partial differential problem in an ordinary differential equation:

$$F + \xi F'(\xi) + 2DF''(\xi) = 0,$$

which gives after integration

$$\xi F + 2DF' = a,$$

with a a constant of integration. Since the solution should be symmetric about $x = 0$ (thus $\xi = 0$), we have $F' = 0$ at $x = 0$ (F has a horizontal tangent at this point), hence $a = 0$. A new integration yields

$$F(\xi) = be^{-\frac{\xi^2}{4D}} \Rightarrow f(x, t) = \frac{b}{\sqrt{t}} e^{-\frac{x^2}{4Dt}},$$

with b another constant of integration. since $\int_{-\infty}^{\infty} e^{-\frac{x^2}{4D}} \mathrm{d}x = 2\sqrt{D\pi}$, we deduce $b = V/2\sqrt{D\pi}$. The solution reads

$$f(x, t) = \frac{V}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}. \tag{2.10}$$

As shown in Fig. 2.3, the shape of the diffusion front does not change with time (it is bell-shaped), although the front spreads. Note that the resulting solution is of great interest because it is the particular solution of the Green problem. For example, assume that the initial condition is more complex $f(x, 0) = g(x)$. Since the differential equation is linear, the sum of two solutions is also a solution. The general solution is then

$$f(x, t) = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} g(\zeta) e^{-\frac{(x-\zeta)^2}{4Dt}} \mathrm{d}\zeta.$$

This means that the concentration f at any time t and for any x is the sum of elementary contributions induced by the distribution of source intensity $g(\zeta)$ per unit length.

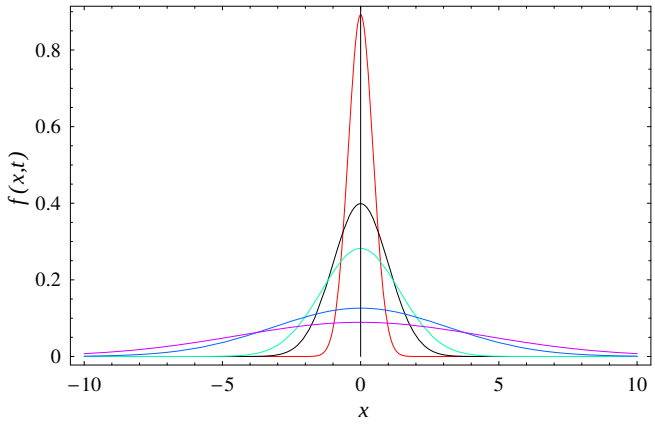

Figure 2.3: *diffusion of f. Calculation done with $D = 1$ m^2/s and at times $t = 0.1$, $t = 0.5$, $t = 1$, $t = 5$, and $t = 10$ s.*

Laplace transform

We wish to solve the diffusion equation:

$$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2}, \tag{2.11}$$

with D the diffusion coefficient (which is constant), subject to the following initial and boundary conditions

$$f(x,\ 0) = 0, \tag{2.12}$$
$$f(0,\ t) = a \text{ for } t > 0, \tag{2.13}$$
$$f(x,\ t) = 0 \text{ for } x \to \infty \text{ and } t > 0, \tag{2.14}$$

with a a constant. We transform it using the Laplace transform in t

$$\hat{f}(x,\ s) = \int_0^\infty e^{-st} f(x,\ t)\mathrm{d}t.$$

To transform (2.11), we just have to multiply it by e^{-st}, then integrate it from 0 to ∞ with respect to t. We get

$$\int_0^\infty De^{-st}\frac{\partial^2 f}{\partial x^2}\mathrm{d}t = D\frac{\partial^2}{\partial x^2}\int_0^\infty e^{-st} f\mathrm{d}t, \tag{2.15}$$
$$\int_0^\infty e^{-st}\frac{\partial f}{\partial t}\mathrm{d}t = \left[fe^{-st}\right]_0^\infty + \int_0^\infty se^{-st} f\mathrm{d}t, \tag{2.16}$$

where the term between brackets vanishes (given the initial condition). The Laplace transform of the linear diffusion equation (2.11) is

$$s\hat{f} = D\frac{\partial^2 \hat{f}}{\partial x^2}, \tag{2.17}$$

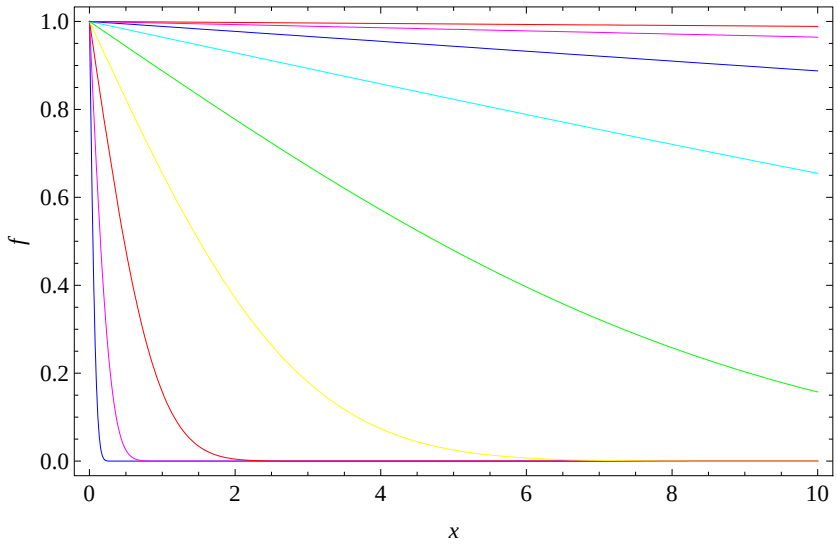

Figure 2.4: *variation in f for $t = 10^{-2}$, 10^{-2}, 1, $10^{+1}\ldots$, 10^{+6}. Calculation done for $a = 1$ and $D = 1$ m^2/s.*

which, despite the partial derivatives, behaves like an ordinary differential equation in x. The Laplace transform of the boundary conditions (2.13) and (2.14) yields

$$\hat{f}(0,\ s) = \int_0^\infty a e^{-st} = \frac{a}{s}, \tag{2.18}$$

$$\hat{f}(x,\ s) = 0 \text{ when } x \to \infty. \tag{2.19}$$

The solution to (2.17) is then

$$\hat{f}(x,\ s) = \frac{a}{s} \exp\left(-x\sqrt{\frac{s}{D}}\right),$$

whose inverse Laplace transform is

$$f(x,\ t) = a\left(1 - \text{Erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right),$$

with Erf the error function. Figure 2.4 shows f profiles at different times. At long time, we get

$$\lim_{t\to\infty} f(x,\ t) = a,$$

whose profile tends to a uniform profile $f = a$.

2.2.3 Convection-diffusion equation

Convection-diffusion is a combination of two phenomena. This is the phenomenon commonly encountered in hydraulics. For example, the discharge of a pollutant

into a river leads to a transport of this pollutant by diffusion (due to turbulence) and convection (advection speed of the water). The characteristic equation is

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}, \tag{2.20}$$

where D and u are assumed constant. This equation can be reduced to a linear diffusion problem by making the following change of variable (which amounts to changing the reference frame and placing us in the frame attached to the stream)

$$\begin{aligned}\zeta &= x - ut,\\ \tau &= t.\end{aligned}$$

We get

$$\begin{aligned}\frac{\partial \cdot}{\partial x} &= \frac{\partial \cdot}{\partial \zeta}\frac{\partial \zeta}{\partial x} + \frac{\partial \cdot}{\partial \tau}\frac{\partial \tau}{\partial x},\\ &= \frac{\partial \cdot}{\partial \zeta},\\ \frac{\partial \cdot}{\partial t} &= \frac{\partial \cdot}{\partial \zeta}\frac{\partial \zeta}{\partial t} + \frac{\partial \cdot}{\partial \tau}\frac{\partial \tau}{\partial t},\\ &= -u\frac{\partial \cdot}{\partial \zeta} + \frac{\partial \cdot}{\partial \tau}.\end{aligned}$$

Equation (2.20) becomes

$$\frac{\partial f}{\partial \tau} = D\frac{\partial^2 f}{\partial \zeta^2},$$

which is similar to the linear diffusion equation (2.8) seen above.

A special case of convection-diffusion is met with the Burgers equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = D\frac{\partial^2 u}{\partial x^2}, \tag{2.21}$$

which can also be transformed into a diffusion equation using the Cole-Hopf transformation:

$$u = -\frac{2D}{\phi}\frac{\partial \phi}{\partial x},$$

with $\phi(x,\, t)$ an auxiliary function. Indeed we have

$$\begin{aligned}\frac{\partial u}{\partial x} &= -\frac{2D}{\phi}\frac{\partial^2 \phi}{\partial x^2} + \frac{2D}{\phi^2}\left(\frac{\partial \phi}{\partial x}\right)^2,\\ \frac{\partial u}{\partial t} &= -\frac{2D}{\phi}\frac{\partial^2 \phi}{\partial x \partial t} + \frac{2D}{\phi^2}\frac{\partial \phi}{\partial x}\frac{\partial \phi}{\partial t},\\ \frac{\partial^2 u}{\partial x^2} &= -\frac{2D}{\phi}\frac{\partial^3 \phi}{\partial x^3} - \frac{4D}{\phi^3}\left(\frac{\partial \phi}{\partial x}\right)^3 + \frac{6D}{\phi^2}\frac{\partial^2 \phi}{\partial x^2}\frac{\partial \phi}{\partial x}.\end{aligned}$$

After simplification, we obtain

$$\frac{\partial\phi}{\partial t}\frac{\partial\phi}{\partial x} - \phi\frac{\partial^2\phi}{\partial x\partial t} + 2D\left(\phi\frac{\partial^3\phi}{\partial x^3} - \frac{\partial\phi}{\partial x}\frac{\partial^2\phi}{\partial x^2}\right) = 0,$$

which can be transformed—by dividing it by ϕ^2, then integrating with respect to x, and ultimately by multiplying it again by ϕ—into a linear diffusion equation

$$\frac{\partial\phi}{\partial t} = D\frac{\partial^2\phi}{\partial x^2}.$$

2.2.4 Wave

Dynamic waves are solutions to a differential equation such as the following (second-order) partial differential equation:

$$\frac{\partial^2\phi}{\partial t^2} = c^2\frac{\partial^2\phi}{\partial x^2}, \tag{2.22}$$

with c the (phase) velocity. This form is not exhaustive; for example, the equation of gravity waves reads

$$\frac{\partial^2\phi}{\partial t^2} = -g\frac{\partial\phi}{\partial y},$$

with here ϕ the velocity potentiel ($\mathbf{u}(x,\, y,\, t) = \nabla\phi$) and g gravity acceleration.

Often solutions are sought in the form of harmonics (periodic wave)

$$\phi(t) = A\exp[\imath(kx - \omega t)] = \mathrm{Re}(A)\cos(kx - \omega t) - \mathrm{Im}(A)\sin(kx - \omega t),$$

where A is the *amplitude*, k *wave number* ($\lambda = 2\pi/k$ *wavelength*), ω *angular frequency*; we also introduce a frequency f defined as $f = \omega/(2\pi)$: the number of complete oscillations during a second at a given position. The period is defined as $T = \lambda/c$.

The *wave velocity* is $c = \omega/k$. This means that for an interval δt, the wave has moved a distance $c\delta t$. The dispersion relation $\omega(k)$ is here linear because we have: $\omega(k) = ck$, i.e. the wave crests move at a constant speed, which is independent of the wavelength. In most systems, the relation is not linear, which in practice means that the crest velocity depends on the wavelength. We then introduce the phase velocity c_p

$$c_p = \frac{\omega(k)}{k}.$$

In a physical process where waves result from the superposition of many harmonic waves of different wavelength, each harmonic component moves at its own speed, which ultimately leads to a separation or *dispersion* of the wave, hence

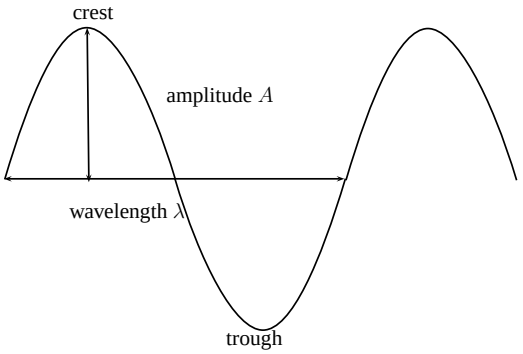

Figure 2.5: *wave length and amplitude of harmonic wave.*

the name *dispersion relation* for $\omega(k)$. There is a third velocity, called *group velocity*, which represents the speed at which the energy associated with the wave propagates:

$$c_g = \frac{\mathrm{d}\omega}{\mathrm{d}k}. \tag{2.23}$$

In general for most physical processes, we have $c_g \leq c_p$.

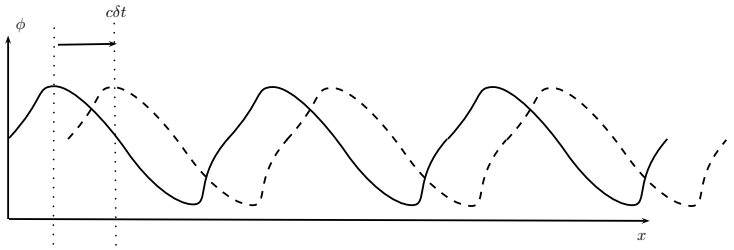

Figure 2.6: *rightward shift of a forward wave a speed c .*

The differential equation (2.22) is linear, which implies that any combination of solutions is also solution (superposition principle). There are two directions of propagation:

- forward wave $f = f(x - ct)$: the wave goes in the $x > 0$ direction;
- backward wave $f = f(x + ct)$: the wave goes in the $x < 0$ direction.

Equation (2.22) can also be cast in the form of products

$$\frac{\partial^2 f}{\partial t^2} - c^2 \frac{\partial^2 f}{\partial x^2} = \left(\frac{\partial}{\partial t} - c\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right) f = 0,$$

which makes it possible to transform a second-order partial differential equation into a system of first-order equations:

$$\begin{cases} f_t - cf_x = v, \\ v_t + cv_x = 0. \end{cases}$$

The general solution to the wave equation (2.22) reads

$$f = a(x - ct) + b(x + ct),$$

with a and b two functions. This is the *d'Alembert* solution.

Note that in many cases of practical interest, the equations are linear, the linearity allows to apply the principle of superposition. A stationary wave results from the superimposition of a backward wave and a forward wave of same amplitude. In this case, time dependence is removed.

2.2.5 Laplace equation

Elliptic equations generally reflect how a process at equilibrium is spatially organized. The prototype of the elliptic equation is the *Laplace* equation:

$$u_{xx} + u_{yy} = 0. \tag{2.24}$$

For example, the heat equation (2.7) in steady state ($\partial_t T = 0$) becomes elliptical. The Laplace equation is used to describe a large number of steady flows in environmental problems. For instance, the slow flow of water in a porous medium is also a Laplace equation. Indeed, if the velocity $\mathbf{u}$ follows Darcy's law, then it is connected to the pressure gradient p by: $\mathbf{u} = -k\nabla p/\mu$ with μ the viscosity and k the permeability of the medium. We can recast this equation as follows $\mathbf{u} = -\nabla\psi$ with $\psi = -kp/\mu$. We say that $\mathbf{u}$ is derived from the potential ψ. The continuity equation (incompressible fluid) requires that $\operatorname{div}\mathbf{u} = 0$, hence

$$\nabla \cdot \nabla\psi = 0 \Rightarrow \Delta\psi = 0.$$

Exercises

Exercice 2.1 Calculate the phase velocity and group velocity of the following equation:

$$u_t + u_x + u_{xxx} = 0.$$

$\rightsquigarrow$ *Answer.*

We seek harmonic solutions of the form:

$$u(x,\ t) = A\mathrm{e}^{\imath(kx-\omega t)}.$$

The dispersion relation is:

$$\omega = k - k^3.$$

We deduce that the phase velocity is

$$c = \frac{\omega}{k} = 1 - k^2,$$

i.e. a function of k. This is thus a dispersive wave. The group velocity

$$c_g = \frac{\mathrm{d}\omega}{\mathrm{d}k} = 1 - 3k^2,$$

which is lower than the phase velocity, as expected. □

Exercice 2.2 Consider the following initial-value problem

$$t\frac{\partial u}{\partial x} - x\frac{\partial u}{\partial t} = 0,$$

with $u(x,\ 0) = f(x)$ for $x > 0$. What type is this equation? Solve it after determining the associate characteristic equation.

Exercice 2.3 A function $u(x,\ t)$ decreases like

$$\frac{\mathrm{d}u}{\mathrm{d}t} = -k,$$

along a curve $x = x_s(t)$ in the $x-t$ plane. Which partial differential equation does u satisfy? Conversely, show that any partial differential equation of the form

$$\frac{\partial u}{\partial t} + a(u,\ x,\ t)\frac{\partial u}{\partial x} = b(u,\ x,\ t),$$

can be transformed into a first-order ordinary differential equation

$$\frac{\mathrm{d}u}{\mathrm{d}t} = g$$

along a curve whose equation has to be specified.

Exercice 2.4 The Euler-Darboux equation reads

$$u_{xy} + \frac{au_x - bu_y}{x - y} = 0.$$

Characterize this equation.

Exercice 2.5 The Helmholtz equation reads

$$\nabla^2 u + k^2 u = 0.$$

Characterize this equation.

Exercice 2.6 The Klein-Gordon equation is a variant of the Schrödinger equation, which described how an elementary particle behaves. It reads

$$\frac{\partial^2 u}{\partial t^2} - \gamma^2 \frac{\partial^2 u}{\partial x^2} + c^2 u = 0.$$

Characterize this equation. Seek periodic solutions in the form $u(x,\ t) = a(k)\exp(\imath kx + \lambda(k)t)$ with a the amplitude of the wave and where λ and k are the modes. Determine the mode λ? Is the solution stable?

Exercice 2.7 Consider the equation:

$$\dot{y} = -\frac{y(y^2 - x)}{x^2},$$

with initial condition $y(1) = 0$. Answer the following equations:

- which type is this equation?
- solve it numerically;
- put the equation in the form $A\mathrm{d}x + B\mathrm{d}y = 0$. Is it an exact differential?
- multiply the equation above $2/(2xy^3 - x^2 y)$. Is it an exact differential?

- integrate the equation and compare with the numerical solution.

Exercice 2.8 Find the function $y(x)$ that minimize the functional

$$J[y] = \int_0^1 (y^2 + y'^2)\mathrm{d}x,$$

given that $y(0) = 0$ and $y(1) = 1$.

3 Analytical tools

3.1 Overview

Several methods are available for solving differential equations. If there is no universal solving technique that can solve any type of equation, there are a number of methods that work in most cases of practical interest. Exact methods include:

- *variable separation*: this technique can transform a partial differential equation into a set of differential equations;
- *integral transformation*: Fourier or Laplace transform can be used to transform a PDE into a linear ordinary differential equation when the domain of integration is infinite (or semi-infinite). An example is given with the diffusion equation in § 2.2.2;
- *Green method*: for linear equations with boundary conditions that are also linear, it is possible to exploit the linearity by first seeking to solve a Green problem, that is, the same differential equation but with boundary conditions involving impulse (Dirac) functions. The final solution is obtained by summing the response to each elementary impulse. An example is given with the diffusion equation in § 2.2.2;
- *invariance group*: the idea is to exploit geometric transformations (forming what is called a group in mathematics) which leave an equation invariant. Among the most frequent, the translation invariance and stretching group can find self-similar solutions. These methods simplify the problem by transforming the partial differential equation into an ordinary differential equation;
- *hodograph method*: some equations are simpler to solve when the role of dependent and independent variables is swapped;

- *eigenfunction expansion*: the solution to a linear differential equation (with linear boundary conditions) is sought in the form of an infinite series of eigenfunctions.

For some equations, there are specific methods that we do not describe here. For example, conformal transformations offer an application of the theory of complex-valued functions to solve the Laplace equation.

Approximate methods include:

- *perturbation techniques*: we transform a nonlinear problem into a (hierarchical) set of linear equations that can approximate the nonlinear equation;
- *asymptotic methods*: we simplify the equations by removing terms whose order of magnitude is small compared to other terms;
- *numerical methods*: equations are discretized and solved by iterative methods using a computer. Other numerical methods: Galerkin methods seek numerical solutions by decomposing the form of known functions (spline, polynomial, wavelet, etc.).

3.1.1 Perturbation techniques

It is quite common in mechanics to obtain rather complex differential equations, whose some terms are weighted by coefficients that take values relatively low compared to other contributions. The idea is then

- to approximate the solution by a series of functions, whose order of magnitude decreases;
- to substitute this expression into the original equation;
- to group terms of same order to form a hierarchy of equations;
- to solve the equations iteratively.

♣ **Example.** – Let us take an example with this second-order differential equation

$$y'' + \epsilon y' + y = 0, \tag{3.1}$$

with the initial conditions $y(0) = 1$ and $y'(0) = 0$; ϵ is much smaller than unity (e.g., $\epsilon = 0.1$). We consider the following expansion in ϵ

$$y(x) = y_0(x) + \epsilon y_1(x) + \epsilon^2 y_2 + \ldots \epsilon^n y_n + \ldots,$$

with y_k a function of x such that $O(y_k) = 1$ over the interval $[0,\ 1]$. This expression is substituted into equation (3.1), which gives

$$\begin{aligned}(y_0(x) + \epsilon y_1(x) + \epsilon^2 y_2 + \ldots \epsilon^n y_n + \ldots)''+\\ \epsilon(y_0(x) + \epsilon y_1(x) + \epsilon^2 y_2 + \ldots \epsilon^n y_n + \ldots)'+\\ (y_0(x) + \epsilon y_1(x) + \epsilon^2 y_2 + \ldots \epsilon^n y_n + \ldots) = 0\end{aligned}$$

The boundary conditions yield

$$\begin{aligned}y_0(0) + \epsilon y_1(0) + \epsilon^2 y_2(0) + \ldots \epsilon^n y_n(0) + \ldots = 1,\\ y_0'(0) + \epsilon y_1'(0) + \epsilon^2 y_2'(0) + \ldots \epsilon^n y_n'(0) + \ldots = 0.\end{aligned}$$

To order ϵ^0, we obtain

$$y_0'' + y_0 = 0,$$

with boundary conditions $y_0(0) = 1$ and $y_0'(0) = 0$. Integrating this equation gives: $y_0(x) = \cos x$. To ϵ^1, we get

$$y_1'' + y_1 = -y_0',$$

with boundary conditions $y_1(0) = 0$ and $y_1'(0) = 0$ and whose integration gives: $y_1(x) = \frac{1}{2}(\sin x - x\cos x)$. This computation can be iterated indefinitely. The solution to order $O(\epsilon^2)$ is

$$y = \cos x + \frac{1}{2}\epsilon(\sin x - x\cos x) + O(\epsilon^2).$$

Figure 3.1 shows good agreement between exact and approximate solutions. □

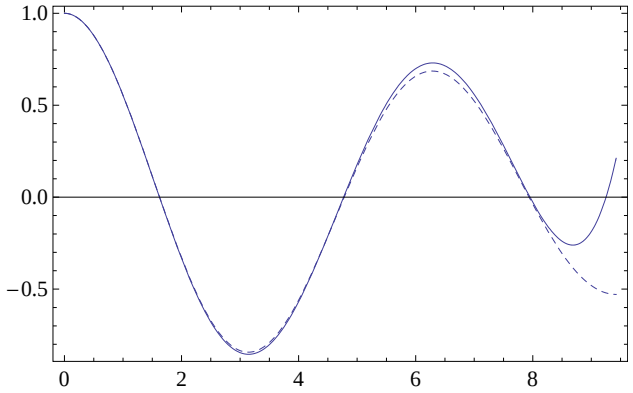

Figure 3.1: *comparison between the exact solution (solid line) and approximate solution to order 2 (dashed line) of equation (3.1) with* $\epsilon = 0.1$.

3.1.2 Asymptotic methods

In equations where several contributions come up, it is rare that all terms have the same importance. In seeking what are the dominant terms, we may obtain an asymptotic solution towards which the true solution tends. In general, we seek a balance between two, exceptionally three terms.

♣ **Example.** – Let us consider the differential equation

$$y'' + xy' + y = 0, \tag{3.2}$$

with initial conditions: $y(0) = 1$ and $y'(0) = 0$. The solution is $y = \exp(-x^2/2)$. We would like to approximate the solution for $x \to 0$ without using our knowledge of the true solution. To do this we will examine the contributions of the equation two by two:

- let us assume that $y'' \ll y$. We have to solve $x\tilde{y}' + \tilde{y} = 0$, whose first integral is $x\tilde{y} = a$, with a a constant. It is not possible to satisfy the boundary conditions. This balance is not possible;
- let us assume that $y \ll y''$. The dominant balance is $\tilde{y}'' + x\tilde{y}' = 0$, whose solution is $\tilde{y} = 1$. The assumption $y \ll y''$ is not satisfied, which means that this balance does not make sense;
- the only possibility is then $xy' \ll y$, which leads us to $\tilde{y}'' + \tilde{y} = 0$, whose solution is $\tilde{y} = \cos x$. We deduce that $x\tilde{y}' = -x \sin x$ is smaller than $\tilde{y}$ when $x \to 0$.

The approximate solution to equation (3.2) is $\tilde{y} = \cos x$, which provides a relatively accurate representation of the solution when $x \to 0$, as shown in Figure 3.2. □

3.1.3 Similarity solutions

Here we will see two techniques for working out self-similar solutions to a partial differential equation (if such solutions exist):

- in the first method, we will see that when dimensional analysis of the partial differential equation and of its boundary/initial conditions shows that there are only two dimensionless numbers that define the problem, i.e. when the solution can be written as $\Pi_1 = \phi(\Pi_2)$, then we can work out a self-similar solution;
- in the second method, we first make equations dimensionless, then ask whether they are invariant to a "stretching" transformation. In this case, we can reduce the order of the partial differential equation and transform

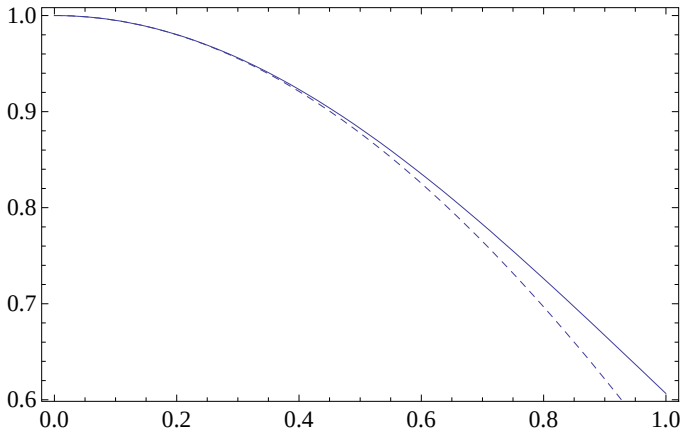

Figure 3.2: *Comparison between the exact solution* $y = \exp(-x^2/2)$ *(solid line) and approximate* $\tilde{y} = \cos x$ *(dashed line) of Equation (3.2).*

partial differential equations into ordinary equations, which are far easier to solve.

These two methods are studied through the example of the heat equation (see also § 2.2.2).

Insight from dimensional analysis

Let us consider the heat equation (2.7) in dimension 1 for a bar of section S

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}, \tag{3.3}$$

with α thermal diffusion, $T(x,\, t)$ temperature, x abscissa in the bar direction. Thermal energy E is conserved

$$\int_{-\infty}^{\infty} T(x,\ t)\mathrm{d}x = V = \frac{E}{cS}, \tag{3.4}$$

with c heat capacity. There are $n = 5$ variables: T, x, t, α, and V; the other variables (E, c, and S) are introduced through V.

The dimensional matrix is the following

	T	x	t	α	V
homogeneous to	K	m	s	m^2/s	m· K
power decomposition :					
power of m	0	1	0	2	1
power of s	0	0	1	-1	0
power of K	1	0	0	0	1

This is a 3×5 matrix of rank 3 (the fourth column is obtained by linear combination of columns 2 and 3, column 5 is the sum of columns 1 and 2). We can therefore form $k = n - r = 2$ dimensionless numbers. Let

$$\Pi_1 = x\alpha^a t^b V^c \text{ et } \Pi_2 = T\alpha^{a'} t^{b'} V^{c'}.$$

To get $[\Pi_1] = 0$, we must have

$$[\text{m } (\text{m}^2/\text{s})^a \text{ s}^b \text{ (mK)}^c] = 0,$$

which leads to the following system of equations

$$\begin{aligned} \text{for m} &: 0 = 2a + c + 1, \\ \text{for s} &: 0 = -a + b, \\ \text{for K} &: 0 = c, \end{aligned}$$

whose solution is $a = -\frac{1}{2}$, $b = -\frac{1}{2}$, and $c = 0$. The first dimensionless group is

$$\Pi_1 = \frac{x}{\sqrt{\alpha t}}.$$

To get $[\Pi_2] = 0$, we must have

$$[\text{K } (\text{m}^2/\text{s})^{a'} \text{ s}^{b'} \text{ (mK)}^{c'}] = 0,$$

which leads to the following system of equations

$$\begin{aligned} \text{for m} &: 0 = 2a' + c', \\ \text{for s} &: 0 = -a' + b', \\ \text{for K} &: 0 = c' + 1, \end{aligned}$$

whose solution is $a' = \frac{1}{2}$, $b' = \frac{1}{2}$, and $c' = -1$. The second dimensionless group is

$$\Pi_2 = \frac{T\sqrt{\alpha t}}{V}.$$

Dimensional analysis leads us to pose the solution in the form $\Pi_2 = F(\Pi_1)$. We substitute T into (3.3), with T defined by

$$T = \frac{V}{\sqrt{\alpha t}} F(\xi),$$

with $\xi = x/\sqrt{\alpha t}$. We get

$$\begin{aligned} \frac{\partial T}{\partial t} &= -\frac{1}{2}\frac{V}{t^{3/2}\sqrt{\alpha}} F(\xi) - \frac{1}{2}\xi \frac{V}{t^{3/2}\sqrt{\alpha}} F'(\xi) \\ \frac{\partial T}{\partial x} &= \frac{V}{t\alpha} F'(\xi), \\ \frac{\partial^2 T}{\partial x^2} &= \frac{V}{(t\alpha)^{3/2}} F''(\xi), \end{aligned}$$

which leads to write the heat equation in the form of a second-order ordinary differential equation

$$-\frac{1}{2}F - \frac{1}{2}\xi F' = F'',$$

which is easy to integrate

$$\frac{1}{2}\xi F + F' = a_0,$$

with a_0 a constant of integration. If propagation occurs in both directions $x \to \infty$ et $x \to -\infty$, then the solution is even and for $\xi = 0$, $F' = 0$ (horizontal tangent). Eventually we get $a_0 = 0$. A new integration leads to

$$\frac{F'}{F} = -\frac{1}{2}\xi \Rightarrow F = a_1 \exp\left(-\frac{1}{4}\xi^2\right)$$

with a_1 a constant of integration. Using Equation (3.4) and since $\int_{\mathbb{R}} F \mathrm{d}\xi = 1$, we deduce $a_1 = 1/(2\sqrt{\pi})$.

The solution reads

$$T = \frac{V}{2\sqrt{\pi\alpha t}} \exp\left(-\frac{1}{4}\frac{x^2}{\alpha t}\right).$$

Mathematical derivation of similarity solution

We first make Equation (3.3) dimensionless by introducing dimensionless variables

$$\begin{aligned} T &= T_* \hat{T}, \\ t &= \tau_* \hat{t}, \\ x &= L_* \hat{x}, \end{aligned}$$

with T_*, τ_*, and L_* temperature, time, and length scales; $\hat{T}$, $\hat{t}$, and $\hat{x}$ are dimensionless temperature, time, and length. When substituting these variables into (3.3), we get $L_*^2 = \alpha\tau_*$ while the boundary condition (3.4) imposes $L_* T_* = V$. A third condition is needed to determine all scales; we assume that τ_* is known, which makes it possible to derive the two other scales above.

When written in a dimensionless form, (3.3) and (3.4) read

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}, \tag{3.5}$$

$$\int_{-\infty}^{\infty} T(x,\ t)\mathrm{d}x = 1, \tag{3.6}$$

where the hat has been removed for the sake of simplicity.

A solution to a partial differential equation of the form $G(x,\ t,\ T) = 0$ is said to to be *self similar* if we can find a set of coefficients a and b such that for any scalar λ we have $G(\lambda x,\ \lambda^a t,\ \lambda^b T) = 0$. This means that the solution $T(x,\ t)$ to the

equation $G = 0$ is invariant when we stretch the variables by multiplying them by a factor of proportionality. Let us seek these factors by considering the following stretching, whose intensity depends on the parameter λ:

$$\begin{aligned} x &\to \lambda x', \\ t &\to \lambda^a t', \\ T &\to \lambda^b T', \end{aligned}$$

with a and b two constants to be determined. We substitute these expressions into the heat equation (3.5), which yields

$$\frac{\lambda^b}{\lambda^a}\frac{\partial T'}{\partial t'} = \frac{\lambda^b}{\lambda^2}\frac{\partial^2 T'}{\partial x'^2}. \tag{3.7}$$

This equation is identical to Equation (3.5) if we take $a = 2$. The boundary condition (3.6) gives

$$\int_{-\infty}^{\infty} \lambda^b \lambda T(x,\ t)\mathrm{d}x = 1, \tag{3.8}$$

which imposes $b = -1$.

It can be shown that the solutions invariant to the *stretching* transformation is then given by the characteristic equation

$$\frac{\mathrm{d}x}{x} = \frac{\mathrm{d}t}{at} = \frac{\mathrm{d}T}{bT}. \tag{3.9}$$

☣ **Proof**. If a solution to $G(x,\ t,\ T) = 0$ is self-similar, then we have $G(\lambda x,\ \lambda^a t,\ \lambda^b T) = 0$. Let us differentiate this equation with respect to λ and set $\lambda = 1$; we deduce the relation:

$$x'\frac{\partial G}{\partial x'} + at'\frac{\partial G}{\partial t'} + bT'\frac{\partial G}{\partial T'} = 0.$$

The geometric interpretation is simple: the vector ∇G is normal to the vector $(x',\ at',\ bT')$. If a point M of coordinates $(x',\ t',\ T')$ lies on the solution surface and a neighboring point M' $(x' + \mathrm{d}x',\ t' + \mathrm{d}t',\ T' + \mathrm{d}T')$ lies also on this surface, then the increment vector between M and M' $(\mathrm{d}x',\ \mathrm{d}t',\ \mathrm{d}T')$ is normal to ∇G

$$\mathrm{d}x'\frac{\partial G}{\partial x'} + \mathrm{d}t'\frac{\partial G}{\partial t'} + \mathrm{d}T'\frac{\partial G}{\partial T'} = 0.$$

Comparing both equations leads to deducing that the equations are equivalent to within a proportionality coefficient if $(\mathrm{d}x',\ \mathrm{d}t',\ \mathrm{d}T')$ and $(x',\ at',\ bT')$ are collinear. Equation (3.9) simply expresses the parallelism condition between both vectors. This may seem more complex than the original equation since it replaces a partial differential equation by a system of 3 differential equations. In fact, we have made our life easier because we know how to solve the above equations two by two. □

The characteristic equation associated with Equation (3.5) is

$$\frac{\mathrm{d}x}{x} = \frac{\mathrm{d}t}{2t} = -\frac{\mathrm{d}T}{T},$$

which admits two first integral: $\xi = x/t^{1/2}$ (obtained with the left-hand terms) and $\tau = Tt^{1/2}$. Similarity solutions are of the form $\tau(\xi)$:

$$T = \frac{1}{\sqrt{t}} H(\xi).$$

Substituting this expression into Equation (3.5), we find

$$-\frac{1}{2}H - \frac{1}{2}\xi H' = H'',$$

whose solution is $a_2 \exp\left(-\frac{1}{4}\xi^2\right)$, with a_2 a constant of integration. The boundary condition (3.6) provides the value: $a_2 = 1/(2\sqrt{\pi})$. The dimensionless solution is

$$\hat{T} = \frac{1}{2\sqrt{\pi\hat{t}}} \exp\left(-\frac{1}{4}\frac{\hat{x}^2}{\hat{t}}\right),$$

while its dimensional form is

$$T = \frac{V}{2\sqrt{\pi\alpha t}} \exp\left(-\frac{1}{4}\frac{x^2}{\alpha t}\right).$$

Summary

The first method is used to build self-similar solutions (when they exist) step by step and has the advantage of being a physical approach, but requires a lot of work. The second method, somewhat more mathematical, can quickly determine whether self-similar solutions exist and, when appropriate, to work it out.

In practice, if we consider a partial differential equation of the form $F(u,\ x,\ t)$ with u the dependent variable x and t independent variables, we use a *stretching* transformation for a parameter λ:

$$u \to u' = \lambda^{\alpha} u, \tag{3.10}$$

$$t \to t' = \lambda^{\beta} t, \tag{3.11}$$

$$x \to x' = \lambda x. \tag{3.12}$$

where α and β are two constants to be determined; they are determined by substituting these expressions into equation $F(u,\ x,\ t)$ and the boundary/initial conditions and then by seeking for what values of α and β, the transformed equations are independent of λ. Once these parameters have been found, we can solve the *characteristic equation*

$$\frac{\mathrm{d}x}{x} = \frac{\mathrm{d}t}{\beta t} = \frac{\mathrm{d}u}{\alpha u}.$$

This equation shows that the self-similar solution of $F(u,\ x,\ t)$ can be written as

$$u(x,\ t) = t^{\alpha/\beta} f(x/t^{1/\beta}). \tag{3.13}$$

3.2 First-order hyperbolic differential equations

In fluid mechanics, we are often faced with hyperbolic equations or systems of n hyperbolic equations:

- dimension 1: nonlinear convection equation, for example the kinematic wave equation, which describes flood propagation in rivers

$$\frac{\partial h}{\partial t} + K\sqrt{i}\frac{\partial h^{5/3}}{\partial x} = 0,$$

  with h flow depth, K Manning-Strickler coefficient, et i bed gradient;

- dimension 2: Saint-Venant equations

$$\frac{\partial h}{\partial t} + \frac{\partial h\bar{u}}{\partial x} = 0, \tag{3.14}$$

$$\frac{\partial \bar{u}}{\partial t} + \bar{u}\frac{\partial \bar{u}}{\partial x} = g\sin\theta - g\cos\theta\frac{\partial h}{\partial x} - \frac{\tau_p}{\varrho h}, \tag{3.15}$$

  with $\bar{u}$ flow-depth averaged velocity, h flow depth, θ bed slope, τ_p bottom shear stress;

- dimension 3 : Saint-Venant equations with advection of pollutant

$$\frac{\partial h}{\partial t} + \frac{\partial h\bar{u}}{\partial x} = 0, \tag{3.16}$$

$$\frac{\partial \bar{u}}{\partial t} + \bar{u}\frac{\partial \bar{u}}{\partial x} = g\sin\theta - g\cos\theta\frac{\partial h}{\partial x} - \frac{\tau_p}{\varrho h}, \tag{3.17}$$

$$\frac{\partial \varphi}{\partial t} + \bar{u}\frac{\partial \varphi}{\partial x} = 0, \tag{3.18}$$

  with φ pollutant concentration.

All these differential equations are first-order equations that reflect evolution and transport of various flow variables. Here we will focus on problems with one space variable x, but what we will say can be generalized to two (or more) space variables.

The key element in solving hyperbolic differential equations hinges upon the concept of information. Through the example of the wave equation and the convection equation, we have already seen that a partial differential equation expresses a physical process in which information spreads. The questions that arise are: in which direction does this information propagate? Is information conserved or attenuated? The answer these questions, we will go through the notions of *characteristic curve* (information propagation) and *Riemann variables* (quantity of information conveyed).

3.2.1 Characteristic equation

Let us first consider the following advection equation with $n = 1$ space variable:

$$\partial_t u(x,\ t) + a(u)\partial_x u(x,\ t) = 0, \tag{3.19}$$

subject to one boundary condition of the form:

$$u(x,\ 0) = u_0(x) \text{ at } t = 0, \tag{3.20}$$

A characteristic curve is a curve $x = x_c(t)$ along which the partial differential equation $\partial_f U + a\partial_x U = 0$ is equivalent to an ordinary differential equation. Consider a solution $u(x,\ t)$ of the differential system. Along the curve $\mathcal{C}$ of equation $x = x_c(t)$ we have: $u(x,\ t) = u(x_c(t),\ t)$ and the rate change is:

$$\frac{\mathrm{d}u(x_c(t),\ t)}{\mathrm{d}t} = \frac{\partial u(x,\ t)}{\partial t} + \frac{\mathrm{d}x_c}{\mathrm{d}t}\frac{\partial u(x,\ t)}{\partial x}.$$

Suppose now that the curve $\mathcal{C}$ satisfies the equation $\mathrm{d}x_c/\mathrm{d}t = a(u)$. So we immediately obtain:

$$\frac{\mathrm{d}u(x,\ t)}{\mathrm{d}t} = \frac{\partial u(x,\ t)}{\partial t} + a\frac{\partial u(x,\ t)}{\partial x} = 0. \tag{3.21}$$

Since $\mathrm{d}u(x,\ t)/\mathrm{d}t = 0$ along $x_c(t)$, this means that $u(x,\ t)$ is conserved along this curve. Since u is constant $a(u)$ is also constant, so the curves $\mathcal{C}$ are straight lines. In Fig. 3.3, we have plotted three characteristics: the slope of these lines is given by the initial condition $u_0(x)$.

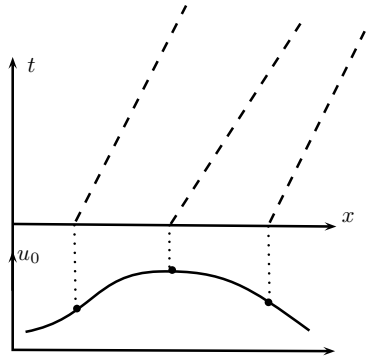

Figure 3.3: *characteristic curves (dashed lines) for the one-dimensional problem.*

From these transformations, we can deduce that Equations (3.19) and (3.21) are equivalent. Any convection equation can be cast in a characteristic form:

$$\boxed{\frac{\partial}{\partial t}u(x,\ t) + a(u)\frac{\partial}{\partial x}u(x,\ t) = 0 \Leftrightarrow \frac{\mathrm{d}u(x,\ t)}{\mathrm{d}t} = 0 \text{ along straight lines } \mathcal{C} \text{ of equation } \frac{\mathrm{d}x}{\mathrm{d}t} = a(u).} \tag{3.22}$$

When this equation is subject to an initial condition of the form (3.20), the characteristic equation (3.21) can be easily solved. Let us first seek the equation of (straight) characteristics by integrating the differential characteristic equation, knowing that u is constant along the characteristic line:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = a(u) \Rightarrow x - x_0 = a(u)(t - t_0),$$

with the initial condition $t_0 = 0$, $u(x,\ t) = u_0(x)$. We then infer

$$x - x_0 = a(u_0(x_0))t \tag{3.23}$$

is the equation for the (straight) characteristic line emanating from point x_0. Furthermore, we have for $t \geq 0$ $u(x,\ t) = u_0(x_0)$ since u is conserved. Since after equation (3.23), we have: $x_0 = x - a(u_0(x_0))t$, we eventually deduce :

$$\boxed{u(x,\ t) = u_0(x - a(u_0(x_0))t).} \tag{3.24}$$

3.2.2 Shock formation

A feature of hyperbolic equations is that they can propagate an initial discontinuity or generate a discontinuity after a finite time. It is therefore necessary to spend some time on characterizing discontinuities, which here we call *shock*.

We study the formation of a shock for a problem as simple as possible. We consider the convective nonlinear equation:

$$\frac{\partial}{\partial t}u(x,\, t) + \frac{\partial}{\partial x}f[u(x,\, t)] = 0, \tag{3.25}$$

with initial condition $u(x,\ 0) = u_0(x)$ and f a given function of u. This equation can be solved simply by the method of characteristics. Indeed, we have seen that a convection equation such as (3.25) can be cast in the following form

$$\frac{\mathrm{d}u}{\mathrm{d}t} = 0 \text{ along curves } \frac{\mathrm{d}x}{\mathrm{d}t} = \lambda(u),$$

We deduce that u is constant along the characteristic curves. So $\mathrm{d}x/\mathrm{d}t = \lambda(u) = c$, with c a constant that can be determined using the initial condition: the characteristics are straight lines with slopes $\lambda(u_0(x_0))$ depending on the initial condition:

$$x = x_0 + \lambda(u_0(x_0))t.$$

Since u is constant along a characteristic curve, we find:

$$u(x,\ t) = u_0(x_0) = u_0\left(x - \lambda(u_0(x_0))t\right)$$

As shown in Fig. 3.4, the characteristic lines can intersect in some cases, particularly when the characteristic velocity decreases (the $x - t$ diagram is in a fact

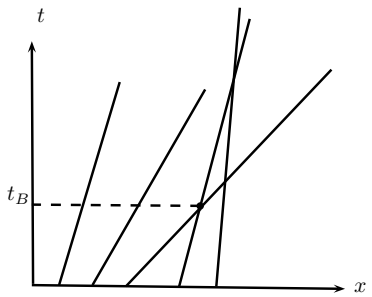

Figure 3.4: *characteristic curves and shock formation.*

a $t-x$ diagram, this slowdown is reflected in a steepening of the characteristic curves): $\lambda'(u) < 0$. What happens then? When two characteristic curves intersect, this means that potentially, u takes two different values, which is not possible for a continuous solution. The solution becomes discontinuous: a shock is formed.

When two characteristic curves interest, the differential u_x becomes infinite (since u takes two values at the same time). We can write u_x as follows

$$u_x = u_0'(x_0)\frac{\partial x_0}{\partial x} = u_0'(x_0)\frac{1}{1+\lambda'(u_0(x_0))u'(x_0)t} = \frac{u_0'(x_0)}{1+\partial_x\lambda(x_0)t},$$

where we used the relation: $\lambda'(u_0(x_0))u'(x_0) = \partial_u\lambda\partial_x u = \partial_x\lambda$. The differential u_x tends to infinity when the denominator tends to 0, i.e. at time: $t_b = -1/\lambda'(x_0)$. At the crossing point, u changes its value very fast: a shock is formed. The $s = s(t)$ line in the $x-t$ plane is the shock locus. A necessary condition for shock occurrence is then $t_b > 0$:

$$\boxed{\lambda'(x_0) < 0.}$$

Therefore there is a slower speed characteristic (see Fig. 3.4).

The characteristic curves that are causing the shock form an envelope curve whose implicit equation is given by:

$$x = x_0 + \lambda(u_0(x_0))t \quad \text{et} \quad \lambda'(u_0(x_0)) + 1 = 0. \tag{3.26}$$

After the shock, the solution is multivalued (see Fig. 3.5), which is impossible from a physical standpoint. The multivalued part of the curve is then replaced by a discontinuity positioned so that the lobes of both sides are of equal area.

Generally, we do not attempt to calculate the envelope of characteristic curves, because there is a much simpler method to calculate the trajectory of the shock. Indeed, Eq. (3.25) can also be cast in the integral form:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{x_L}^{x_R} u(x,\,t)\mathrm{d}x = f(u(x_L,\,t)) - (u(x_R,\,t)),$$

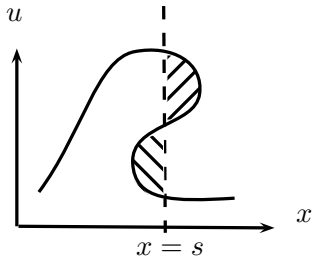

Figure 3.5: *shock position.*

where x_L and x_R are abscissa of fixed point of a control volume. If the solution admits a discontinuity in $x = s(t)$ on the interval $[x_L,\, x_R]$, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{x_L}^{x_R} u(x,\, t)\mathrm{d}x = \frac{\mathrm{d}}{\mathrm{d}t}\left(\int_{x_L}^{s} u(x,\, t)\mathrm{d}x + \int_{s}^{x_R} u(x,\, t)\mathrm{d}x\right),$$

That is:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{x_L}^{x_R} u(x,\, t)\mathrm{d}x = \int_{x_L}^{s} \frac{\partial}{\partial t}u(x,\, t)\mathrm{d}x + \int_{s}^{x_R} \frac{\partial}{\partial t}u(x,\, t)\mathrm{d}x + \dot{s}u(x_L, t) - \dot{s}u(x_R, t).$$

Taking the limit $x_R \to s$ and $x_L \to s$, we deduce:

$$\dot{s}[\![u]\!] = [\![f(u)]\!], \tag{3.27}$$

where

$$[\![u]\!] = u^+ - u^- = \lim_{x\to s, x>s} u - \lim_{x\to s, x<s} u,$$

The $+$ and $-$ signs are used to describe what is happening on the right and left, respectively, of the discontinuity at $x = s(t)$.

In conclusion, the short computations that we just made show that if there is a discontinuity at a point $x = s(t)$, then we must have on both sides of $x = s(t)$:

$$\boxed{\dot{s}[\![u]\!] = [\![f(u)]\!]} \tag{3.28}$$

This relationship is called *Rankine-Hugoniot*. It is fundamental in gas dynamics (it is used to calculate the propagation of a supersonic shock wave) and hydraulics (it is used to calculate the propagation of a hydraulic jump).

3.2.3 Riemann problem for one-dimensional equations ($n = 1$)

We call *Riemann problem* an initial-value problem of the following form:

$$\partial_t u + \partial_x[f(u)] = 0,$$

$$u(x,\ 0) = u_0(x) = \begin{cases} u_L & \text{if } x < 0, \\ u_R & \text{if } x > 0, \end{cases}$$

with u_L et u_R two constants. This problem describes how an initially piecewise constant function u, with a discontinuity in $x = 0$ changes over time. This problem is fundamental to solving theoretical problems and to solving hyperbolic equations numerically. In hydraulics, it is also important because the configuration studied corresponds to the rupture of a dam on dry or wet bottom. In the linear case, an initial discontinuity propagates and never disappears; conversely, for a solution to be discontinuous, the initial condition must include a discontinuity. The nonlinear case is somewhat more complex. We shall see that depending on u_R being larger or smaller than u_L, different solutions may be generated. When $f'(u)$ is an increasing function ($f''(u) > 0$) and $u_L < u_r$, the solution initially discontinuous becomes continuous since a continuous wave called *rarefaction wave* allows to link the two initial states and thus reduce the initial discontinuity. Conversely if $u_L > u_r$, the initial discontinuity propagates and the solution remains discontinuous. Recall also that even if the solution is initially continuous, nonlinear equations can generate discontinuities over time (see § 3.2.2). When the function f is complicated, more or less complicated solutions to the Riemann problem may arise.

Linear case

First let us consider the linear case $f(u) = au$, with a a constant. The solution is straightforward:

$$u(x,\ t) = u_0(x - at) = \begin{cases} u_L & \text{if } x - at < 0, \\ u_R & \text{if } x - at > 0. \end{cases}$$

The discontinuity propagates with a speed a.

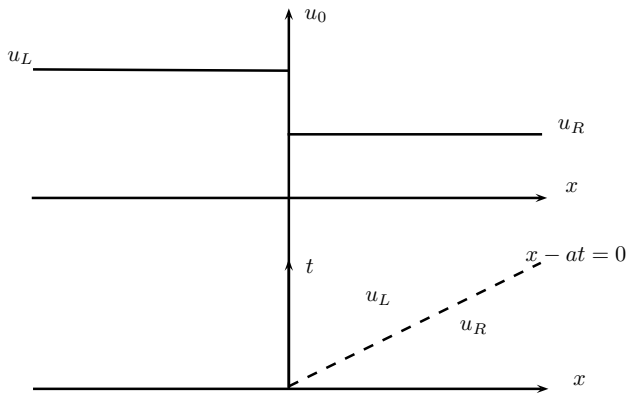

Figure 3.6: *Riemann problem for the linear case.*

Nonlinear case

Convex flux ($f'' > 0$) In the general case (where $f'' \neq 0$), the Riemann problem is an initial-value problem of the following form:

$$\partial_t u + \partial_x [f(u)] = 0,$$

$$u(x,\ 0) = u_0(x) = \begin{cases} u_L & \text{if } x < 0, \\ u_R & \text{if } x > 0. \end{cases}$$

with u_L and u_R two constants. Assume that $f'' > 0$ (the case of a non-convex flow will not be treated here). We will show that there are two possible solutions:

- a solution called *rarefaction wave* (or simple wave), which is continuous;
- a discontinuous solution which represents the spread of the initial discontinuity (*shock*).

Physically, only one of these solutions is possible and the choice will be dictated by a condition (called *entropy*) depending on the respective value of u_L and u_R. Essentially, the idea is that shocks cause energy dissipation and cannot create energy!

Rarefaction wave. Note first that this equation is invariant under the transformation $x \to \lambda x$ and $t \to \lambda t$. A general solution can be sought in the form $U(\xi)$ with $\xi = x/t$. Substituting this general form into the partial differential equation, we obtain an ordinary differential equation of the form:

$$\left(f'(U(\xi)) - \xi\right) U' = 0.$$

There are two types of solution to this equation:

- *rarefaction wave*: $(f'(U(\xi)) - \xi) = 0$. If $f'' > 0$, then $f'(u_R) > f'(u_L)$; equation $f'(U) = \xi$ admits a single solution when $f'(u_R) > \xi > f'(u_L)$. In this case, u_L is connected to u_R through a *rarefaction wave*: $\xi = f'(U(\xi))$. Inverting f', we find out the desired solution

$$u(x,\ t) = f'^{(-1)}(\xi)\ ;$$

- *constant state* : $U'(\xi) = 0$. This is the trivial solution $u(x,\ t) = \text{cte}$. This solution does not satisfy the initial problem.

The solution reads

$$u(x,\ t) = \begin{cases} u_L & \text{if } \dfrac{x}{t} \leq f'(u_L), \\ f'^{(-1)}(\xi) & \text{si } f'(u_L) \leq \dfrac{x}{t} \leq f'(u_R) \\ u_R & \text{if } \dfrac{x}{t} \geq f'(u_R). \end{cases}$$

Shock wave. We have previously seen that weak solutions (discontinues) to the hyperbolic differential equation (3.25) may exist. Assuming a discontinuity along a line $x = s(t) = \dot{s}t$, we get: $[\![f(u)]\!] = \dot{s}[\![u]\!]$. The solution is then:

$$u(x,\ t) = \begin{cases} u_L & \text{if } x < \dot{s}t, \\ u_R & \text{if } x > \dot{s}t. \end{cases}$$

Then there is formation of a shock wave velocity $\dot{s}$ given by:

$$\dot{s} = \frac{f(u_L) - f(u_R)}{u_L - u_R}.$$

Selection of the physical solution. Two cases may arise (remember that $f'' > 0$). We call $\lambda(u) = f'(u)$ the *characteristic velocity* (see section below), which is the slope of the characteristic curve (straight line) of the problem.

- 1st case: $u_R > u_L$. Since $f'' > 0$, then $\lambda(u_R) > \lambda(u_L)$. At initial time $t = 0$, the two characteristic lines form a fan. Equation $\xi = f'(U(\xi))$ admits a solution over the interval $\lambda(u_R) > \xi > \lambda(u_L)$. See Fig. 3.7;
- 2nd case: $u_R < u_L$. Characteristic lines intersect as of $t = 0$. The shock propagates at rate $\lambda(u_R) < \dot{s} < \lambda(u_L)$. This last condition is called *Lax condition*; it allows to determining whether the shock velocity is physically admissible.

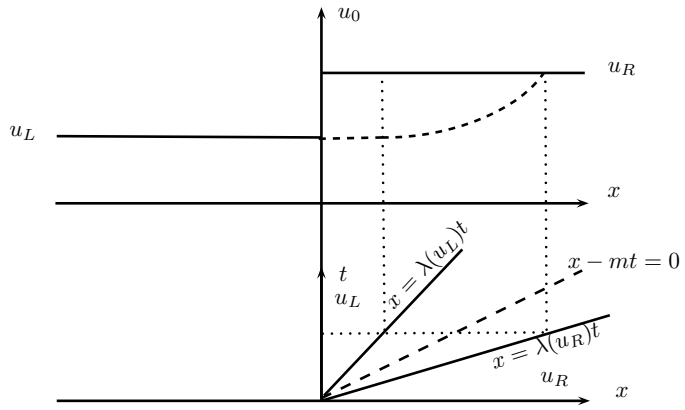

Figure 3.7: *Riemann problem for $u_R > u_L$.*

Non-convex flux For some applications, the flux is not convex. An example is given by the equation of Buckley-Leverett, reflecting changes in water concentration ϕ in a pressure-driven flow of oil in a porous medium:

$$\phi_t + f(\phi)_x = 0,$$

with $f(\phi) = \phi^2(\phi^2 + a(1-\phi)^2)^{-1}$ and a a parameter $(0 < a < 1)$. This fonction has an inflexion point. Contrary to the convex case, for which the solution involves shock and rarefaction waves, the solution is here made up of compose de chocs et *compound wave*) resulting from the superimposition of one shock wave and one rarefaction wave (LeVeque, 2002, see pp. 350–356).

Exercises

Exercice 3.1 We would like to solve the following equation over [0, 1]:

$$\epsilon y'' + y' + y = 0,$$

with initial conditions $y(0) = 1$ and $y(1) = 1$. Show that there is no regular expansion to this equation. Can you find the reason why the regular perturbation techniques does not work here?

Exercice 3.2 (Homework)

The Boussinesq equation is used to calculate the level of an aquifer in the ground; for example, as shown in Figure 3.8, a water flow in a channel, where the water height varies with time causes groundwater flow. For one-dimensional problem, the Boussinesq equation reads

$$\theta \frac{\partial h}{\partial t} = K_s \frac{\partial}{\partial x}\left(h \frac{\partial h}{\partial x}\right),$$

with θ soil porosity, K_s hydraulic conductivity, h water level. The boundary conditions are

$$h(0,\ t) = h_0(t),$$
$$\lim_{x \to \infty} h(x,\ t) = 0.$$

The initial condition is $h(x,\ 0) = 0$ for $x \geq 0$. Reply to the following questions:

- put the Boussinesq equation in a dimensionless form;
- search how to write the similarity solutions when $H_0(t) = At^n$ (i.e., show that solutions can be sought in the form $h = t^\alpha H(\xi)$ with $\xi = xt^{-\beta}$);
- show that the initial differential problem can be transformed into an ordinary differential problem in H;
- we consider the case where the level in the channel is constant $H_0 = A$ ($n = 0$). Show that the governing differential equation in H can be reduced to a quasi-linear equation of first order by making of the following change of variable $z = H/\xi^2$ and $p = H'/\xi$;
- write this equation in the form $\mathrm{d}p/\mathrm{d}z = f(p,\ z)$ with f a function to be determined;

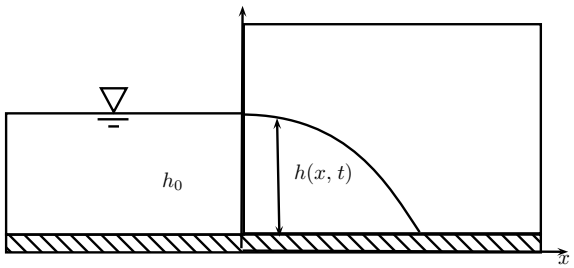

Figure 3.8: *groundwater propagation.*

- show that there is front propagation, c'est-à-dire a point x_f where $h(x_f) = 0$ and $h = 0$ beyond this point.

Exercice 3.3 Solve the initial value problem:

$$u_x + u_t = 0,$$

for $x \in \mathbb{R}$ and with $u(x,\ 0) = \cos x$.

Exercice 3.4 Solve analytically, then approximately to order ϵ the following equation

$$\frac{\mathrm{d}y(x)}{\mathrm{d}x} + \epsilon y(x) = 1,$$

with boundary conditions $y(0) = 1$ and where $\epsilon = 0.01$ is a small parameter.

$\rightsquigarrow$ *Answer.* The analytical solution is

$$y(x) = \frac{e^{-x\epsilon}\,(\epsilon + e^{x\epsilon} - 1)}{\epsilon}.$$

We use the following expansion $y = y_0 + \epsilon y_1 + \ldots$. To order ϵ^0, we have to solve $y_0' = 1$ with $y_0(0) = 1$, that is, $y(x) = x + 1$. To order ϵ^1, we have to solve $y_1' + y_0 = 0$ with $y_1(0) = 0$, that is, $y_1(x) = -x - \frac{1}{2}x^2$.

As shown on Fig. 3.9, the deviation between the theoretical and approximate solutions is low, even at order ϵ^0. □

Exercice 3.5 Solve Huppert's equation, which describes fluid motion over an inclined plane in the low Reynolds-number limit:

$$\frac{\partial h}{\partial t} + \frac{\rho g h^2 \sin\theta}{\mu}\frac{\partial h}{\partial x} = 0. \tag{3.29}$$

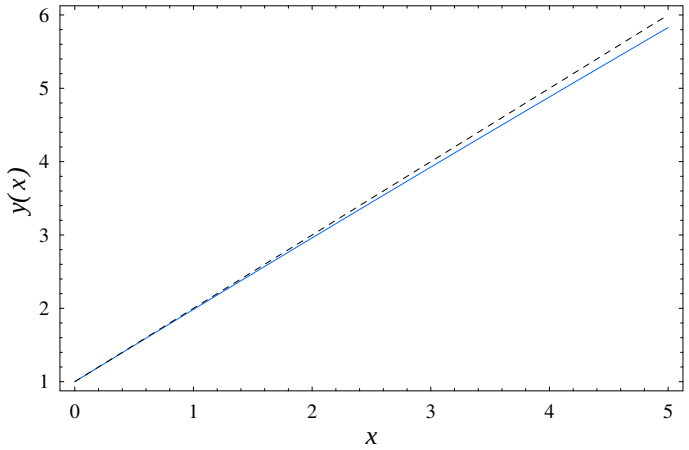

Figure 3.9: *comparison between the theoretical solution (solid line) and approximate solution (to order ϵ^0) $y = x + 1$ (dashed line) over $0 \leq x \leq 5$.*

Note that this equation is obtained from the Navier-Stokes equations assuming that the inertial terms are negligible and using the approximation of long wave (Huppert, 1982). The boundary conditions are given in Figure 3.10: it is the release of a finite volume of fluid.

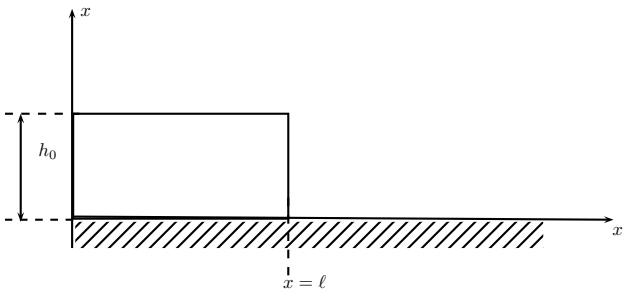

Figure 3.10: *initial flow configuration.*

$\rightsquigarrow$ *Answer.* This is a nonlinear convection equation of the form: $\partial_t h + c(h)\partial_x h = 0$ with $c(h) = \rho g h^2 \sin\theta/\mu$ or equivalently $\partial_t h + \partial_x f(h) = 0$ with $f(h) = \rho g h^3 \sin\theta/(3\mu)$.

This initial boundary-value problem can be solved straightforwardly. It is indeed a double Riemann problem, a first Riemann problem at $x = 0$ and another one $x = \ell$. We must therefore seek weak solutions (shock) and rarefaction waves that are associated with this equation. For weak solutions with a discontinuity in $x = s(t)$, there is a relation that gives h on both sides of $x = s$

$$\dot{s}[\![h]\!] = [\![f(h)]\!] \tag{3.30}$$

as a function of $\dot{s}$, the shock speed. Rarefaction waves are similarity solutions of the form $\mathcal{H}(\xi)$ with $\xi = x/t$. Here, substituting $h(x,\, t)$ with $\mathcal{H}(\xi)$ into (3.29), we obtain

$$\mathcal{H}'(-\xi + c(\mathcal{H})) = 0,$$

which implies that we have either $\mathcal{H}' = 0$, or

$$\mathcal{H} = \sqrt{\frac{\mu}{\rho g \sin\theta}}\xi. \tag{3.31}$$

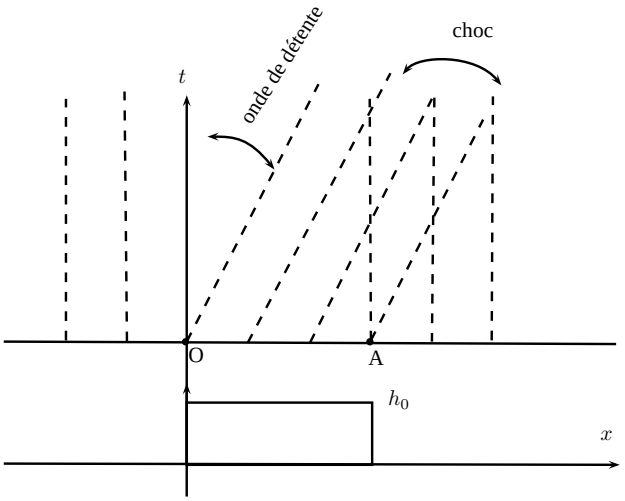

Figure 3.11: *characteristic curves.*

When put in a characteristic form, (3.29) becomes

$$\frac{\mathrm{d}h}{\mathrm{d}t} = 0 \text{ le long de } \frac{\mathrm{d}x}{\mathrm{d}t} = c(h). \tag{3.32}$$

It follows that initially the characteristics are straight lines, whose slope is given by $c(h_0)$, as shown in Fig. 3.11.

At short times, there is

- a shock on the right. According to (3.28), we have

$$\begin{aligned} \dot{s}_0[\![h]\!] &= [\![f(h)]\!], \\ \dot{s}_0(0 - h_0) &= f(0) - f(h_0), \\ \dot{s}_0 &= \frac{f(h_0)}{h_0} = \frac{\rho g h_0^2 \sin\theta}{3\mu} \end{aligned}$$

  whose characteristic curve emanating from point A has the following equation

$$x = \ell + \dot{s}_0 t = \ell + \frac{1}{3}\frac{\rho g h_0^2 \sin\theta}{\mu} t.$$

- a rarefaction wave on the left. Point O is the apex of a fan made up of straight characteristic lines:

$$x = mt,$$

with m a real parameter varying from 0 to $m_0 = \rho g h_0^2 \sin\theta/\mu$.

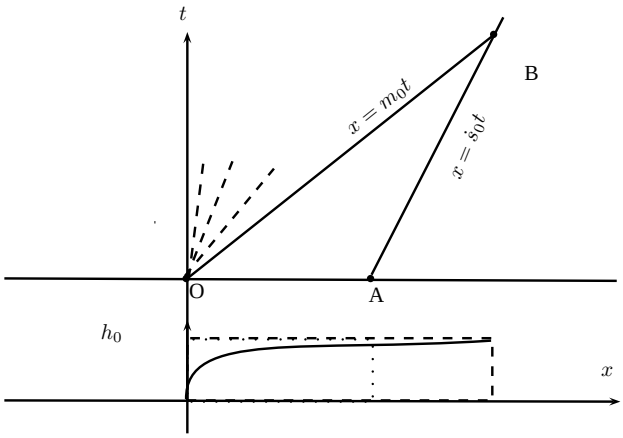

Figure 3.12: *crossing of two characteristics.*

The two characteristic lines $x = m_0 t$ and $x = \ell + \dot{s}_0 t$ cross at point B and time t_B

$$t_B = \frac{\ell}{m_0 - \dot{s}_0} = \frac{3}{2}\frac{\mu\ell}{\rho g h_0^2 \sin\theta}.$$

The abscissa of B is

$$x_B = m_0 t_B = \frac{3}{2}\ell.$$

The short-time solution is then ($0 \le t \le t_B$)

$$h(x,\, t) = \sqrt{\frac{\mu}{\rho g \sin\theta}\frac{x}{t}} \text{ for } 0 \le x \le m_0 t, \tag{3.33}$$

$$h(x,\, t) = h_0 \text{ for } m_0 t \le x \le \ell + \dot{s}_0 t \tag{3.34}$$

$$h(x,\, t) = 0 \text{ for } x > s(t) = \ell + \dot{s}_0 t \text{ or } x < 0. \tag{3.35}$$

Note that the volume is well conserved over time.

For $t > t_B$, the flow depth on the right of $x = s(t)$ is still 0, but leftwards, it diminishes. According to (3.29), this flow depth is

$$h_s = \sqrt{\frac{\mu}{\rho g \sin\theta}\frac{s}{t}}$$

which leads to the following shock speed

$$\begin{aligned} \dot{s}[\![h]\!] &= [\![f(h)]\!], \\ \dot{s}(0 - h_s) &= f(0) - f(h_s), \\ \dot{s} &= \frac{f(h_s)}{h_s} = \frac{\rho g h_s^2 \sin\theta}{3\mu} = \frac{1}{3}\frac{s}{t}. \end{aligned}$$

Integrating this equation, we find that the characteristic curve associated with the shock is

$$s(t) = x_B \left(\frac{t}{t_B}\right)^{1/3} = \frac{3}{2}\left(\frac{2}{3}\frac{\rho g h_0^2 \ell^2 \sin\theta}{\mu} t\right)^{1/3} = A t^{1/3},$$

with $A = \left(\frac{9}{4}\frac{\rho g h_0^2 \ell^2 \sin\theta}{\mu}\right)^{1/3}$. The long-time solution is then ($t > t_B$)

$$h(x,\, t) = \sqrt{\frac{\mu}{\rho g \sin\theta}\frac{x}{t}} \text{ for } 0 \le x \le A t^{1/3}, \tag{3.36}$$

$$h(x,\, t) = 0 \text{ pour } x > s(t) = A t^{1/3} \text{ for } x < 0. \tag{3.37}$$

Exercice 3.6 The Emden-Fowler equation arises in the context of equilibrium-mass distribution of a cloud of gas with adiabatic exponent

$$\ddot{y} + \frac{2}{x}\dot{y} + y^n = 0,$$

with $n = 5$ (corresponding to an adiabatic exponent 6/5).

- Seek similarity variables (hint: show that the equation is invariant under stretching group).
- Plot the phase portrait after a change of variable (with the similarity variable).
- Try to find an analytical solution.

4 Propriétés des fluides

4.1 Diffusion

4.1.1 Équations de diffusion

Une propriété assez générale aux fluides est la diffusion liée à l'agitation moléculaire et/ou au mouvement fluide. Si l'on place dans de l'eau un volume fini d'une solution d'une espèce diffusante (c'est-à-dire qu'elle ne va pas sédimenter tout de suite) comme par exemple de l'encre ou du sucre fin, on va observer une redistribution et un transport progressif de cette espèce dans tout le volume. Il en est de même si l'on chauffe localement un fluide, la chaleur va se propager progressivement dans tout le volume. Dans les deux cas de figure, on parle de *diffusion*.

Un cas typique de diffusion est rencontré lorsqu'il y a un gradient de concentration. Par exemple, soit $n(x,\ t)$ le nombre de particules en x, à l'instant t le long d'un barreau de section S. Expérimentalement, on observe que le flux de particules à travers ce barreau peut être défini à l'aide d'une relation dite (première) *loi de Fick*[1]

$$J = \frac{\delta n}{S\delta t} = -D\frac{\mathrm{d}n}{\mathrm{d}x},$$

avec D le coefficient de diffusion moléculaire (supposé constant), S la surface du barreau, δn la différence entre le nombre de particules entrant en x et sortant en $x + \Delta x$ (voir figure 4.1) pendant δt. Cette loi empirique est l'équivalent de la loi d'Ohm pour une résistance : $I = U/R$; le coefficient de diffusion correspond à la conductivité $(1/R)$, δn à la différence de potentiel U, et I et J sont deux « courants ».

[1] Adolf Eugen Fick (1829–1901) était un médecin allemand spécialisé en physiologie. Il proposa la loi qui porte aujourd'hui son nom et qui fut établie à partir d'expériences de diffusion d'un gaz à travers une membrane. Il est à l'origine des lentilles de contact et des premières mesures du débit cardiaque.

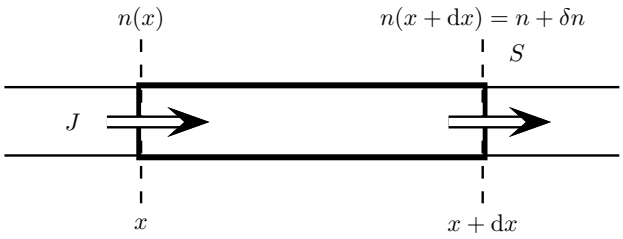

Figure 4.1: *bilan de matière dans un barreau.*

Si on fait un bilan dans le barreau considéré comme un milieu unidimensionnel et qu'on applique le principe « variation de n au cours du temps = ce qui entre – moins de ce qui sort », on aboutit à une équation de diffusion pour $n(x,\ t)$, qui est en tout point semblable à l'équation de la chaleur

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2}. \tag{4.1}$$

L'exemple typique de solution est celle obtenue en considérant qu'à l'instant $t = 0$, on lâche une quantité N de particules, qui seraient concentrées initialement dans une bande infiniment fine autour de $x = 0$. Les particules vont ensuite se propager dans les deux directions. Comme on peut le montrer (voir annexe 2), la solution mathématique à l'équation de diffusion est une gaussienne

$$n(x,\ t) = \frac{N}{2\sqrt{\pi D t}}\mathrm{e}^{-\frac{x^2}{4Dt}}.$$

Comme le montre la figure 4.2, l'effet de la diffusion moléculaire est d'adoucir le profil de concentration en n : au cours du temps, le profil est de plus en plus plat.

Comme pour la loi de Fourier vue (voir annexe 2), on peut généraliser cette loi scalaire pour obtenir une loi tensorielle (en dimension 3) en interprétant la dérivée comme un gradient :

$$\mathbf{J} = -D\nabla n,$$

où $\mathbf{J}$ est appelé aussi le vecteur « densité de courant » et cette équation est appelée seconde loi de Fick. On peut obtenir une équation linéaire tridimensionnelle de diffusion

$$\frac{\partial n}{\partial t} = -D\nabla \cdot \mathbf{J}.$$

Aussi bien pour les cas scalaire que tridimensionnel, on considère que la diffusion a lieu dans un fluide au repos. Si le fluide est en mouvement, il faut tenir compte de l'advection de matière ; mathématiquement, on remplace la dérivée locale par rapport au temps par une dérivée totale

$$\frac{\mathrm{d}n}{\mathrm{d}t} = \frac{\partial n}{\partial t} + \mathbf{u} \cdot \nabla n = D\nabla \cdot \mathbf{J} = D\triangle n,$$

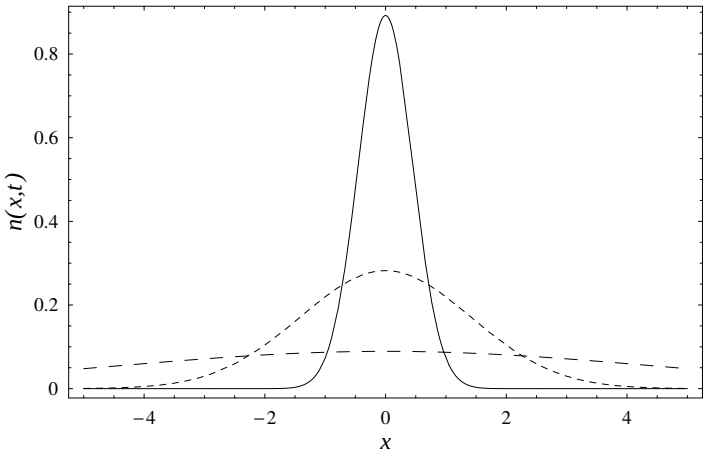

Figure 4.2: *solution à l'équation de diffusion dans le cas où la condition initiale correspond à la diffusion d'une tache ponctuelle, avec ici $N = 1$ et $D = 1$ m^2/s. Trait continu : solution à $t = 0,1$ s ; trait à tiret court : solution à $t = 1$ s ; trait à tiret long : solution à $t = 10$ s.*

$\triangle n$ le laplacien de n.

4.1.2 Origine physique

Il s'agit là d'une description empirique de la diffusion, mais il existe une description plus théorique du phénomène. Les mécanismes de la diffusion peuvent être appréhendés de façon indirecte par un processus dit d'auto-diffusion que l'on retrouve dans le mouvement brownien. Le mouvement brownien est le mouvement aléatoire d'une petite particule (du pollen, des poussières, des sables de taille micrométrique) immergée dans un fluide. Cette particle est soumise à des chocs avec les molécules du fluide, ce qui explique le mouvement erratique de la particule. Ce phénomène a été décrit pour la première fois en 1827 par Brown[2] alors qu'il observait avec un microscope du pollen en suspension dans l'eau. Physiquement, le mouvement brownien peut se comprendre comme suit (voir figure 4.3) :

- entre deux chocs, la particule se déplace en ligne droite avec une vitesse à peu près constante ;

[2]Robert Brown (1773–1858) était un botaniste anglais. En 1827, en observant du pollen avec un microscope, il constata que le pollen bougeait dans tous les sens. Il renouvela l'observation sur d'autres plantes, interprétant dans un premier temps ce phénomène comme la manifestation d'un organisme vivant. Cependant, il observa la même chose sur des particules inertes. L'explication du phénomène ne sera donné que bien plus tard par la théorie d'Einstein en 1905 (Smoluchowski, Bachelier, et Langevin), puis par les expériences de Perrin à la veille de la première guerre mondiale.

- la particule est accélérée instantanément lorsqu'elle est percutée par une molécule ou bien rencontre une paroi. Sa trajectoire marque alors un changement net de direction.

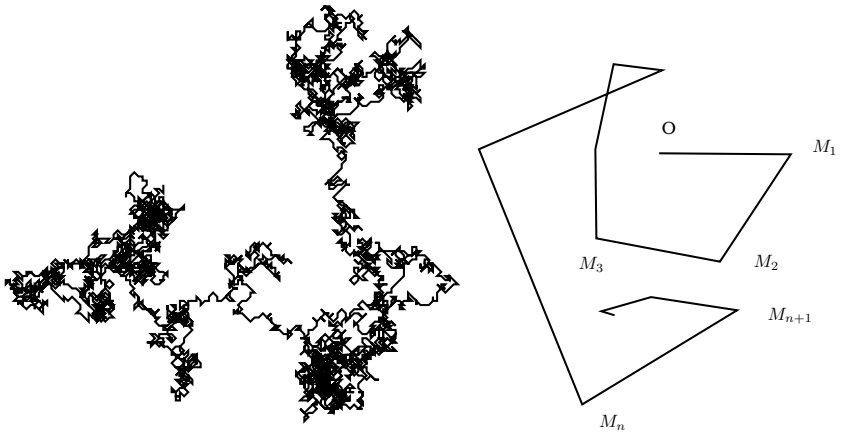

Figure 4.3: *idéalisation du mouvement brownien. (a) vue générale ; (b) agrandissement.*

Puisque la particule supposée au repos réalise des déplacements aléatoires au gré des collisions, il n'y a pas de raison pour qu'il y ait un sens de déplacement favorisé, donc en valeur moyenne, le déplacement $\mathbf{r}(t)$ est nul, ce que l'on note par

$$\langle \mathbf{r}(t) \rangle = 0$$

où les crochets $\langle \cdot \rangle$ renvoient à une moyenne (dans le temps). En revanche, le moment du second ordre[3] ou la variance du déplacement n'est pas nul. Ce moment s'écrit $\langle \mathbf{r}^2(t) \rangle$ et peut s'interpréter comme la moyenne du carré du déplacement. On va montrer assez simplement que ce moment du second ordre s'écrit[4]

$$\langle \mathbf{r}^2(t) \rangle = n\ell^2,$$

avec n le nombre de chocs subit par la particule. On suppose ici qu'en moyenne, tous les bouts de trajectoires sont de même longueur ℓ. Il s'ensuit aussi que si t_c désigne le temps moyen entre deux collisions, on a $n = t/t_c$ (on a aussi $t_c = \ell/w$,

[3] Si f désigne une densité de probabilité d'une variable X, alors la moyenne de X est $\int x f(x) \mathrm{d}x$ et est appelé moment du premier ordre ; le moment d'ordre n est simplement $\int x^n f(x) \mathrm{d}x$.

[4] Il suffit pour cela d'écrire qu'à l'instant t, $\mathbf{r}(t) = \mathbf{OM}_n = \sum_{i=0}^{n} \mathbf{M}_{i-1}\mathbf{M}_n$, puis de calculer la moyenne de $\langle \mathbf{r}^2(t) \rangle$ en faisant la décomposition.

avec w la vitesse de la particule entre chaque collision), d'où

$$\langle \mathbf{r}^2(t) \rangle = n\ell^2 = \frac{\ell^2}{t_c} t.$$

Si on définit le coefficient de diffusion comme étant $D = \ell^2/t_c = w\ell$, on trouve que $\langle \mathbf{r}^2(t) \rangle = Dt$. La particule « diffuse » donc en $\sqrt{t}$ autour de sa position initiale $\mathbf{r} = \mathbf{0}$.

Notons que le raisonnement réalisé en dimension 2 peut être mené dans le cas d'une propagation aléatoire dans une seule direction de l'espace, ce qui va permettre d'apporter un éclairage différent au problème de la figure 4.1, où l'on étudiait un transport de particules dans un barreau. Considérons une particule parmi les n particules présentes dans le barreau et supposons qu'elle soit en mouvement aléatoire. La probabilité qu'elle aille dans une direction équivaut à celle qu'elle aille dans la direction opposée ; la probabilité qu'elle change de direction à l'instant t est indépendante de tout ce qui a pu se passer jusqu'à l'instant t. La direction est donc aléatoire et peut prendre deux valeurs équiprobables $\epsilon = \pm 1$; le temps t est continu ; la vitesse de la particule est supposée constante et égale à w. On écrit donc tout cela sous forme mathématique

$$P(x - \delta x,\ t + \delta t | x,\ t) = \frac{1}{2},$$

$$P(x + \delta x,\ t + \delta t | x,\ t) = \frac{1}{2},$$

avec δx et δt de petits intervalles d'espace et temps, qui sont fixes. Ce que l'on peut traduire : la probabilité que la particule soit à l'instant $t+\delta t$ en $x-\delta x$ sachant qu'elle était en x à l'instant t vaut $1/2$. En se servant des lois de composition des probabilités[5]

$$\begin{aligned} P(x,\ t + \delta t) &= P(x,\ t + \delta t | x - \delta x,\ t) P(x - \delta x,\ t) + P(x,\ t + \delta t | x + \delta x,\ t) P(x + \delta x,\ t) \\ &= \frac{1}{2} P(x - \delta x,\ t) + \frac{1}{2} P(x + \delta x,\ t). \end{aligned}$$

En faisant un développement limité au second ordre[6] en x, on trouve que P vérifie l'équation

$$P(x,\ t + \delta t) - P(x,\ t) = \frac{1}{2} \delta x^2 \frac{\partial^2 P}{\partial x^2},$$

puis un développement au premier ordre en δt amène finalement à

$$\frac{\partial P}{\partial t} = \frac{\delta x^2}{2\delta t} \frac{\partial^2 P}{\partial x^2}.$$

[5] Rappelons que $P(x,\ y) = P(x|y)P(y)$ par définition de la probabilité conditionnelle.
[6] Rappel $f(x + \delta x) = f(x) + \delta x f'(x) + \delta x^2 f''(x)/2 + \cdots$.

On note que c'est la même équation que celle de la chaleur ou celle de la diffusion (4.1) sous réserve que $\delta x^2/\delta t$ soit constant. On pose donc $\delta x = \sqrt{2D\delta t}$. On aboutit donc à l'équation suivante pour la probabilité $P(x,\ t)$

$$\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2},$$

qui est une forme particulière de l'*équation de Fokker-Planck*. Une solution de cette équation est la loi de Gauss. Puisqu'en moyenne le déplacement moyen est nul (aucune direction favorisée), on déduit que

$$P(x,\ t) = \frac{1}{\sqrt{4\pi Dt}}\mathrm{e}^{-\frac{x^2}{4Dt}}.$$

On note dans ce cas particulier la correspondante des équations et des solutions pour $n(x,\ t)$ et $P(x,\ t)$.

Un point important également à noter dans notre explication du mouvement brownien est qu'encore une fois, c'est l'agitation thermique des atomes qui explique le comportement observé à l'échelle macroscopique. L'agitation est donc responsable à la fois d'une force continue (force de viscosité) et d'une force erratique (collisions donnant naissance au mouvement brownien). C'est cette analyse qui a permis à Einstein[7] de calculer le coefficient de diffusion d'une particule sphérique de rayon a dans un fluide newtonien de viscosité μ

$$D = \frac{kT}{6\pi\mu a},$$

qui montre que le coefficient de diffusion est un rapport entre l'énergie cinétique fluctuante kT et la force de frottement visqueuse $6\pi\mu a$.

Dans les expériences de Brown, on a précisé que le mouvement brownien affecte des particules de petite taille, typiquement de taille micrométrique pour une particule dans de l'eau. On peut caractériser plus finement l'échelle de taille et les caractéristiques du fluide pour lesquelles le mouvement brownien est important. Cela peut se faire par exemple en considérant la (seconde) loi de Fick pour calculer la diffusion de particules dans un fluide en mouvement avec une vitesse caractéristique u_*

$$\underbrace{\frac{\partial n}{\partial t}}_{\text{variation locale}} + \underbrace{\mathbf{u}\cdot\nabla n}_{\text{convection}} = \underbrace{D\triangle n}_{\text{diffusion}}.$$

[7]Albert Einstein (1879-1955) a été le physicien le plus célèbre du XX$^{\text{e}}$ siècle siècle, principalement pour ses travaux sur la relativité, qui remettait en cause notre conception du monde. Einstein a également eu des contributions importantes en physique des fluides en expliquant le mouvement brownien et en calculant la viscosité équivalente d'une suspension diluée de particules dans un fluide newtonien.

Si l'on compare dans cette équation différentielle, la part jouée par la convection et celle jouée par la diffusion, on peut former un rapport sans dimension appelé *nombre de Péclet*[8]

$$\mathrm{Pe} = \frac{\text{convection}}{\text{diffusion}} \sim \frac{u_* n/\ell_*}{Dn/\ell_*^2} \sim \frac{u_*\ell_*}{D},$$

où ℓ_* est une échelle caractéristique du système étudié (taille de la particule ou libre parcours moyen). Lorsque $\mathrm{Pe} \gg 1$, la convection l'emporte sur la diffusion. Les particules sont donc transportées (advectées) par le fluide. Dans le cas contraire, lorsque $\mathrm{Pe} \ll 1$, la diffusion l'emporte sur la convection.

[8]Jean Claude Eugène Péclet (1793–1857) était un physicien français, essentiellement tourné vers l'enseignement. Il est à l'origine de l'École Centrale des Arts et Manufactures.

A Phase portrait

A.1 Introduction

A number of nonlinear equations of first order as well as second-order autonomous equations can be cast in the following form:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{f(x,\ y)}{g(x,\ y)}, \tag{A.1}$$

with f and g two functions that may vanish. The points that are both zeros of f and g are called *singular points* [1] since the differential term $\mathrm{d}y/\mathrm{d}x$ is *a priori* indeterminate at these points. The behavior of the integral curves depends strongly on the structure of curves $f(x,\ y) = 0$ and $g(x,\ y) = 0$ around these critical points, c'est-à-dire the multiplicity of critical curves generated by the equations $f(x,\ y) = 0$ and $g(x,\ y) = 0$ and by the sign of f/g in the different areas delineated by these critical curves.

The simplest case is encountered when, near the singularity, it is possible to linearize Equation (A.1). We can then write: $f(x,\ y) = ax + by + o(x,\ y)$ et $g(x,\ y) = cx + dy + o(x,\ y)$. Let us assume that $ad - bc \neq 0$ and these coefficients are not all zero. There are two critical curves in the vicinity of the singularity:

- $y = -ax/b$ where the curves admit a horizontal tangent;
- $y = -cx/d$ where the curves admit a vertical tangent.

Introducing dummy variable t, we can transform (A.1) into the matrix form:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{u} = \mathbf{M} \cdot \mathbf{u}, \text{ with } \mathbf{M} = \begin{bmatrix} c & d \\ a & b \end{bmatrix}. \tag{A.2}$$

[1] They are also called *critical* points or *equilibrium* points.

We seek a solution in the form $\mathbf{v} = \mathbf{v}_0 \exp(\lambda t)$, with $\mathbf{v}_0$ the initial-condition vector (at $t = 0$). We deduce that λ must be an eigenvalue of the matrix $\mathbf{M}$ and $\mathbf{v}_0$ an associate eigenvector; λ is solution to the second order equation $\lambda^2 - 2h\lambda + k = 0$, with $2h = b + c$ and $k = \det \mathbf{M} = -ad + bc$, that is:

$$\lambda = h \pm \sqrt{h^2 - k}.$$

The principal directions principales are: $b - c \mp \sqrt{(b-c)^2 + 4ad}$. Depending on the value taken by λ, different behaviors arise:

- when $\Delta = h^2 - k > 0$ and $k > 0$, the two eigenvalues are real and of the same sign. Assume that $h > 0$, then the two eigenvalues are positive, which means that either both solutions to (A.2) tend to 0 as $t \to -\infty$ (resp. when $h < 0$, the solutions tend to 0 as $t \to +\infty$). Hence, if every initial condition lies on one of the principal axes, each solution tends to the origin point, the solution is a part of a straight line with slope equal to one of the principal directions. What happens if the initial condition does not lie on one of the principal directions? Let us assume that an integral curve tends towards the origin point. The limit of $\mathrm{d}y/\mathrm{d}x$ at 0 in the equation (A.1) is not defined. Applying Rule's Hospital (see below), the slope of the solution at point O must satisfy:
$$m = \frac{a + bm}{c + dm},$$
i.e., $m = b - c \pm \sqrt{(b-c)^2 + 4ad}$ and m coincide with one of the main directions. Given the sign of $\mathrm{d}y/\mathrm{d}x$ around the origin point, only one of these solutions is possible: the curves reach the origin point, following an asymptotic curve of equation $y = mx$. This singularity is called a *node*. Figure A.1 shows an example.

- if $\Delta > 0$ and $k > 0$, the two eigenvalues are real and of opposite sign. The two solutions of system (A.2) behave differently when $t \to \infty$: one tends towards the singular point while the other tends to infinity. There are always two curves that pass through the singular point and that coincide with the principal directions. If now the initial point (initial condition of the differential equation) does not lie on one of the principal directions, then it is not possible to find an integral curve emanating from that point to the singular point because of the sign of $\mathrm{d}y/\mathrm{d}x$ in the close vicinity of the singular point. The paths diverge when approaching the singular point. We refer to this point as a *saddle*. Figure A.2 shows an example.

- if $\Delta = 0$, the singular point is a node.

- if $\Delta < 0$, both eigenvalues are imaginary. The curves coiled like a spiral around the singular point. This point is called *focal point*. Figure A.3 shows an example.

♣ **Example.** – When solving the equation:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{x+2y}{2x+y}, \tag{A.3}$$

we find out that there are two eigenvalues 3 and 1 associated with principal directions 1 and et -1 respectively. It is a node.

♣ **Example.** – When solving the equation:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{2x+y}{x+2y}, \tag{A.4}$$

we find out that there are two eigenvalues 3 and -1 associated with principal directions 1 and et -1 respectively. It is a saddle.

♣ **Example.** – When solving the equation:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{2x+y}{x-y}, \tag{A.5}$$

we find out that there are two complex eigenvalues $(3 \pm \imath\sqrt{3})/2$. It is a focal point.

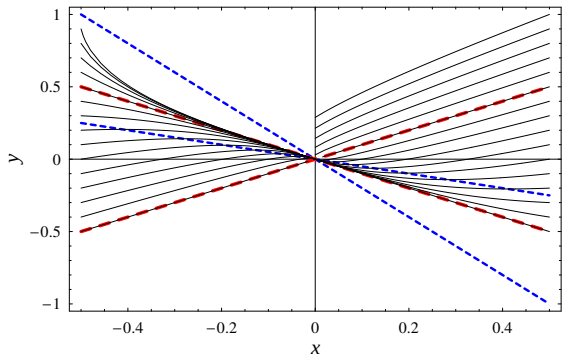

Figure A.1: *Example of node. Solid lines are solutions to the differential equation (A.3). Blue dashed lines represent singular curves while the red lines stand for the principal directions.*

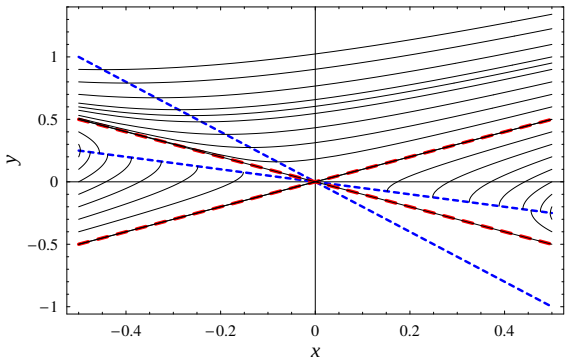

Figure A.2: *Example of saddle. Solid lines are solutions to the differential equation (A.4). Blue dashed lines represent singular curves while the red lines stand for the principal directions.*

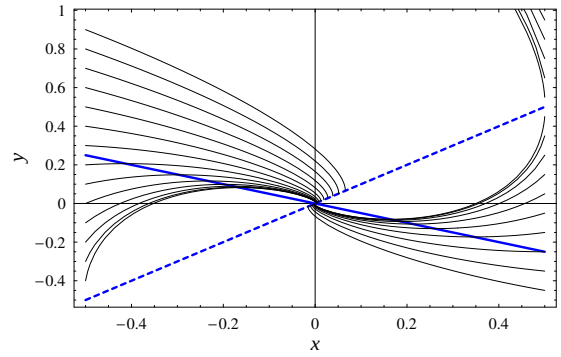

Figure A.3: *Example of focal point. Solid lines are solutions to the differential equation (A.5). Blue dashed lines represent singular curves.*

A.2 Typology of singular points

The preceding discussion can be generalized to forms of differential equations that are much more complex than the linear system (A.2). We note that there are three

possible types of behavior:

- *node* where the integral curves (there exists an infinity of such curves) are directed towards the singular point, usually following an asymptotic curve that can be deduced from the differential equation;
- *saddle* where the integral curves diverge as they approach the singular point, except one who is able to cross it;
- *focal point* where the curves wrap up like spirals or make loop around the singular point.

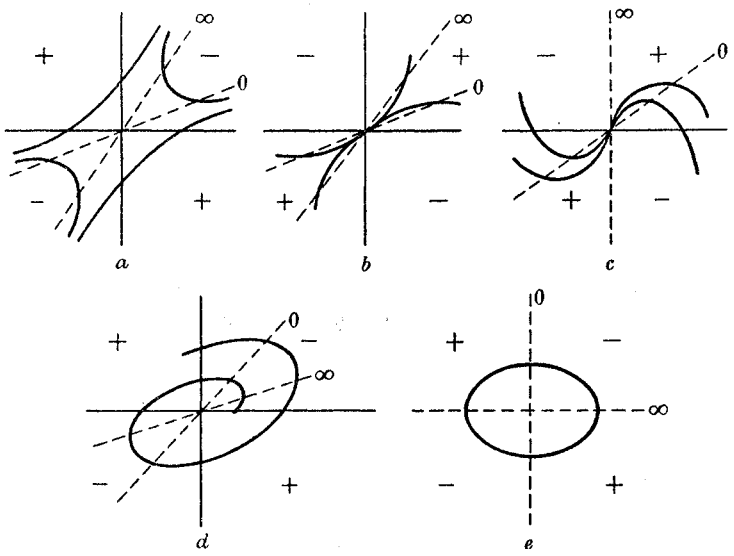

Figure A.4: *Typology of singular points where there are two critical curves. After (Jones, 1953).*

In the general case, the behavior of functions is a combination of these three basic forms, which is more or less complex depending on the number of critical curves $f = 0$ and $g = 0$. Figure A.4 recalls the possible behaviors when there are two critical curves. Figure A.5 shows the possible combinations when there are three critical curves (two corresponding to $f = 0$ et a single one to $g = 0$). Figure A.6 shows the possible combinations when four critical curves, two of which coincide with the coordinate axes.

A.3 Computation of the asymptotic curve

When the singularity is a node, there is an asymptotic curve to which any curve passing through the singularity tends. Similarly, when the singular point is a

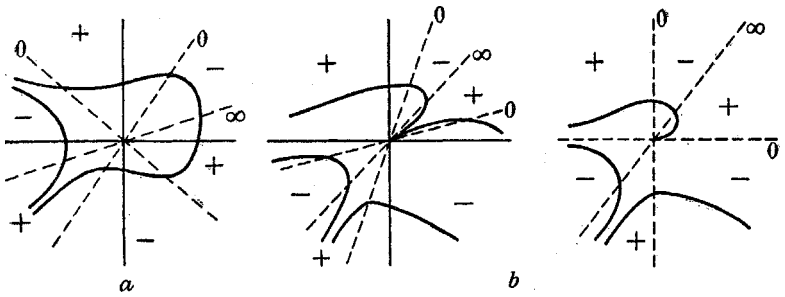

Figure A.5: *Typology of singular points where there are three critical curves. After (Jones, 1953).*

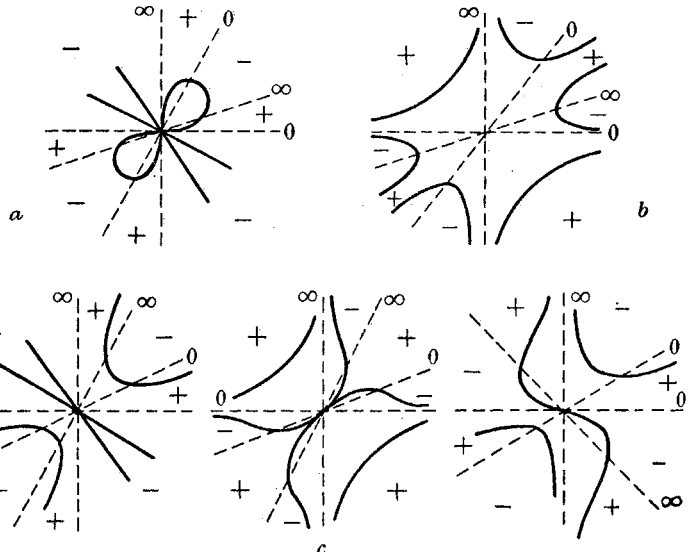

Figure A.6: *Typology of singular points where there are four critical curves. After (Jones, 1953).*

saddle, there is a (single) curve solution that arrives at the singular point. The exceptional curve is called *separatrix*. because it also separates two regions of space, each characterized by a specific behavior near the singular point. We can use several methods to work out the equation of this curve.

A.3.1 Numerical computation

Using l'Hôpital's rule, we can obtain the asymptotic curve toward which the integral curves moving towards a node converge or the single curve passing through a

saddle. Indeed we can write:

$$F(x) = f(x,\ y(x)) \ \text{ and } \ G(x) = g(x,\ y(x)).$$

By making a first-order expansion around a singular point $\mathbf{x}_s$, we have:

$$\dot{y}_s + x\ddot{y}_s + \cdots = \frac{x\dot{F}_s + \frac{x^2}{2}\ddot{F}_s + \cdots}{x\dot{G}_s + \frac{x^2}{2}\ddot{G}_s + \cdots} = \frac{\dot{F}_s + \frac{x}{2}\ddot{F}_s + \cdots}{\dot{G}_s + \frac{x}{2}\ddot{G}_s + \cdots},$$

with $\dot{y}_s = \dot{y}(\mathbf{x}_s)$ et $\ddot{y}_s = \ddot{y}(\mathbf{x}_s)$. Computing $\dot{F}_s$ requires the computation of compound derivatives:

$$\dot{F} = \frac{\partial f}{\partial x} + \dot{y}\frac{\partial f}{\partial y},$$

$$\ddot{F} = \frac{\partial \dot{F}}{\partial x} + \dot{y}\frac{\partial \dot{F}}{\partial y} + \ddot{y}\frac{\partial \dot{F}}{\partial \dot{y}}.$$

We do the same with G. We wish to compute the series expansion of the asymptotic curve at the singular point, that is, an equation of the form $y = y_s + m(x - x_s) + p(x - x_s)^2/2$, with $m = \dot{y}_s = \dot{y}(x_s)$ and $p = \ddot{y}_s = \ddot{y}(x_s)$. To order 0, we must solve the second-order equation:

$$m = \frac{f_x + m\ f_y}{g_x + m\ g_y}, \tag{A.6}$$

to find m. Once m is known, we can infer p, which is solution to the following equation:

$$\ddot{F}_s = m\ddot{G}_s + 2p\dot{G}_s. \tag{A.7}$$

♣ **Example.** – Let us consider the differential equation

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{x + 3xy + 3(1-y)y}{3x(2x+3y)}.$$

We would like to determine how the integral curves behave close the origin point (which is singular). We find:

$$\dot{F}(0) = 1 + 3m \ \text{ et } \ \dot{G}(0) = 0,$$

and the solution to (A.6) is $m = -1/3$. To order 1, we get

$$\ddot{F}(0) = -\frac{8}{3}p \ \text{ et } \ \ddot{G}(0) = 6,$$

and the solution to ((A.7) is $p = 2/9$. The equation of the asymptotic curve is then:

$$y = -\frac{1}{3}x\left(1 - \frac{2}{3}x + \cdots\right).$$

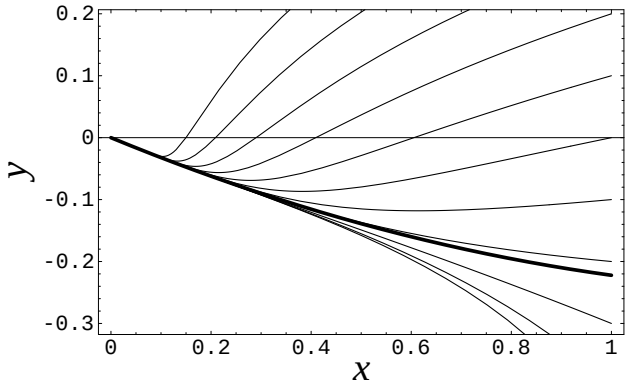

Figure A.7: *Convergence of integral curves towards the asymptotic curve.*

A.3.2 Analytical calculation

The separatrix is a curve, which is solution to the differential equation (A.1) for all Lie groups admitted by the same equation. An implicit curve equation $\phi(x,\ y) = 0$ is invariant under a Lie group $X = \xi\partial_x + \eta\partial_y$ if $X\phi = 0$. Using the condition

$$X\phi = \xi\partial_x\phi + \eta\partial_y\phi = 0,$$

we deduce that ϕ is also solution to the following first-order differential equation

$$y' = \frac{\eta(x,\ y)}{\xi(x,\ y)}.$$

The equation of the separatrix is then obtained by substituting y' by η/ξ into (A.1) (Dressler, 1983; Bluman, 1990) :

$$\frac{\eta(x,\ y)}{\xi(x,\ y)} = \frac{f(x,\ y)}{g(x,\ y)}.$$

To find the equation of the separatrix, we must then find all groups that leave Equation (A.1) invariant. This is beyond the scope of the lecture notes and we mention this technique just for completeness.

♣ **Example.** – Let us consider the differential equation

$$y' = \frac{y(x - y^2)}{x^2},$$

which is invariant under transformation $x_1 = \lambda x$ and $y_1 = \sqrt{\lambda}y$, whose infinitesimal generator is $X = 2x\partial_x + y\partial_y$. We then deduce $\xi = 2x$ and $\eta = y$. The equation of the separatrix is

$$\frac{y}{2x} = \frac{y(x - y^2)}{x^2},$$

or, equivalently,

$$y^2 = \frac{x}{2}.$$

□

A.4 Singular points located at infinity

In many cases, we have $f(x,\ y) \to \infty$ and $g(x,\ y) \to \infty$ when $x \to \infty$ and $y \to \infty$, which implies that the behavior of $\mathrm{d}y/\mathrm{d}x$ is indefinite there. One way to find the proper limit is to use the dominant-balance technique, i.e. $y \ll x$, $y \sim x$, or $y \gg x$, then integrate the resulting differential equation to check whether the assumption is consistent *a posteriori* or not. In some cases, singular points expelled to infinity may actually represent a single point; a change of variable can usually show that (Lacey *et al.*, 1982). For example, with the following variable change

$$x_1 = \frac{x}{x^2 + y^2} \text{ et } y_1 = -\frac{y}{x^2 + y^2},$$

then by analyzing behavior at $(0,\ 0)$ in the $(x_1,\ y_1)$ plane, we can determine the behavior of a singular at infinity (note that it is equivalent to making the change $z_1 = 1/z$ with $z = x + \imath y$).

♣ **Example.** – Let us consider the differential equation

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{3y(x - 2y)}{(1 - 3x)y - x - x^2},$$

for which we consider one of the following possibilities when $x \to \infty$ and $y \to \infty$:

- $y \ll x$, then we find $\dot{y} \propto 3y/x$, i.e., $y \propto x^3$, which contrasts with the initial assumption;
- $y \sim x$, then we set $y \propto mx$, we deduce $m = 4/3$, which is consistent with our assumption;
- $y \gg x$, then $\dot{y}/y \propto 2y/x)$, i.e. $y \propto x^2$, which is consistent with our assumption.

For the first quadrant $(x,\ y) > 0$, $x \to \infty$ and $y \to \infty$, there are two singular points at infinity corresponding to two asymptotic curves $y = 4x/3$ and $y = x^2$. For the second quadrant $x \to -\infty$ and $y \to \infty$, there is one singular point corresponding to the curve $y = x^2$, identical to the asymptotic curve we have found previously. It is in fact the same point and in practice, this means that one path may escape from the first quadrant along the curve $y = x^2$ to return via the second quadrant and following the same curve. To show this, we can make the change of variable

$$u = \frac{1}{x} \text{ and } v = \frac{x^2}{y},$$

such that both singular points of the first problem collapse onto a single point $A(0,\ 1)$. We then conclude:

$$\frac{\mathrm{d}v}{\mathrm{d}u} = \frac{v\ \ (2-(5+2\ u)\ \ v)}{3+u\ \ (-1+v)+u^2\ v}.$$

Point A is not a singular point of this equation; therefore, for A and for points in the near vicinity of A, only one curve passes.

A.5 Singular points with horizontal/vertical tangent

We can find differential equations with singularities satisfying $m = 0$ or $m = \pm\infty$ and in this case, the behavior is deduced by approximation and integration of the solution (argument like the one used in the *dominant balance* technique).

♣ **Example.** – Let us consider the differential equation:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{8-3x}{x(4-x)-2}y, \tag{A.8}$$

for which we note that the denominator vanishes at A_- $(2-\sqrt{2},\ 0)$ and A_+ $(2+\sqrt{2},\ 0)$, which are two singular points (nodes). The numerator vanishes at A_0 $(8/\ 3,\ 0)$, which corresponds to an extremum in the integral curve. The solution has the following behavior:

		A_-		A_0		A_+	
numerator	+	|	+	|	−	|	−
denominator	−	|	+	|	+	|	−
function	−	|	+	|	−	|	+

The behavior around the nodes is then given by:

- for A_-, we get:
$$\frac{\mathrm{d}y}{\mathrm{d}x} \approx n\frac{y}{x-x_{A-}},$$
with $x_{A-} = 2-\sqrt{2}$ and $n = (8-3x_{A-})/(x_{A+}-x_{A-}) = 3/2+1/\sqrt{2} \approx 2,20 > 1$. After integration, we find: $y = c(x-x_{A-})^n$, with c an integration constante, thus at point A_-, the curve admits a horizontal tangent.

- for A_+, we have:
$$\frac{\mathrm{d}y}{\mathrm{d}x} \approx n'\frac{y}{x-x_{A+}},$$

avec $n' = (3x_{A+} - 8)/(x_{A+} - x_{A-}) = -3/2 + 1/\sqrt{2} \approx 0,79 < 1$. After integration, we get: $y = c|x_{A+} - x|^{n'}$, thus at point A_+, the curve admits a vertical tangent.

Note that in this case, there is an analytic solution of the form:

$$y(x) = c|2 - ax + x^2|^{3/2} \exp\left[-\sqrt{2}\,\operatorname{arctanh}\frac{x-2}{\sqrt{2}}\right].$$

The result (numerical integration) is reported on the following figure. Note that the vertical tangent at point A_+ is not very apparent because the interval over which the derivative is very large is narrow. □

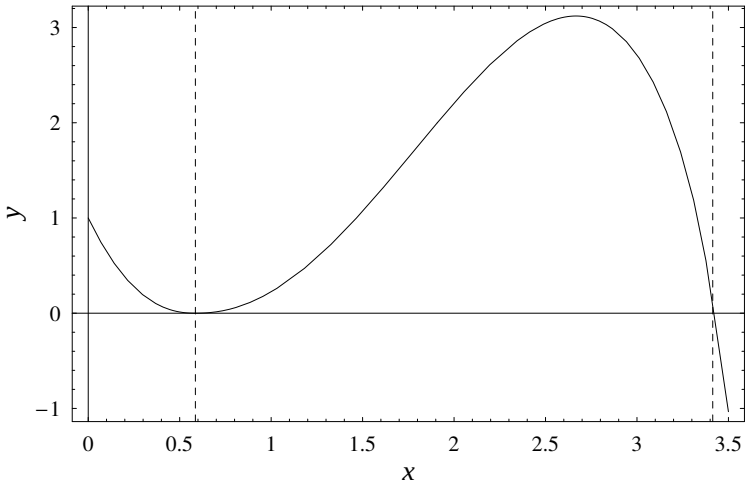

Figure A.8: *Solution to equation (A.8).*

♣ **Example.** – Let us consider the differential equation:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{6y(2y-x)}{2q^2 + 6yx + x}.$$

It is singular at point O and A $(0,\ -1/2)$ At O, we find that $m = 0$. To work out the asymptotic-curve equation, we try to approximate the solution. We assume $x \ll y$ when $y \to 0$. This therefore gives

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{6y(2y-x)}{2q^2 + 6yx + x} \approx \frac{12y^2}{x},$$

whose first integral is the family of curves

$$x = K \exp\left(-\frac{1}{12y}\right),$$

with K an integration constant.

B Approximation

B.1 Definitions

We are concerned with the scalar function (u, ϵ), which takes value x on an interval D and depends on a parameter ϵ over an interval I: $0 < \epsilon < \epsilon_1$.

The notation

$$u(x, \epsilon) = O(v(x, \epsilon)) \text{ sur } I \tag{B.1}$$

means that for all x over D, there exists a number $k(x)$ such that

$$u(x, \epsilon) \leq k(x)|v(x, \epsilon)|, \text{ pour tout } \epsilon \in I.$$

Similarly we have

$$u(x, \epsilon) = O(v(x, \epsilon)) \text{ quand } \epsilon \to 0,$$

for any x of D, when there exists a positive real $k(x)$ and a neighborhood N of $\epsilon = 0$ such that $u(x, \epsilon) = k(x)|v(x, \epsilon)|$ for any ϵ over I. The relation (B.1) is said to be *uniformly valid* when k does not depend on x.

♣ **Example.** – The relation

$$\frac{1}{x + \epsilon} = O(1),$$

is correct because if we take $k(x) = 1/x$ and since $(x + \epsilon)^{-1} < x^{-1}$, the relation $u(x,\ \epsilon) < k(x) \times 1$ holds. However, this relation is not uniformly valide since there is no constant k such that $u(x,\ \epsilon) < k \times 1$. □

The notation $u = O(v)$ does not mean that u and v must have the same order of magnitude. This notation implies tat u is bounded. If u and v have the same order of magnitude, then the limit u/v (when $\epsilon \to 0$) exists and is finite; we have $u = O(v)$ and $v = O(u)$. We can make use of the following notation $u = \text{ord}(v)$ (this notation is, however, not universally accepted).

$$u(x,\epsilon) = o(v(x,\epsilon)) \text{ quand } \epsilon \to 0 \tag{B.2}$$

means that for any x over D and for any constant $k > 0$, there is an interval N_ϵ $(0 < \epsilon < \epsilon_1(x,k))$ such that

$$u(x,\epsilon) \leq k|v(x,\epsilon)|, \text{ for any } \epsilon \in N_\epsilon.$$

u becomes arbitrarily small compared to $|v|$. We also note that $u \ll v$. The relation (B.2) is said to be uniformly valid if ϵ_1 depends on k, but not on x.

A sequence of functions $\phi_n(\epsilon)$ is called *asymptotic series* if

$$\phi_{n+1}(\epsilon) = o(\phi_n(\epsilon)) \text{ quand } \epsilon \to 0.$$

♣ **Example.** – The sequence $\phi_n(\epsilon) = \epsilon^{n-1}$ with $n = 1, 2, \ldots$ is an asymptotic series. □

For a function (u, ϵ), its asymptotic expansion to order N means that when $\epsilon \to 0$, we are able to build a function $\sum_{n=1}^{N} u_n(x)\phi_n(\epsilon)$ such that

$$u(x,\epsilon) - \sum_{n=1}^{N} u_n(x)\phi_n(\epsilon) = o(\phi_M) \text{ quand } \epsilon \to 0,$$

for $M = 1, 2, \ldots, N$ and where $\phi_n(\epsilon)$ is a sequence of functions.

When the function u is known and if the asymptotic series $\phi_n(\epsilon)$ is specified, we can easily construct the sequence of functions $u_n(x)$

$$\begin{aligned}
u_1(x) &= \lim_{\epsilon\to 0} \frac{u(x,\epsilon)}{\phi_1(\epsilon)}, \\
u_2(x) &= \lim_{\epsilon\to 0} \frac{u(x,\epsilon) - u_1(x)\phi_1(\epsilon)}{\phi_2(\epsilon)}, \\
u_k(x) &= \lim_{\epsilon\to 0} \frac{u(x,\epsilon) - \sum_{n=1}^{k-1} u_n(x)\phi_n(\epsilon)}{\phi_k(\epsilon)}.
\end{aligned}$$

B.2 Regular perturbation techniques

Let us consider a projectile launched vertically from the Earth surface (sphere of radius R). Its equation of motion is

$$\frac{\mathrm{d}^2 z}{\mathrm{d}\tau^2} = -\frac{gR^2}{(z+R)^2}, \tag{B.3}$$

with g gravitational acceleration, $\tau > 0$ the time, and with the initial conditions $z(0) = 0$ and $\dot{z}(0) = v_0$. This problem is formally equivalent to

$$\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} = -\frac{1}{(\epsilon y + 1)^2}, \tag{B.4}$$

where $\epsilon = v_0^2/Rg$ is a small parameter ($\epsilon \ll 1$), $t = \tau/T_*$, $z = y/L_*$, $T_* = v_0/g$, and $L_* = v_0^2/g$. We seek an asymptotic approximation to

$$y = y_0 + \epsilon y_1 + \epsilon^2 y_2 + \dots$$

Substituting this expression into (B.3), we have

$$1 + \left(y_1{}''(t) - 2y_0(t)\right)\epsilon + \left(3y_0(t)^2 - 2y_1(t) + y_2{}''(t)\right)\epsilon^2 + + \dots = -y_0{}''(x).$$

To order ϵ^0, we have

$$y_0'' + 1 = 0,$$

whose solution is

$$y_0 = t - \frac{1}{2}t^2.$$

To order ϵ, we get

$$y_1'' = 2y_0 = 2t - t^2,$$

whose solution is

$$y_1 = \frac{1}{12}\left(4t^3 - t^4\right).$$

To order ϵ^2, we get

$$y_2'' = 2y_1 - 3y_0^3 = \frac{1}{12}t^2\left(7t^2 - 28t + 36\right),$$

whose solution is

$$y_2 = \frac{1}{360}\left(-7t^6 + 42t^5 - 90t^4\right).$$

The second-order approximation is then

$$y \sim t - \frac{1}{2}t^2 + \frac{\epsilon}{12}\left(4t^3 - t^4\right) + \frac{\epsilon^2}{360}\left(-7t^6 + 42t^5 - 90t^4\right).$$

B.3 Non regular techniques

Let us consider the following differential equation [0, 1]

$$(x + \epsilon f)f' + f = 1,$$

with boundary condition $f[1] = 2$. Note that at $x = -\epsilon f$, the differential problem becomes singular. We use the following expansion

$$f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \dots$$

After substitution, we find that to order 0, we have

$$-1 + f_0 + x f_0' = 0,$$

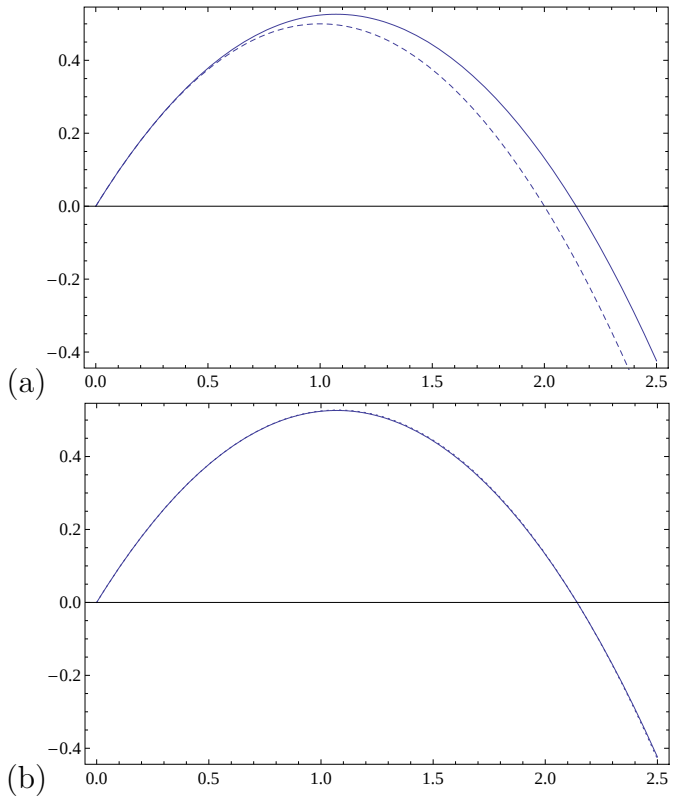

Figure B.1: *Solution to Equation (B.4); dashed line: numerical solution, dashed line (a) solution to order ϵ^0; dotted line (b) solution to order ϵ. Computation done for $\epsilon = 0.1$.*

subject to the condition $f_0(1) = 2$, which yields: $f_0(x) = (1+x)/x$. To order 1, we find

$$f_1 + x f_1' = \frac{1+x}{x^3},$$

subject to the condition $f_1(1) = 0$, which gives: $f_1(x) = (3x^2 - 2x - 1)/(2x^3)$. To order 1, we get

$$9 + \frac{4}{x} + 2x^4 f_2 + 2x^5 f_2' = x(2+3x),$$

subject to the condition $f_2(1) = 0$, which gives: $f_2(x) = (1+3x-x^2-3x^3)/(2x^5)$. We finally obtain

$$f(x) = \frac{1+x}{x} + \epsilon \frac{3x^2 - 2x - 1}{2x^3} + \epsilon^2 \frac{1+3x-x^2-3x^3}{2x^5} + o(\epsilon^2). \tag{B.5}$$

This approximation is asymptotic when x is fixed and $\epsilon \to 0$, but is no longer asymptotic when $x = \mathcal{O}(\epsilon^{1/2})$. Indeed, the second term in the approximation, which should be $O(\epsilon)$ becomes $O(1)$. To address this issue more carefully, we

can compare the approximate solution with the exact solution. The latter could be easily obtained by making use of $(x+\epsilon f)f' + f = 1$, which is equivalent to $\epsilon\frac{1}{2}(f^2)' + (xf)' = 1$. It is easy to integrate this equation: $\epsilon\frac{1}{2}f^2 + xf = x + c$, with c a constant. We find

$$f(x) = \frac{\sqrt{x^2 + 2\epsilon x + 4\epsilon^2 + 2\epsilon} - x}{\epsilon}.$$

The solution comparison reported on Fig. B.2 shows that the approximate solution diverges when approaching the origin point, whereas the exact solution does not do so. The approximate solution is singular at 0.

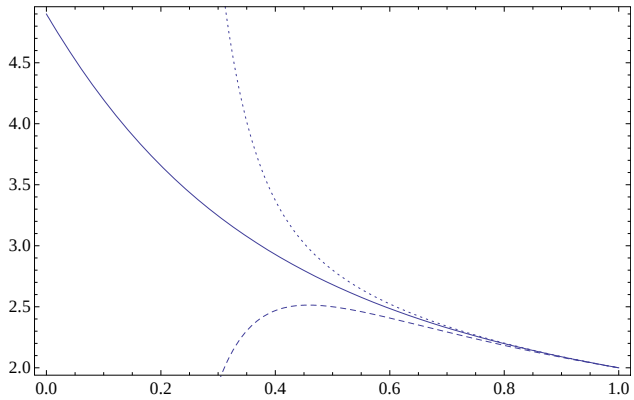

Figure B.2: *Solution to Equation* $(x+\epsilon f)f' + f = 1$. *Solid line: exact solution. Dashed line: approximate solution to ordre 1. Dotted line: approximate solution to ordre 2. Computation done for* $\epsilon = 0.1$.

We can get around this delicate issue using two different methods.

B.3.1 Stretched-coordinate method

We make use of the two following expansions

$$f(x,\epsilon) = f_0(s) + \epsilon f_1(s) + \ldots,$$
$$x(s,\epsilon) = s + \epsilon x_1(s) + \ldots,$$

with f_0 that must be uniformly asymptotic over $[0,1]$. The differential operator

$$\frac{\mathrm{d}}{\mathrm{d}x} = \frac{\mathrm{d}s}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}s} = \frac{1}{\mathrm{d}x/\mathrm{d}s}\frac{\mathrm{d}}{\mathrm{d}s} = (1 - \epsilon x_1' + \epsilon^2(x_1'^2 - x_2')\ldots)\frac{\mathrm{d}}{\mathrm{d}s}.$$

To order 0, we find

$$sf_0' + f_0 = 1,$$

with $f_0(1) = 2$, which yields: $f_0(s) = (1+s)/s$. To order ϵ, we get:

$$f_1 + sf_1' + (f_0 + x_1)f_0' - sf_0'x_1' = 0,$$

subject to boundary conditions

$$\begin{aligned} 2 &= f_0(s) + \epsilon f_1(s) + \dots \\ &= f_0(1 - \epsilon x_1(s)) + \epsilon f_1(1 - \epsilon x_1(s)) + \dots \\ &= f_0(1) + \epsilon \left(-x_1(1)f_0'(1) + f_1(1)\right) + O(\epsilon^2), \\ 1 &= s + \epsilon x_1(s) + \dots . \end{aligned}$$

We then derive $f_1(1) = -x_1(1)$. Substituting f_0 into this expression leads to

$$f_1 + sf_1' = \frac{x_1}{s^2} - \frac{x_1'}{s} + \frac{1}{s^2} + \frac{1}{s^3}, \tag{B.6}$$

One way of proceeding is to select x_1 such that the governing equation of f_1 is homogeneous. Solving

$$\frac{x_1}{s^2} - \frac{x_1'}{s} + \frac{1}{s^2} + \frac{1}{s^3} = 0$$

gives us

$$x_1 = \frac{3s^2 - 2s - 1}{2s}.$$

Integrating Equation (B.6) provides $f_1 = 0$. When we invert $x = s + \epsilon x_1(s)$, we find

$$s = \frac{-x + \epsilon + \sqrt{x^2 + 4\epsilon^2 - 2(x+1)\epsilon}}{3\epsilon - 2},$$

which, once substituted into the equation of f_0, gives us

$$f \sim \frac{x + \sqrt{x^2 + 4\epsilon^2 - 2(x+1)\epsilon}}{\epsilon},$$

which is, in fact, identical to the analytical solution.

There is no unique choice of x_1. We could have proceeded differently. For instance, we can integrate Equation (B.6) easily

$$(sf_1)' = \left(-\frac{x_1}{s} - \frac{1}{s} - \frac{1}{2s^2}\right)',$$

that is,

$$f_1 = \frac{A}{s} - \frac{x_1}{s^2} - \frac{1}{s^2} - \frac{1}{2s^3},$$

for which the boundary conditions yield $A = 0$. To get rid of the singularities (i.e., terms of order of magnitude larger than $1/x$), we set

$$x_1 = -\frac{1+2s}{2s},$$

which yields $f_1(s) = 3/(2s)$. We can invert $x = s + \epsilon x_1(s)$ and substitute into f_0

$$f(x) \sim \frac{x + \epsilon + \sqrt{x^2 + 2\epsilon x + \epsilon(\epsilon+2)} + 2}{x + \epsilon + \sqrt{x^2 + 2\epsilon x + \epsilon(\epsilon+2)}} = -\frac{x}{\epsilon} + \frac{1}{\epsilon}\sqrt{x^2 + 2\epsilon x + \epsilon(\epsilon+2)}.$$

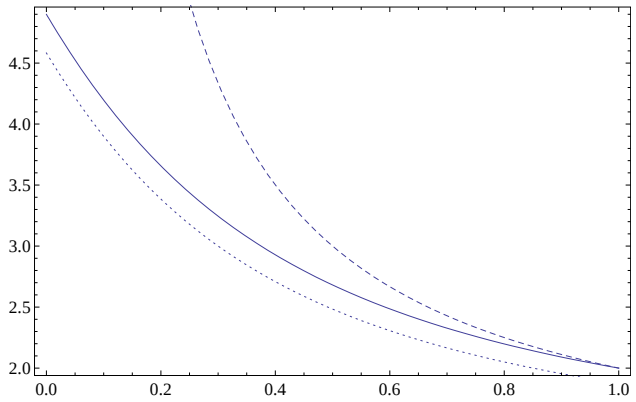

Figure B.3: *Solution to Equation* $(x + \epsilon f)f' + f = 1$. *Solid line: exact solution. Dashed line: approximate solution to ordre 1. Dotted line: approximate solution to ordre 2. Computation done for* $\epsilon = 0.1$.

B.3.2 Matched perturbation technique

The approximate solution is no longer valid for $x = \mathcal{O}(\epsilon^{1/2})$ where $f = \mathcal{O}(\epsilon^{-1/2})$. This leads us to make use of new variables, which will be used for the *inner solution*, i.e., the solution close to the singular point:

$$\begin{aligned} x &= \epsilon^{1/2}\xi, \\ f_i(x) &= \epsilon^{-1/2}F_0(\xi) + F_1(\xi) + \epsilon^{1/2}F_2(\xi) + \dots. \end{aligned}$$

Since $\mathrm{d}/\mathrm{d}x = \epsilon^{-1/2}\mathrm{d}/\mathrm{d}\xi$, we deduce that to order $\epsilon^{-1/2}$, we have

$$F_0 + \xi F0' + F_0F_0' = 0,$$

whose general solution is

$$F_0 = \sqrt{\xi^2 + A_0} - \xi,$$

with A_0 a constant of integration. To order ϵ^0, we get

$$-1 + F_1 + F_1F_0' + \xi F_1' + F_0F_1' = 0,$$

whose general solution is

$$F_1 = \frac{A_1 + \xi}{\sqrt{\xi^2 + A_0}},$$

with A_1 a constant of integration To order $\epsilon^{1/2}$, we have

$$F_2 + F_2F_0' + F_1F_1' + \xi F_2' + F_0F_2' = 0,$$

whose general solution is

$$F_2 = \frac{-A_1^2 - 2\xi A_1 + 2A_2\xi^2 + A_0 + 2A_0A_2}{2\left(\xi^2 + A_0\right)^{3/2}},$$

with A_2 a constant of integration.

We now have to determine the constants of integration. Take a closer look at the *outer solution*

$$f(x) = \frac{1+x}{x} + \epsilon\frac{3x^2 - 2x - 1}{2x^3} + O(\epsilon^2).$$

The change of variable $x = \epsilon^{1/2}\xi$ shows that

- to order $\epsilon^{-1/2}$ and in the limit $\xi \to \infty$, we have $f_{\epsilon^{-1/2}} \sim \xi^{-1}$ while $F_0 \sim A_0/(2\xi)$ hence $A_0 = 2$;
- to order ϵ^0 and in the limit $\xi \to \infty$, we have $f_{\epsilon^0} \sim 1$ while $F_1 \sim 1$ hence we set $A_1 = 0$;
- to order $\epsilon^{1/2}$ and in the limit $\xi \to \infty$, we have $f_{\epsilon^{1/2}} \sim 3/(2\xi)$ while $F_2 \sim A_2/(\xi)$ hence $A_2 = 3/2$.

The inner solution is

$$f_i(\xi) = \epsilon^{-1/2}\left(\sqrt{\xi^2+2} - \xi\right) + \frac{\xi}{\sqrt{\xi^2 + A_0}} + \epsilon^{1/2}\frac{3\xi^2 + 8}{2\left(\xi^2+2\right)^{3/2}},$$

while the outer solution f_e is given by (B.5). The composite solution is

$$f = f_i + f_e - f_r,$$

with f_r the matching value between f_i and f_e

$$f_r = \lim_{\xi\to\infty} f_i = \epsilon^{-1/2}\xi^{-1} + 1 = \frac{1}{x} + 1.$$

We note that $f_e = f_r$. The solution is plotted on Fig. B.4. Note that reasonably good agreement is obtained.

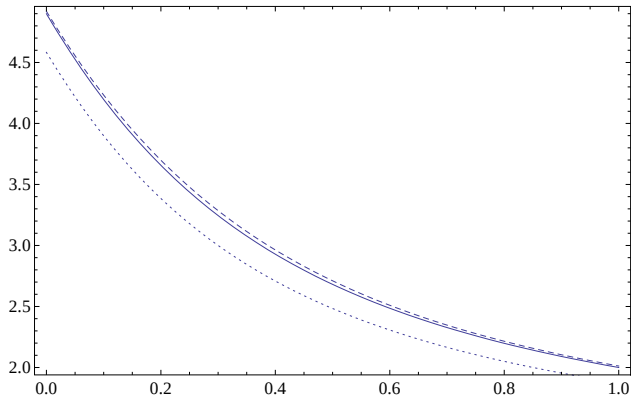

Figure B.4: *Solution to Equation* $(x + \epsilon f)f' + f = 1$. *Solid line: exact solution. Dashed line: approximate solution to ordre* $\epsilon^{1/2}$. *Dotted line: approximate solution to ordre 1 using the stretched coordinate method. Computation done for* $\epsilon = 0.1$.

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