Lecture Notes on Mathematical Modelling From Applied Sciences to Complex Systems

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Lecture Notes on Mathematical Modelling From Applied Sciences to Complex Systems

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Preface

The Lecture Notes collected in this book refer to a university course delivered at the Politecnico of Torino to students of the Master Graduation in Mathematical Engineering. Ph.D. students attending programs in engineering sciences have been attending the same lectures.

The monograph corresponds to the first part of the course devoted to modelling issues to show how the application of models to describe real world phenomena generates mathematical problems to be solved by appropriate mathematical methods. Mathematical models are quite simple being proposed with tutorial aims.

The contents are developed through four chapters. The first one proposes an introduction to the science of mathematical modelling focusing on the three representation scales of physical reality: microscopic, macroscopic and statistical over the microscopic states. The three chapters which follow deal with the derivation and applications of models related to each of the aforementioned scales. Different mathematical structures correspond to each scale. Specifically models at the microscopic scale are generally stated in terms of ordinary differential equations, while models at the macroscopic scale are stated in terms of partial differential equations. Models of the mathematical kinetic theory, presented in Chapter 4, are stated in terms of integro-differential equations.

The above different structures generate a variety of analytic and computational problems. The contents are devoted to understand how computational methods can be developed starting from an appropriate discretization of the dependent variables.

The Lecture Notes look at applications focussing on modelling and computational issues, while the pertinent literature on analytic methods is brought to the attention of the interested reader for additional education.

After the above introduction to the contents and aims of the Lecture Notes, a few remarks are stated to make a little more precise the guidelines followed by the authors.

• All real systems can be observed and represented at different scales by mathematical equations. The selection of a scale with respect to others belong, on one side, to the strategy of the scientists

in charge of deriving mathematical models, and on the other hand to the specific application of the model.

• Systems of the real world are generally nonlinear. Linearity has to be regarded either as a very special case, or as an approximation of physical reality. Then methods of nonlinear analysis need to be developed to deal with the application of models. Computational methods are necessary to solve mathematical problems generated by the application of models to the analysis and interpretation of systems of real world.

• Computational methods can be developed only after a deep analysis of the qualitative properties of a model and of the related mathematical problems. Different methods may correspond to different models and problems.

• Modelling is a science which needs creative ability linked to a deep knowledge of the whole variety of methods offered by applied mathematics. Indeed, the design of a model has to be precisely related to the methods to be used to deal with the mathematical problems generated by the application of the model.

• Modeling systems of the inert matter can generally take advantage of first principles related to well defined physical theories. On the other hand, models of the living matter need looking at the complexity of living entities and at their ability to express specific strategies.

These Lectures Notes attempt to provide an introduction to the above issues and will exploit the use of electronic diffusion to update periodically the contents also on the basis of interactions with students. The authors aim at taking advantage of suggestions, generally useful, from students involved in the master graduation in mathematics for engineering sciences. This edition is a revisiting of the Lecture Notes published by SIMAI with the slightly different title. The main novelty consists in enlarging the horizons of applied mathematics to modeling and simulation of living, and hence complex, living systems.

Nicola Bellomo, Elena De Angelis, Marcello Delitala

Chapter 1

An Introduction to the Science of Mathematical Modelling

1.1 An Intuitive Introduction to Modelling

The analysis of systems of applied and natural sciences, for instance technology, economy, biology etc., needs a constantly growing use of methods of mathematics and computer sciences. In fact, once a physical system has been observed and phenomenologically analyzed, it is often useful to use mathematical models to describe its evolution in time and space. Indeed, the interpretation of systems and phenomena, which occasionally show complex features, is generally developed on the basis of methods which organize their interpretation toward simulation. When simulations related to the behavior of the real system are available and reliable, it may be possible, in most cases, to reduce time devoted to observation and experiments.

Bearing in mind the above reasoning, one can state that there exists a strong link between applied sciences and mathematics represented by mathematical models designed and applied, with the aid of computer sciences and devices, to the simulation of systems of real world. The term mathematical sciences refers to various aspects of mathematics, specifically analytic and computational methods, which both cooperate to the design of models and to the development of simulations.

Before going on with specific technical aspects, let us pose some preliminary questions:

1 • What is the aim of **mathematical modelling**, and what is a mathematical model ?

2 • There exists a link between **models** and **mathematical structures** ?

3 • There exists a correlation between **models** and **mathematical methods** ?

4 • Which is the relation between **models** and **computer sciences** ?

Moreover:

5 • Can mathematical **models** contribute to a deeper understanding of **physical reality** ?

6 • Is it possible to reason about a **science of mathematical modelling** ?

7 • Can *education in mathematics* take some advantage of the above mentioned science of mathematical modelling ?

8 • Is it possible designing models of living systems by an approach that retains the complexity of the living matter ?

Additional questions may be posed. However, it is reasonable to stop here considering that specific tools and methods are needed to answer precisely to the above questions. A deeper understanding of the above topics will be achieved going through the chapters of these Lecture Notes also taking advantage of the methods which will be developed in the next chapters. Nevertheless an intuitive reasoning can be developed and some preliminary answers can be given:

• Mathematical models are designed to describe physical systems by equations or, more in general, by logical and computational structures.

• The above issue indicates that **mathematical modelling** operates as a science by means of methods and mathematical structures with well defined objectives.

• Intuitively, it can be stated that education in mathematics may take advantage of the science of mathematical modelling. Indeed, linking mathematical structures and methods to the interpretation and simulation of real physical systems is already a strong motivation related to an inner feature of mathematics, otherwise too much abstract. Still, one has to understand if modelling provides a method for reasoning about mathematics.

• At this preliminary stage, it is difficult to reason about the possibility that mathematical models may contribute to a deeper understanding of physical reality. At present, we simply trust that this idea will be clarified all along the contents of these Lectures Notes. The goal consists in depicting, by mathematical models, behaviors that have not yet been observed in reality.

• Far more difficult is a reply, although preliminary, to the last question 8. We simply observe that deterministic causality principles are lost in the case of living system, as observed by May (2004) and Reed (2004). This delicate matter will be treated more deeply in the last chapter of this monograph.

This chapter has to be regarded as an introduction to the science of mathematical modelling which will be developed through these Lecture Notes with reference to well defined mathematical structures and with the help of several applications intended to clarify the above concepts. Specifically it deals with general introduction to mathematical modelling, and is organized into six more sections which follow this introduction:

– Section 1.2 deals with the presentation of some simple examples of mathematical models which act as a preliminary reference for the various concepts introduced in the following sections. Then, the definition of mathematical model is given as an equation suitable to define the evolution in time and space of the variable charged to describe (at each specific scale) the physical state of the real system.

– Section 1.3 deals with a preliminary aspect of the modelling process, that is the identification of the representation scales, microscopic, macroscopic and statistical, needed to observe and represent a real system. The above concepts are related to a variety of examples of models at each one of the above scales. Simple examples are chosen with tutorial aims, while more sophisticated models are treated in the next chapters.

– Section 1.4 deals with the dimensional analysis of mathematical models. It is shown how writing the model in terms of dimensionless variables is useful towards computational analysis and allows to extract suitable scaling parameters which can be properly used towards a qualitative understanding of the properties of the model.

– Section 1.5 analyzes the various concepts proposed in the preceding sections by means of models of vehicular traffic flow. Such a system can be described by different models and scales, all of them are analyzed with reference to the above mentioned definitions and scaling methods.

– Section 1.6 deals with a classification of models and mathematical problems still referring to the various aspects of the modelling process dealt with in the preceding sections.

– Section 1.7 provides a description and critical analysis of the contents of this chapter with special attention to complexity problems. This section introduces the contents of the last chapter, devoted to the modeling of living systems.

1.2 Elementary Examples and Definitions

This section deals with the description of three simple examples of mathematical models which will be a technical reference for the definitions given in the following sections. The models are derived by an intuitive approach, while well defined modelling methods will be developed in the chapters which follow and applied to the design of relatively more sophisticated models.

The first example describes linear oscillations of a mass constrained to move along a line, while the second one refers to modelling heat diffusion phenomena. The third example is a generalization of the second one to a nonlinear case. As already mentioned, very simple examples are selected to reason, according to tutorials aims, with classification of models and mathematical structures.

Example 1.2.1
Linear Elastic Wire-Mass System

Consider, with reference to Figure 1.2.1, a mechanical system constituted by a mass m constrained to translate along an horizontal line, say the x-axis. The location of the mass is identified by the coordinate of its center of mass P, which is attached to an elastic wire stretched with ends in A and P. The assumptions defining the mechanical model are the following:

- The system behaves as a point mass with localization identified by the variable x.
- The action of the wire is a force directed toward the point A with module: $T = k\,x$.
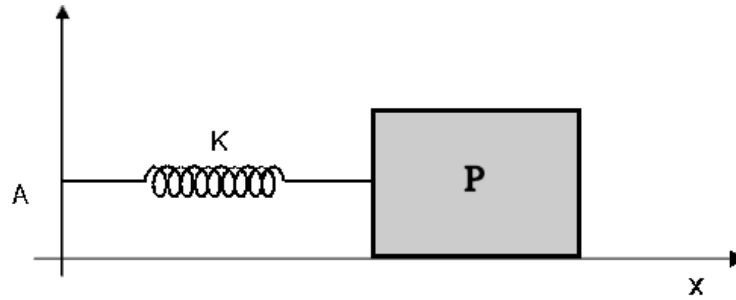
Figure 1.2.1 – Elastic wire–mass system

• Friction forces are negligible with respect to the action of the wire.

Application of Newton's principles of classical mechanics yields:

$$m\,\frac{d^2x}{dt^2} = -kx\,. \tag{1.2.1}$$

The mathematical model is an evolution equation for the following vector variable:

$$\mathbf{u} = \left(u_1 = x\,,\ u_2 = \frac{dx}{dt}\right)\,. \tag{1.2.2}$$

Using the above variables, the second order ordinary differential equation (1.2.1) reads:

$$\begin{cases} \dfrac{du_1}{dt} = u_2\,, \\[2mm] \dfrac{du_2}{dt} = -\dfrac{k}{m}u_1\,, \end{cases} \tag{1.2.3}$$

which is a linear equation.

□

<div align="center">

Example 1.2.2

Linear Heat Diffusion Model
</div>

Consider the one-dimensional linear heat diffusion model in a rod. The assumptions defining the mechanical model are the following:

• The state of the system is described by the temperature $u = u(t, x)$ along the axis of the rod identified by the variable $x \in [0, 1]$. Variations orthogonal to the axis of the rod are neglected as the walls of the rod are perfectly isolated.

• The heat flow q per unit area is proportional to the temperature gradient:

$$q = -h_0\,\frac{\partial u}{\partial x}\,, \tag{1.2.4}$$

where h_0 is the heat conduction coefficient.

• The material properties of the conductor are identified by the heat conduction coefficient h_0 and heat capacity c_0.

The mathematical model can be obtained equating the net heat flux in a volume element to the rate of increase of the heat capacity in the volume. Let q^+ and q^- be, respectively, the ingoing and outgoing heat fluxes for unit area, see Figure 1.2.2 The above balance writes:

$$c_0\, A \frac{\partial u}{\partial t}\, dx = -A(q^+ - q^-) = -A\, \frac{\partial q}{\partial x} dx\,, \qquad (1.2.5)$$

where A is the cross section of the rod.
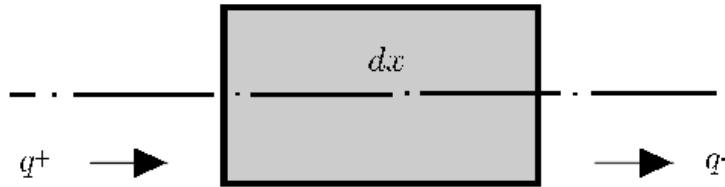
Figure 1.2.2 – Diffusion in one space dimension

Using Eq. 1.2.4 yields:

$$\frac{\partial u}{\partial t} = k_0 \frac{\partial^2 u}{\partial x^2}\,, \qquad k_0 = \frac{h_0}{c_0}\,. \qquad (1.2.6)$$

The above model can also be used to describe the steady temperature distribution, which is obtained equating to zero the right-hand side term:

$$k_0 \frac{d^2 u}{dx^2} = 0\,, \qquad (1.2.7)$$

which can also be written as a system of two coupled equations in normal form:

$$\begin{cases} \dfrac{du}{dx} = v\,, \\[2mm] \dfrac{dv}{dx} = 0\,. \end{cases} \qquad (1.2.8)$$

□

Example 1.2.3
Nonlinear Heat Diffusion Model

Nonlinearity may be related to the modelling of the heat flux phenomenon. For instance, if the heat flux coefficient depends on the temperature, say $h = h(u)$, the same balance equation generates the following model:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left[k(u)\frac{\partial u}{\partial x}\right], \qquad k(u) = \frac{h(u)}{c_0}. \tag{1.2.9}$$

$\square$

The reader with a basic knowledge of elementary theory of differential equations will be soon aware that the above two simple models generate interesting mathematical problems. In fact, Model 1.2.1 needs initial conditions for $t = t_0$ both for $u_1 = u_1(t)$ and $u_2 = u_2(t)$, while Models 1.2.2 and 1.2.3 need initial conditions at $t = t_0$ and boundary conditions at $x = 0$ and $x = 1$ for $u = u(t, x)$.

The solution of the above mathematical problems ends up with simulations which visualize the behavior of the real system according to the description of the mathematical model.

After the above examples, a definition of **mathematical model** can be introduced. This concept needs some preliminary definitions referring to:

- *Independent variables*, generally time and space.

- *State variables* which are the *dependent variables*, that take values corresponding to the independent variables.

Then the following concept can be introduced:

- *Mathematical model*, that is a set of equations which define the evolution of the state variable over the dependent variables.

The general idea is to observe the phenomenology of a real system in order to extract its main features and to provide a model suitable to describe the evolution in time and space of its relevant aspects. Bearing this in mind, the following definitions are proposed:

Independent variables

*The evolution of the real system is referred to the **independent variables** which, unless differently specified, are time t, defined in an interval ($t \in [t_0, T]$), which refers the observation period; and space $\mathbf{x}$, related to the volume $\mathcal{V}$, ($\mathbf{x} \in \mathcal{V}$) which contains the system.*

State variable

The **state variable** is the finite dimensional vector variable

$$\mathbf{u} = \mathbf{u}(t, \mathbf{x}) : \quad [t_0, T] \times \mathcal{V} \to \mathbb{R}^n \,, \tag{1.2.10}$$

where $\mathbf{u} = \{u_1, \dots, u_i, \dots, u_n\}$ is deemed as sufficient to describe the evolution of the physical state of the real system in terms of the **independent variables.**

Mathematical model

A **mathematical model** of a real physical system is an **evolution equation** suitable to define the evolution of the state variable $\mathbf{u}$ in charge to describe the physical state of the system itself.

In order to handle properly a mathematical model, the number of equations and the dimension of the state variable must be the same. In this case the model is defined consistent:

Consistency

The mathematical model is said to be **consistent** if the number of unknown dependent variables is equal to the number of independent equations.

This means that one has to verify whether an equation belonging to the model can be obtained combining the remaining ones. If this is the case, that equation must be eliminated.

The space variable may be referred to a suitable system of orthogonal axes, $0(x, y, z)$ with unit vectors $\mathbf{i}$, $\mathbf{j}$, $\mathbf{k}$, so that a point $\mathbf{P}$ is identified by its coordinates

$$\mathbf{P} = \mathbf{P}(\mathbf{x}) = x\,\mathbf{i} + y\,\mathbf{j} + z\,\mathbf{k}\,. \tag{1.2.11}$$

The real physical system may be interacting with the outer environment or may be isolated. In the first case the interactions has to be modelled.

Closed and Open Systems

A **real physical system** is **closed** if it does not interact with the outer environment, while it is **open** if it does.

The above definitions can be applied to real systems in all fields of applied sciences: engineering, natural sciences, economy, and so on. Actually, almost all systems have a continuous distribution in space. Therefore, their discretization, that amounts to the fact that $\mathbf{u}$ is a finite dimensional vector, can be regarded as an **approximation** of physical reality.

In principle, one can always hope to develop a model which can reproduce exactly physical reality. On the other hand, this idealistic program cannot be practically obtained considering that real systems are characterized by an enormous number of physical variables. This reasoning applies to Example 1.2.1, where it is plain that translational dynamics in absence of frictional forces is only a crude approximation of reality. The observation of the real behavior of the

system will definitively bring to identify a gap between the observed values of u_1 and u_2 and those predicted by the model.

Uncertainty may be related also to the mathematical problem. Referring again to the above example, it was shown that the statement of mathematical problems need u_{10} and u_{20}, i.e. the initial position and velocity of P, respectively. Their measurements are affected by errors so that their knowledge may be uncertain.

In some cases this aspect can be dealt with by using in the model and/or in the mathematical problems randomness modelled by suitable stochastic variables. The solution of the problem will also be represented by random variables, and methods of probability theory will have to be used.

As we have seen, mathematical models are stated in terms of evolution equations. Examples have been given for ordinary and partial differential equations. The above equations cannot be solved without complementing them with suitable information on the behavior of the system corresponding to some values of the independent variables. In other words the solution refers to the mathematical problem obtained linking the model to the above mentioned conditions. Once a problem is stated suitable mathematical methods have to be developed to obtain solutions and simulations, which are the prediction provided by the model.

The analysis of the above crucial problems, which is a fundamental step of applied mathematics, will be dealt with in the next chapters with reference to specific classes of equations.

1.3 Modelling Scales and Representation

As we have seen by the examples and definitions proposed in Section 1.2, the design of a mathematical model consists in deriving an evolution equation for the dependent variable, which may be called state variable, which describes the physical state of the real system, that is the object of the modelling process.

The selection of the state variable and the derivation of the evolution equation starts from the phenomenological and experimental observation of the real system. This means that the first stage of the whole modelling method is the selection of the observation scale. For instance one may look at the system by distinguishing all its microscopic components, or averaging locally the dynamics of all microscopic components, or even looking at the system as a whole by averaging their dynamics in the whole space occupied by the system.

For instance, if the system is a gas of particles inside a container, one may either model the dynamics of each single particle, or consider some macroscopic quantities, such as mass density, momentum and energy, obtained averaging locally (in a small volume to be properly defined: possibly an infinitesimal volume) the behavior of the particles. Moreover, one may average the physical variables related to the microscopic state of the particles and/or the local macroscopic variables over the whole domain of the container thus obtaining gross quantities which represent the system as a whole.

Specifically, let us concentrate the attention to the energy and let us assume that energy may be related to temperature. In the first case one has to study the dynamics of the particles and then obtain the temperature by a suitable averaging locally or globally. On the other hand, in the other two cases the averaging is developed before deriving a model, then the model should provide the evolution of already averaged quantities. It is plain that the above different way of observing the system generates different models corresponding to different choices of the state variable. Discussing the validity of one approach with respect to the other is definitively a difficult, however crucial, problem to deal with. The above approaches will be called, respectively, ***microscopic modelling*** and ***macroscopic modelling***.

As an alternative, one may consider the microscopic state of each microscopic component and then model the evolution of the statistical distribution over each microscopic description. Then one deals with the ***kinetic type*** (***mesoscopic***) modelling which will be introduced in this chapter and then properly dealt with later in Chapter 4. Modelling by methods of the mathematical kinetic theory requires a detailed analysis of microscopic models for the dynamics of the interacting components of the system, while macroscopic quantities are obtained, as we shall see, by suitable moments weighted by the above distribution function.

This section deals with a preliminary derivation of mathematical framework related to the scaling process which has been described above. This process will ends up with a classification both of state variables and mathematical equations. Simple examples will be given for each class of observation scales and models. The whole topic will be specialized in the following chapters with the aim of a deeper understanding on the aforementioned structures.

Both observation and simulation of system of real world need the definition of suitable observation and modelling scales. Different models and descriptions may correspond to different scales. For instance, if the motion of a fluid in a duct is observed at a microscopic scale, each particle is singularly observed. Consequently the motion can be described within the framework of Newtonian mechanics, namely by ordinary differential equations which relate the force applied to each particle to its mass times acceleration. Applied forces are generated by the external field and by interactions with the other particles.

On the other hand, the same system can be observed and described at a larger scale considering suitable averages of the mechanical quantities linked to a large number of particles, and the model refers to macroscopic quantities such as mass density and velocity of the fluid. A similar definition can be given for the mass velocity, namely the ratio between the momentum of the particles in the reference volume and their mass. Both quantities can be measured by suitable experimental devices operating at a scale of a greater order than the one of the single particle. This class of models is generally stated by partial differential equations.

Actually, the definition of ***small*** or ***large*** scale has a meaning which has to be related to the size of the object and of the volume containing them. For instance, a planet observed as a rigid homogeneous whole is a single object which is small with respect to the galaxy containing the planet, but large with respect to the particles constituting its matter. So that the galaxy can be regarded as a system of a large number of planets, or as a fluid where distances between

planets are neglected with respect to the size of the galaxy. Bearing all above in mind, the following definitions are given:

> **Microscopic scale**
>
> *A real system can be observed, measured, and modelled at the **microscopic scale** if all single objects composing the system are individually considered, each as a whole.*

> **Macroscopic scale**
>
> *A real system can be observed, measured, and modelled at the **macroscopic scale** if suitable averaged quantities related to the physical state of the objects composing the system are considered.*

> **Mesoscopic scale**
>
> *A real system can be observed, measured, and modelled at the **mesoscopic (kinetic) scale** if it is composed by a large number of interacting objects and the macroscopic observable quantities related to the system can be recovered from moments weighted by the distribution function of the state of the system.*

As already mentioned, microscopic models are generally stated in terms of ordinary differential equations, while macroscopic models are generally stated in terms of partial differential equations. This is the case of the first two examples proposed in the section which follows. The contents will generally be developed, unless otherwise specified, within the framework of deterministic causality principles. This means that once a cause is given, the effect is deterministically identified, however, even in the case of deterministic behavior, the measurement of quantities needed to assess the model or the mathematical problem may be affected by errors and uncertainty.

The above reasoning and definitions can be referred to some simple examples of models, this also anticipating a few additional concepts which will be dealt in a relatively deeper way in the chapters which follow.

Example 1.3.1
Elastic Wire-Mass System with Friction

Following Example 1.2.1, let us consider a mechanical system constituted by a mass m constrained to translate along a horizontal line, say the x-axis. The location of the mass is identified by the coordinate of its center of mass P, which is attached to an elastic wire stretched with ends in A and P. The following assumption needs to be added to those of Model 1.2.1 defining the mechanical model:

• Friction forces depend on the p-th power of the velocity and are direct in opposition with it.

Application of Newton's model yields:

$$m \frac{d^2 x}{dt^2} = -kx - c \left(\frac{dx}{dt} \right)^p .$$
(1.3.1)

The mathematical model, according to the definitions proposed in Section 1.2, is an evolution equation for the variable **u** defined as follows:

$$\mathbf{u} = \left(u_1 = x \, , \, u_2 = \frac{dx}{dt} \right) .$$
(1.3.2)

Using the above variables, the second order ordinary differential equation (1.3.1) can be written as a system of two first order equations:

$$\begin{cases} \dfrac{du_1}{dt} = u_2 \, , \\[2mm] \dfrac{du_2}{dt} = -\dfrac{k}{m} u_1 - \dfrac{c}{m} u_2^p . \end{cases}$$
(1.3.3)

$\square$

The above example has shown a simple model that can be represented by an ordinary differential equation, Eq. (1.3.3), which is nonlinear for values of p different from zero or one.

Observing Eq. (1.3.3), one may state that the model is consistent, namely there are two independent equations corresponding to the two components of the state variable. The physical system is observed singularly, i.e. at a microscopic scale, while it can be observed that the model is stated in terms of ordinary differential equations.

Linearity of the model is obtained if $c = 0$. On the other hand, if k is not a constant, but depends on the elongation of the wire, say $k = k_0 x^q$ a nonlinear model is obtained:

$$\begin{cases} \dfrac{du_1}{dt} = u_2 \, , \\[2mm] \dfrac{du_2}{dt} = -\dfrac{k_0}{m} u_1^{q+1} . \end{cases}$$
(1.3.4)

Independently of linearity properties, which will be properly discussed in the next Chapter 2, the system is isolated, namely it is a closed system. One should add, in the case of open systems, to the second equation the action of the outer environment over the inner system. A simple example is the following:

$$\begin{cases} \dfrac{du_1}{dt} = u_2 \, , \\[2mm] \dfrac{du_2}{dt} = -\dfrac{k_0}{m} u_1^{q+1} + \dfrac{1}{m} F(t) \, , \end{cases}$$
(1.3.5)

where $F = F(t)$ models the above mentioned action.

The above models, both linear and nonlinear, have been obtained linking a general background model valid for large variety of mechanical systems, that is the fundamental principles of Newtonian mechanics, to a phenomenological model suitable to describe, by simple analytic expressions, the elastic behavior of the wire. Such models can be refined for each particular system by relatively more precise empirical data obtained by experiments.

The example which follows is developed at the macroscopic scale and it is related to the heat diffusion model we have seen in Section 1.2. Here, we consider a mathematical model suitable to describe the diffusion of a pollutant of a fluid in one space dimension.

As we shall see, an evolution equation analogous to the one of Example 1.2.2 will be obtained. First the linear case is dealt with, then some generalizations, i.e. non linear models and diffusion in more than one space dimensions, are described.

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Example 1.3.2

Linear Pollutant Diffusion Model

</div>

Consider a duct filled with a fluid at rest and a pollutant diffusing in the duct in the direction x of the axis of the duct. The assumptions which define the mechanical model are the following:

• The physical quantity which defines the state of the system is the concentration of pollutant:

$$c = c(t, x) : \qquad [t_0, T] \times [0, \ell] \to \mathbb{R}_+ \,, \tag{1.3.6}$$

variations of c along coordinates orthogonal to the x-axis are negligible. The mass per unit volume of the pollutant is indicated by ρ_0 and is assumed to be constant.

• There is no dispersion or immersion of pollutant at the walls.

• The fluid is steady, while the velocity of diffusion of the pollutant is described by a phenomenological model which states that the diffusion velocity is directly proportional to the gradient of c and inversely proportional to c.

The evolution model, i.e. an evolution equation for c, can be obtained exploiting mass conservation equation. In order to derive such equation let consider, with reference to Figure 1.2.2, the flux $q = q(t, x)$ along the duct and let q^+ and q^- be the inlet and outlet fluxes, respectively. Under suitable regularity conditions, which are certainly consistent with the physical system we are dealing with, the relation between the above fluxes is given by:

$$q^+ = q^- + \frac{\partial q}{\partial x} \, dx \,. \tag{1.3.7}$$

A balance equation can be written equating the net flux rate to the increase of mass in the volume element $A \, dx$, where A is the section of the duct. The following equation is obtained:

$$\rho_0 \, A \, \frac{\partial c}{\partial t} \, dx + A \, \frac{\partial (cv)}{\partial x} dx = 0 \,, \tag{1.3.8}$$

where v is the diffusion velocity which, according to the above assumptions, can be written as follows:

$$v = -\frac{h_0}{c}\frac{\partial c}{\partial x}\,, \qquad (1.3.9)$$

and h_0 is the diffusion coefficient.

Substituting the above equation into (1.3.8) yields

$$\frac{\partial c}{\partial t} = k_0 \frac{\partial^2 c}{\partial x^2}\,, \qquad k_0 = \frac{h_0}{\rho_0}\,, \qquad (1.3.10)$$

which is a linear model.

□

Nonlinearity related to the above model may occur when the diffusion coefficient depends on the concentration. This phenomenon generates the nonlinear model described in the following example.

Example 1.3.3
Nonlinear Pollutant Diffusion Model

Consider the same phenomenological model where, however, the diffusion velocity depends on the concentration according to the following phenomenological model:

$$v = -h_0 \frac{h(c)}{c}\frac{\partial c}{\partial x}\,, \qquad (1.3.11)$$

where $h(c)$ describes the behavior of the diffusion coefficient with c. The model writes as follows:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(k(c)\frac{\partial c}{\partial x}\right)\,, \qquad k(c) = \frac{h(c)}{\rho_0}\,. \qquad (1.3.12)$$

Phenomenological interpretations suggest:

$$k(0) = k(c_M) = 0\,, \qquad (1.3.13)$$

where c_M is the maximum admissible concentration. For instance:

$$k(c) = c(c_M - c)\,, \qquad (1.3.14)$$

so that the model reads:

$$\frac{\partial c}{\partial t} = c(c_M - c)\frac{\partial^2 c}{\partial x^2} + (c_M - 2c)\left(\frac{\partial c}{\partial x}\right)^2\,. \qquad (1.3.15)$$

□

The above diffusion model can be written in several space dimensions. For instance, technical calculations generate the following linear model:

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Example 1.3.4

Linear Pollutant Diffusion in Space

</div>

Let us consider the linear diffusion model related to Example 1.3.2, and assume that diffusion is isotropic in all space dimensions, and that the diffusion coefficient does not depend on c. In this particular case, simple technical calculations yield:

$$\frac{\partial c}{\partial t} = k_0 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) c = k_0 \, \Delta c \,. \qquad (1.3.16)$$

The steady model is obtained equating to zero the right-hand side of (1.3.16):

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) c = k_0 \, \Delta c = 0 \,. \qquad (1.3.17)$$

□

The above (simple) examples have given an idea of the microscopic and macroscopic modelling. A simple model based on the mesoscopic description will be now given and critically analyzed. Specifically, we consider an example of modelling social behaviors such that the microscopic state is defined by the social state of a certain population, while the model describes the evolution of the probability density distribution over such a state. The above distribution is modified by binary interactions between individuals.

<div align="center">

Example 1.3.5

Population Dynamics with Stochastic Interaction

</div>

Consider a population constituted by interacting individuals, such that:

• The ***microscopic state*** of each individual is described by a real variable $u \in [0, 1]$, that is a variable describing its main physical properties and/or social behaviors. As examples, in the case of a population of tumor cells this state may have the meaning of maturation or progression stage, for a population of immune cells we may consider the state u as their level of activation.

• The statistical description of the system is described by the number density functions

$$N = N(t, u) \,, \qquad (1.3.18)$$

which is such that $N(t, u) \, du$ denotes the number of cells per unit volume whose state is, at time t, in the interval $[u, u + du]$.

If n_0 is the number per unit volume of individuals at $t = 0$, the following normalization of N with respect to n_0 can be applied:

$$f = f(t, u) = \frac{1}{n_0} N(t, u) \,. \tag{1.3.19}$$

If f (which will be called **distribution function**) is given, it is possible to compute, under suitable integrability properties, the **size** of the population still referred to n_0:

$$n(t) = \int_0^1 f(t, u) \, du \,. \tag{1.3.20}$$

The evolution model refers to $f(t, u)$ and is determined by the interactions between pairs of individuals, which modify the probability distribution over the state variable and/or the size of the population. The above ideas can be stated in the following framework:

• Interactions between pairs of individuals are homogeneous in space and instantaneous, i.e. without space structure and delay time. They may change the state of the individuals as well as the population size by shifting individuals into another state or by destroying or creating individuals. Only binary encounters are significant for the evolution of the system.

• The rate of interactions between individuals of the population is modelled by the **encounter rate** which may depend on the state of the interacting individuals

$$\eta = \eta(v, w) \,, \tag{1.3.21}$$

which describes the rate of interaction between pairs of individuals. It is the number of encounters per unit time of individuals with state v with individuals with state w.

• The **interaction-transition probability density**

$$A = A(v \to u \,|\, v, w) \,, \tag{1.3.22}$$

gives the probability density distribution of the transition, due to binary encounters, of the individuals which have state v with the individuals having state w that, after the interaction, manufacture individuals with state u.

The product between η and A is the **transition rate**

$$T(v \to u \,|\, v, w) = \eta(v, w) A(v \to u \,|\, v, w) \,. \tag{1.3.23}$$

• The evolution equations for the density f can be derived by balance equation which equates the time derivative of f to the difference between the **gain** and the **loss** terms. The gain term models the rate of increase of the distribution function due to individuals which fall into the state u due to uncorrelated pair interactions. The loss term models the rate of loss in the distribution function of u-individuals due to transition to another state or due to death.

Combining the above ideas yields the following model

$$\frac{\partial f}{\partial t}(t, u) = \int_0^1 \int_0^1 \eta(v, w) A(v \to u \,|v, w) f(t, v) f(t, w) \, dv \, dw$$

$$- f(t, u) \int_0^1 \eta(u, v) f(t, v) \, dv \,. \tag{1.3.24}$$

□

The above example, as simple as it may appear, gives a preliminary idea of the way a kinetic type modelling can be derived. This topic will be properly revisited in Chapter 4. At present we limit our analysis to observing that a crucial role is defined by the modelling of interactions at the microscopic scale which allows the application of suitable balance equation to obtain the evolution of the probability distribution. At present, we can observe that since $A(v \to u \,|v, w)$ is a probability density, it satisfies

$$\int_0^1 A(v \to u \,|v, w) \, du = 1 \,, \quad \forall v, w \in [0, 1] \,. \tag{1.3.25}$$

As a consequence, Eq. (1.3.24) implies

$$\int_0^1 \frac{\partial f}{\partial t}(t, u) = \frac{\partial}{\partial t} \int_0^1 f(t, u) = 0 \,, \quad \forall t \geq 0 \,, \tag{1.3.26}$$

and, due to the normalization,

$$\int_0^1 f(t, u) \, du = 1 \,. \tag{1.3.27}$$

Therefore, the knowledge of f means knowing the time evolution of the moments

$$E^p(t) = \int_0^1 u^p \, f(t, u) \, du \,, \tag{1.3.28}$$

for $p = 1, 2, \ldots$

1.4 Dimensional Analysis for Mathematical Models

Examples 1.2.1 and 1.3.2 can be properly rewritten using dimensionless variables. This procedure should be generally, may be always, applied. In fact, it is always useful, and in some cases necessary, to write models with all independent and dependent variables written in a dimensionless form by referring them to suitable reference variables. These should be properly chosen in a way that the new variables take value in the domains $[0, 1]$ or $[-1, 1]$.

The above reference variables can be selected by geometrical and/or physical arguments related to the particular system which is modelled. Technically, let w_v be a certain variable

(either independent or dependent), and suppose that the smallest and largest value of w_v, respectively w_m and w_M, are identified by geometrical or physical measurements; then the dimensionless variable is obtained as follows:

$$w = \frac{w_v - w_m}{w_M - w_m}\,, \qquad w \in [0, 1]\,. \tag{1.4.1}$$

For instance, if w_v represents the temperature in a solid material, then one can assume $w_m = 0$, and $w_M = w_c$, where w_c is the melting temperature for the solid.

In principle, the description of the model should define the evolution within the domain $[0, 1]$. When this does not occur, then the model should be critically analyzed.

If w_v corresponds to one of the independent space variables, say it corresponds to x_v, y_v, and z_v for a system with finite dimension, then the said variable can be referred to the smallest and to the largest values of each variable, respectively, x_m, y_m, z_m, and x_M, y_M, and z_M.

In some cases, it may be useful referring all variables with respect to only one space variable, generally the largest one. For instance, suppose that $x_m = y_m = z_m = 0$, and that $y_M = ax_M$, and $z_M = bx_M$, with $a, b < 1$, one has

$$x = \frac{x_v}{x_M}\,, \qquad y = \frac{y_v}{x_M}\,, \qquad z = \frac{z_v}{x_M}\,, \tag{1.4.2}$$

with $x \in [0, 1]$, $\quad y \in [0, a]$, $\quad z \in [0, b]$.

Somehow more delicate is the choice of the reference time. Technically, if the initial time is t_0 and t_v is the real time, one may use the following:

$$t = \frac{t_v - t_0}{T_c - t_0}\,, \qquad t \geq 0\,, \tag{1.4.3}$$

where generally one may have $t_0 = 0$. The choice of T_c has to be related to the actual analytic structure of the model trying to bring to the same order the cause and the effect as both of them are identified in the model. For instance, looking at models in Example 1.2.1, the **cause** is identified by the right-hand side term, while the **effect** is the left-hand term. The model should be referred to the **observation time** during which the system should be observed. This time should be compared with T_c.

Bearing all above in mind let us apply the above concepts to the statement in terms of dimensionless variables of the two models described in Examples 1.2.1 and 1.3.2.

_____ ***Example 1.4.1*** _____
Dimensionless Linear Elastic Wire-Mass System

Let us consider the model described in Example 1.2.1, with the addition of the following assumption:

- A constant force F is directed along the x-axis.

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Therefore, the model can written as follows:

$$m \frac{d^2 x_v}{dt_v^2} = F - k x_v \,. \tag{1.4.4}$$

It is natural assuming $\ell = F/k$, $t = t_v/T_c$, and $x = x_v/\ell$. Then the model writes:

$$\frac{m}{kT_c^2} \frac{d^2 x}{dt^2} = 1 - x \,. \tag{1.4.5}$$

Assuming:

$$\frac{m}{kT_c^2} = 1 \quad \Rightarrow \quad T_c^2 = \frac{m}{k} \,, \tag{1.4.6}$$

yields

$$\frac{d^2 x}{dt^2} = 1 - x \,, \tag{1.4.7}$$

which is a second order model.

The evolution can be analyzed in terms of unit of T_c.

□

Example 1.4.2
Linear Dimensionless Pollutant Diffusion Model

Consider the model described in Example 1.3.2 which, in terms of real variables, can be written as follows:

$$\frac{\partial c_v}{\partial t} = k_0 \frac{d^2 c_v}{\partial x_v^2} \,, \qquad k_0 = \frac{h_0}{\rho_0} \,, \tag{1.4.8}$$

It is natural assuming $u = c_v/c_M$, $\quad t = t_v/T_c$, and $x = x_v/\ell$. Then, the model writes:

$$\frac{1}{T_c} \frac{\partial u}{\partial t} = \frac{k_0}{\ell^2} \frac{\partial^2 u}{\partial x^2} \,, \tag{1.4.9}$$

Moreover, taking:

$$\frac{k_0 T_c}{\ell^2} = 1 \quad \Rightarrow \quad T_c = \frac{\ell^2}{k_0}$$

yields

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \,. \tag{1.4.10}$$

□

In particular Eq. (1.4.10) shows that the same model is obtained, after scaling, to describe linear diffusion phenomena in different media. Indeed, only T_c changes according to the material

properties of the media. This means that the evolution is qualitatively the same, but it evolves in time with different speeds scaled with respect to T_c.

Writing a model in terms of dimensionless variables is useful for various reasons, both from analytical point of view and from the computational one, which will be examined in details in the chapters which follow. One of the above motivations consists in the fact that the procedure may introduce a small dimensionless parameter which characterizes specific features of the evolution equation, e.g. nonlinear terms, time scaling, etc. As we shall see in Chapter 2, the above parameters allow the development of perturbation techniques such that the solution can be sought by suitable power expansion of the small parameter.

1.5 Traffic Flow Modelling

Various models have been proposed in the preceding sections corresponding to the microscopic, macroscopic, and kinetic representation. This section will show how the same physical system can be represented by different models according to the selection of different observation scales.

Let us consider the one dimensional flow of vehicles along a road with length ℓ. First the independent and dependent variables which, in a suitable dimension form, can represent the relevant phenomena related to traffic flow are defined, then some specific models will be described.

In order to define dimensionless quantities, one has to identify characteristic time T and length ℓ, as well as maximum density n_M and maximum mean velocity v_M. Specifically:

n_M is the maximum density of vehicles corresponding to bumper-to-bumper traffic jam;

v_M is the maximum admissible mean velocity which may be reached by vehicles in the empty road.

It is spontaneous to assume $v_M T = \ell$, that means that T is the time necessary to cover the whole road length ℓ at the maximum mean velocity v_M. After the above preliminaries, we can now define dimensionless independent and dependent variables.

The dimensionless independent variables are:

• $t = t_r/T$, the dimensionless time variable referred to the characteristic time T, where t_r is the real time;

• $x = x_r/\ell$, the dimensionless space variable referred to the characteristic length of the road ℓ, where x_r is the real dimensional space.

The dimensionless dependent variables are:

• $\rho = n/n_M$, the dimensionless density referred to the maximum density n_M of vehicles;

• $V = V_R/v_M$, the dimensionless velocity referred to the maximum mean velocity v_M, where V_R is the real velocity of the single vehicle;

• $v = v_R/v_M$, the dimensionless mean velocity referred to the maximum mean velocity v_M, where v_R is the mean velocity of the vehicles;

• q, the dimensionless linear mean flux referred to the maximum admissible mean flux q_M.

Of course a fast isolated vehicle can reach velocities larger that v_M. In particular a limit velocity can be defined

$$V_\ell = (1 + \mu)v_M\,, \qquad \mu > 0\,, \tag{1.5.1}$$

such that no vehicle can reach a velocity larger than V_ℓ. Both v_M and μ may depend on the characteristics of the lane, say a country lane or a highway, as well as to the type of vehicles, say a slow car, a fast car, a lorry, etc.

The above variables can assume different characterization according to the modeling scales which can be adopted for the observation and modeling. In particular, one may consider, according to the indications given in the previous sections, the following types of descriptions:

• **Microscopic description**: the state of each vehicle is defined by position and velocity as dependent variables of time.

• **Kinetic (statistical) description**: the state of the system is still identified by position and velocity of the vehicles however their identification refers to a suitable probability distribution and not to each variable.

• **Macroscopic description**: the state is described by locally averaged quantities, i.e. density, mass velocity and energy, regarded as dependent variables of time and space

In detail, in the **microscopic representation** all vehicles are individually identified. The state of the whole system is defined by dimensionless position and velocity of the vehicles. They can be regarded, neglecting their dimensions, as single points

$$x_i = x_i(t)\,, \qquad V_i = V_i(t)\,, \qquad i = 1, \ldots, N\,, \tag{1.5.2}$$

where the subscript refers to the vehicle.

On the other hand, according to the **kinetic (statistical) description**, the state of the whole system is defined by the statistical distribution of position and velocity of the vehicles. Specifically, it is considered the following distribution over the dimensionless microscopic state

$$f = f(t, x, V)\,, \tag{1.5.3}$$

where $f\,dx\,dV$ is the number of vehicles which at the time t are in the phase domain $[x, x + dx] \times [V, V + dV]$.

Finally, the **macroscopic description** refers to averaged quantities regarded as dependent variables with respect to time and space. Mathematical models are stated in terms of evolution equations for the above variables. If one deals with density and mean velocity, then models will be obtained by conservation equations corresponding to mass and linear momentum:

$$\rho = \rho(t, x) \in [0, 1]\,, \qquad v = v(t, x) \in [0, 1]\,. \tag{1.5.4}$$

Before describing a specific model for each of the above scales, it is necessary to show how the information recovered at the microscopic scale and by the kinetic representation can provide, by suitable averaging processes, gross quantities such as density and mass velocity.

In the microscopic presentation, one can average the physical quantities in (1.5.2) either at fixed time over a certain space domain or at fixed space over a certain time range. For instance the number density $u(t, x)$ is given by the number of vehicles $N(t)$ which at the time t are in $[x - h, x + h]$, say

$$u(t, x) \cong \frac{N(t)}{2h n_M} \, . \tag{1.5.5}$$

A similar reasoning can be applied to the mean velocity

$$v(t, x) \cong \frac{1}{N(t) v_M} \sum_{i=1}^{N(t)} V_i(t) \, , \tag{1.5.6}$$

where, of course, the choice of the space interval is a critical problem and fluctuations may be generated by different choices.

In the kinetic representation, macroscopic observable quantities can be obtained, under suitable integrability assumptions, as momenta of the distribution f, normalized with respect to the maximum density n_M so that all variables are given in a dimensionless form. Specifically, the dimensionless **local density** is given by

$$\rho(t, x) = \int_0^{1+\mu} f(t, x, V) \, dV \, , \tag{1.5.7}$$

while the **mean velocity** can be computed as follows:

$$v(t, x) = E[V](t, x) = \frac{q(t, x)}{u(t, x)} = \frac{1}{\rho(t, x)} \int_0^{1+\mu} V f(t, x, V) \, dV \, . \tag{1.5.8}$$

After the above preliminaries, we can now describe some specific models. Actually very simple ones will be reported in what follows, essentially with tutorials aims. The first model is based on the assumption that the dynamics of each **test** vehicle is determined by the nearest **field** vehicle.

Example 1.5.1
Follow the Leader Microscopic Model

The basic idea of this model, see Klar *et al.* (1996), is that the acceleration $\frac{d^2 x_i}{dt^2}(t + T)$ of the $i - th$ vehicle at time $t + T$ depends on the following quantities:

- The speed $V_i(t)$ of the vehicle at time t,
- The relative speed of the vehicle and of its leading vehicle at time t: $V_{i-1}(t) - V_i(t)$,
- The distance between the vehicle and its leading vehicle at time t: $x_{i-1}(t) - x_i(t)$.

Hence the ordinary differential equation which describes the model is as follows:

$$\frac{d^2 x_i}{dt^2}(t+T) = a\left(V_i(t)\right)^m \frac{V_{i-1}(t) - V_i(t)}{(x_{i-1}(t) - x_i(t))^c},\tag{1.5.9}$$

where T is the reaction time of the driver, and a, m, c, are parameters to be fitted to specifical situations.

□

The model which will be described in what follows was proposed by Prigogine and Hermann (1971), and is based on the assumption that each driver, whatever its speed, has a program in terms of a desired velocity which can be computed by suitable experiments. Specifically $f_d = f_d(V)$ denotes, in what follows, the **desired-velocity distribution function**, meaning that $f_d(V)dx\, dV$ gives the number of vehicles that, at time t and position $x \in [x, x+dx]$, desire to reach a velocity between V and $V + dV$.

Example 1.5.2
Prigogine Kinetic Model

Prigogine's model describes the traffic flow according to the scheme:

$$\frac{\partial f}{\partial t} + V \frac{\partial f}{\partial x} = J_P[f],\tag{1.5.10}$$

where the operator J_P is the sum of two terms:

$$J_P[f] = J_r[f] + J_i[f],\tag{1.5.11}$$

which describe the rate of change of f due to two different contributes:

• The relaxation term J_r, due to the behavior of the drivers of changing spontaneously speed to reach a desired velocity.

• The (slowing down) interaction term J_i, due to the mechanics of the interactions between vehicles with different velocities.

Moreover, it is assumed that the driver's desire also consists in reaching this velocity within a certain relaxation time T_r, related to the normalized density and equal for each driver.

More in details, Prigogine's relaxation term is defined by:

$$J_r[f](t, x, V) = \frac{1}{T_r[f]}\left(f_d(V) - f(t, x, V)\right),\tag{1.5.12}$$

with

$$T_r[f](t, x) = \tau \frac{u(t, x)}{1 - u(t, x)},\tag{1.5.13}$$

where τ is a constant. The relaxation time is smaller the smaller is the density; instead for density approaching to the bumper condition, $u \to 1$, this term grows indefinitely.

The term J_i is due to the interaction between a test (trailing) vehicle and its (field) heading vehicle. It takes into account the changes of $f(t, x, V)$ caused by a braking of the test vehicle due to an ***interaction*** with the heading vehicle: it contains a gain term, when the test vehicle has velocity $W > V$, and a loss term, when the heading vehicle has velocity $W < V$. Moreover, J_i is proportional to the probability P that a fast car passes a slower one; of course this probability depends on the traffic conditions and so on the normalized density. Taking the above probability defined by the local density yields:

$$J_i[f](t, x, V) = u(t, x) f(t, x, V) \int_0^{1+\mu} (W - V) f(t, x, W) \, dW \,. \qquad (1.5.14)$$

Hence the model finally writes:

$$\frac{\partial f}{\partial t} + V \frac{\partial f}{\partial x} = \frac{1 - u(t, x)}{\tau u(t, x)} \left(f_d(V) - f(t, x, V) \right) + u(t, x)$$

$$\times f(t, x, V) \int_0^{1+\mu} (W - V) f(t, x, W) \, dW \,. \qquad (1.5.15)$$

□

Example 1.5.3
Macroscopic Models

The macroscopic model which follows is based on conservation of mass and linear momentum, see Bellomo *et al.* (2002), which can be written as follows:

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial}{\partial x}(uv) = 0 \,, \\[2mm] \dfrac{\partial v}{\partial t} + v \dfrac{\partial v}{\partial x} = g[u, v] \,, \end{cases} \qquad (1.5.16)$$

where g defines the average acceleration referred to each particle. Square brackets are used to indicate that the model of g may be a functional of the arguments. In practice it may be not simply a function of the variables, but also of their first order derivatives. The word ***acceleration*** is used, when dealing with traffic flow models, to avoid the use of the term ***force*** for a system where the mass cannot be properly defined.

It is worth stressing that the above framework simply refers to mass and momentum conservation, while energy is not taken into account. This choice is practically necessary for a system where the individual behavior plays an important role on the overall behavior of the system.

As we have seen, models can be obtained by Eq. (1.5.16) with the addition of a phenomenological relation describing the psycho-mechanic action $g = g[u, v]$ on the vehicles. For instance, if one assumes (in dimensionless variables):

$$g[u, v] \equiv g[u] = -\frac{1}{u}\frac{\partial p}{\partial x}\,, \qquad (1.5.17)$$

then, the following:

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial}{\partial x}(uv) = 0 \\[2mm] \dfrac{\partial v}{\partial t} + v\dfrac{\partial v}{\partial x} = -\dfrac{1}{u}\dfrac{\partial p}{\partial x}\,, \end{cases} \qquad (1.5.18)$$

is obtained, where p is the pressure. A possible relation is the equation of ideal gases: $p = c\,u^{\gamma}$, where c is a constant (in isothermal conditions).

If, instead of (1.5.17), we assume the following:

$$g[u, v] = -\frac{1}{u}\frac{\partial p}{\partial x} + \frac{2}{3uR_e}\frac{\partial^2 v}{\partial x^2}\,, \qquad (1.5.19)$$

we have

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial}{\partial x}(uv) = 0\,, \\[2mm] \dfrac{\partial v}{\partial t} + v\dfrac{\partial v}{\partial x} = -\dfrac{1}{u}\dfrac{\partial p}{\partial x} + \dfrac{2}{3uR_e}\dfrac{\partial^2 v}{\partial x^2}\,. \end{cases} \qquad (1.5.20)$$

Here $R_e = V_0 L u_0/\mu$ with V_0, L and u_0 reference speed, length and density respectively, and $\mu > 0$ a material parameter called viscosity. R_e is a positive constant called Reynolds number, that gives a dimensionless measure of the (inverse of) viscosity. System (1.5.20) defines the equations of motion of a viscous, compressible fluid in one spatial dimension. As it is obvious, the presence or the absence of the viscous term leads to a change in the mathematical structure of the equations, with consequences in the properties of the model.

$\square$

Let us stress again that the above models have to be regarded as simple examples proposed to show how different representation scales generate different models corresponding to the same physical system.

1.6 Classification of Models and Problems

The above sections have shown that the observation and representation at the microscopic scale generates a class of models stated in terms of ordinary differential equations, while the macroscopic representation generates a class of models stated in terms of partial differential equations. In details, the following definitions can be given:

Dynamic and static models			

A mathematical model is **dynamic** if the state variable u depends on the time variable t. Otherwise the mathematical model is **static**.

Finite and continuous models

A mathematical model is **finite** if the state variable does not depend on the space variables. Otherwise the mathematical model is **continuous**.

A conceivable classification can be related to the above definitions and to the structure of the **state variable**, as it is shown in the following table:

finite	static	$\mathbf{u} = \mathbf{u}_e$	Algebric
finite	dynamic	$\mathbf{u} = \mathbf{u}(t)$	ODE
continuous	static	$\mathbf{u} = \mathbf{u}(\mathbf{x})$	PDE
continuous	dynamic	$\mathbf{u} = \mathbf{u}(t, \mathbf{x})$	PDE

Figure 1.6.1 — Classification of mathematical models

The above classification corresponds to well defined classes of equations. Specifically:

• **finite dynamic models** correspond to **ordinary differential equations**, ODEs;

• **continuous dynamic models** correspond to **partial differential equations**, PDEs.

Static models, both finite and continuous, have to be regarded as particular cases of the corresponding dynamic models obtained equating to zero the time derivative. Therefore:

• **finite static models** correspond to **algebraic equations**;

• **continuous static models** correspond to **partial differential equations** with partial derivatives with respect to the space variables only.

As specific examples of static models, the following two examples correspond, respectively, to Example 1.2.1 and Example 1.3.5.

Example 1.6.1

Static Configurations of an Elastic Wire-Mass System

Consider, with reference to Figure 1.2.1, the mechanical system described in Example 1.2.1. Equating to zero the left hand side term, i.e. the time derivatives, yields, in the linear case, the following model:

$$\begin{cases} u_2 = 0\,, \\ -\dfrac{k}{m}u_1 = 0\,. \end{cases} \qquad (1.6.1)$$

Similarly the nonlinear model writes:

$$\begin{cases} u_2 = 0\,, \\ -\dfrac{k_1}{m}u_1 - \dfrac{c}{m}\,u_2^p = 0\,. \end{cases} \qquad (1.6.2)$$

$\square$

Example 1.6.2
_____   *Static Configurations of a Population Dynamics Model*   _____

The static configuration of the stochastic population dynamics model described in Example 1.3.5 are obtained equating to zero the left side term of Eq. (1.3.24)

$$\int_0^1 \int_0^1 \eta(v,w)A(v \to u\,|v,w)f(t,v)f(t,w)\,dv\,dw = f(t,u)\int_0^1 \eta(u,v)f(t,v)\,dv\,. \qquad (1.6.3)$$

$\square$

1.7 Critical Analysis Focusing on Complexity Topics

This chapter has been proposed as an introduction to modelling, classification and organization of mathematical models and equations. It has been stated that a deeper insight into mathematical aspects can be effectively developed only if a well defined class of models (and equations) is effectively specialized. Therefore, the above relatively deeper analysis is postponed to the chapters which follow.

This section simply anticipates some topics and concepts which will be analyzed properly in the chapters which follow. Specifically, we anticipate some ideas concerning ***model validation*** and ***complexity problems in modelling***.

Referring to ***model validation*** one can state, in general, that a model can be regarded ***valid*** if it is able to provide information on the evolution of a real system sufficiently near to those obtained by experiments on the real system. So far a conceivable modelling procedure needs the development of the following steps:

• The real system is modelled by suitable evolution equations able to describe the evolution of the dependent variables with respect to the independent ones.

• Mathematical problems are generated by linking to the model all conditions necessary for its solution. These conditions should be generated by experimental measurements on the real system.

• The above problems can be possibly solved and the output of the simulations is compared with the experimental observations.

• If the distance (according to a concept to be properly defined in mathematical terms) between the above simulations and experiments is less than a critical value fixed *a priori*, then the model can be regarded valid, otherwise revisions and improvements are necessary.

Unfortunately, the concept of validity is not universal, but it refers to the circumstances related to the above comparisons. Indeed, a model which is valid to describe certain phenomena, may loose validity with reference to different phenomena. Therefore development of models and their application needs a constant critical analysis which can go on following a systematic analysis and improvements of each model.

Referring now to ***complexity problems in modelling***, it is worth stating that this concept can be applied to the real system, as well as to the model and to the mathematical problems. In principle all systems of the real world are complex, considering that the number of real variables suitable to describe each system may be extremely large, if not infinite. Once applied mathematicians try to constrain the real system into a mathematical model, i.e. into a mathematical equation, then a selection of the variables suitable to describe the state of the real system is done.

In other words, every model reduces the complexity of the real system through a simplified description by a finite number of variables. Enlarging the number of variables makes the model virtually closer to the real system. On the other hand this enlargement may cause complexity in modelling. In fact a large number of variables may need experiments to identify the phenomenological models related to the material behavior of the system, which may require high costs to be realized, and, in some cases, may be impossible.

However, suppose that the applied mathematician is able to design a model by a large number of variables, then the related mathematical problem may become too difficult to be dealt with. Technically, it may happen that the computational time to obtain a careful solution increases exponentially with the number of variables. In some cases, mathematics may not even be able to solve the above problems. The above concepts refer to ***complexity related to mathematical problems***. Once more, this is a critical aspects of modelling which involves a continuous intellectual effort of applied mathematicians.

It is plain that the attempt to reduce complexity may fall in contrast with the needs posed by validation. Let us anticipate some concepts related to ***validation of models***. Essentially, a validation process consists in the comparison between the prediction delivered by the model and some experimental data available upon observation and measurement of the real system. If this distance is "small", then one may say that the model is valid. Otherwise it is not.

The above distance can be computed by a suitable norm of the difference between the variable which defines the state of the model and the measurement obtained on the real system related to the same variable. Of course, different norms have to be used according to the different classes of models in connection to the different representation scales.

Let us critically focus on some aspects of the validation problems and their interplay with complexity problems:

• The validation of a model is related to a certain experiment. Hence a validity statement holds only in the case of the phenomena related to the experiment. In different physical conditions, the model may become not valid.

• The evaluation of the distance between theoretical prediction and measurements needs the selection of a certain norm which needs to be consistent not only with the analytic structure of the model, but also with the data available by the measurements.

• The concept of **small** and **large** related to the evaluation of the deviations of the theoretical prediction from the experimental data has to be related both to the size (in a suitable norm) of the data, and to the type of approximation needed by the application of the model to the analysis of real phenomena.

• Improving the accuracy (validity) of a model may be contrasted by the complexity problems concerning both modelling and simulations. In some cases accuracy may be completely lost due to errors related to complex computational problems

Mathematical modelling constantly supports the development of applied sciences with the essential contribution of mathematical methods. In the past centuries, a systematic use of modelling methods have generated classical equations of mathematical physics, namely equations describing hydrodynamics, elasticity, electromagnetic phenomena etc. Nowadays, modelling refers to complex systems and phenomena to contribute to the development of technological sciences.

Mathematical models already contribute, and in perspective will be used more and more, to the development of sciences directly related to quality of life, say, among others, biology, medicine, earth sciences.

Modelling processes are developed through well defined methods so that it is correct to talk about the **science of mathematical modelling**. The first stage of this complex process is the observation of the physical system which has to be modelled. Observation also means organization of experiments suitable to provide quantitative information on the real system. Then a mathematical model is generated by proper methods to deal with mathematical methods.

Generally a mathematical model is an evolution equation which can potentially describe the evolution of some selected aspects of the real system. The description is obtained solving mathematical problems generated by the application of the model to the description of real physical behaviors. After simulations it is necessary to go back to **experiments** to validate the model. As we shall see, problems are obtained linking the evolution equation to the so-called **initial and/or boundary conditions**. Indeed, the simplest differential model cannot predict the future if its behavior in the past and on the boundaries of the system are not defined.

The above procedure will be revisited all along these Lecture Notes and it will be particularized with reference to specific models or class of models. However, simply with the aim of introducing the reader to some aspects of the statement of problems and development of math-

ematical methods, the previously described Examples 1.3.1 and 1.2.2 will be revisited with special attention to statement of problems and simulations.

Example 1.7.1
Simulations for the Elastic Wire-Mass Model

Consider the model proposed in Example 1.3.1 as it is described, in the nonlinear case, by Eq. (1.3.3). Simulations should provide the evolution in time of the variables $u_1 = u_1(t)$ and $u_2 = u_2(t)$.

It is plain that the above evolution can be determined from the initial state of the system:

$$u_{10} = u_1(t_0), \qquad u_{20} = u_2(t_0). \tag{1.7.1}$$

In other words, different behaviors correspond to different initial states. A very simple way (actually, as we shall discuss in Chapter 2, too simple) to obtain the above simulation consists in developing a finite difference scheme organized as follows:

i) Consider the discretization of the time variable:

$$I_t = \{t_0, t_1, \ldots, t_i, \ldots\}, \qquad h = t_{i+1} - t_i. \tag{1.7.2}$$

ii) Given the initial state (1.7.1), compute, with reference to Eq. (1.3.3), the state $u_{11} = u_1(t_1)$ and $u_{21} = u_2(t_1)$ by the following scheme:

$$\begin{cases} u_{11} = u_{10} + u_{20}\, h \,, \\[2mm] u_{21} = u_{20} + h\left(-\dfrac{k}{m} u_{10} - \dfrac{c}{m}\, u_{20}^p \right). \end{cases} \tag{1.7.3}$$

iii) Continue the above scheme at the step $(i+1)$ of the discretization by the following scheme:

$$\begin{cases} u_{1(i+1)} = u_{1i} + u_{2i}\, h \,, \\[2mm] u_{2(i+1)} = u_{2i} + h\left(-\dfrac{k}{m} u_{1i} - \dfrac{c}{m}\, u_{2i}^p \right), \end{cases} \tag{1.7.4}$$

where $u_{1i} = u_1(t_i)$ and $u_{2i} = u_2(t_i)$.

The mathematical problem is stated linking conditions (1.7.1) to the mathematical model, while the related mathematical method is developed in items i) – iii).

$\square$

Example 1.7.2
Simulations for Linear Heat Transfer Model

Consider the mathematical model proposed in Example 1.2.2 as it is described by Eq. (1.2.6). Similarly to Example 1.7.1, simulations should provide the evolution in time and space of the variable $u = u(t, x)$. Also in this case, the above simulations can be developed by appropriate mathematical methods, if additional information is given on the behavior of u at the initial time and at the boundaries of the space domain.

Specifically, let us assume it is known the initial state of the system:

$$u_0(x) = u(t_0, x), \quad \forall\, x \in [0, 1], \tag{1.7.5}$$

and the behavior at the boundaries $x = 0$ and $x = 1$, say the fluxes:

$$\alpha(t) = q(t, 0), \quad \beta(t) = q(t, 1), \quad \forall\, t \geq t_0. \tag{1.7.6}$$

Different behaviors correspond to different initial and boundary states. A very simple (actually too simple as we shall discuss in Chapter 3) way to obtain the above simulation consists in developing a finite difference scheme organized as follows:

i) Consider the discretization (1.7.2) of the time variable, and the following discretization for the space variable:

$$I_x = \{x_0 = 0, x_1, \ldots, x_j, \ldots, x_n = 1\}, \qquad d = x_{j+1} - x_j. \tag{1.7.7}$$

ii) Compute, with reference to (1.2.4), the fluxes at the boundary of each tract (finite volume) $[x_j, x_{j+1}]$ by their approximate values $q_{j+1} = q_{j+1}(t)$:

$$q_{j+1} = -\frac{h_0}{d}(u_{j+1} - u_j), \tag{1.7.8}$$

where $u_j = u_j(t) = u(t, x_j)$, $\forall\, j = 1, \cdots n - 1$

iii) Apply the following scheme at each time and for each volume corresponding to the space discretization:

$$\frac{du_{j+1}}{dt} \cong -\frac{1}{c_0\, d}(q_{j+1} - q_j) = \frac{k_0}{d^2}(u_{j+1} - 2u_j + u_{j-1}). \tag{1.7.9}$$

iv) Apply the time discretization to $\dfrac{d\, u_{j+1}}{d\, t}$ as in Example 1.7.1.

The mathematical problem is stated linking conditions (1.7.5)–(1.7.6) to the mathematical model, while the related mathematical method is developed in items i) – iv).

□

The reader should be aware that the above examples have been dealt with at an intuitive and, may be, naive level and that the above topics have to be revisited in a deeper framework.

Then, at this stage, some simple remarks are proposed with the aim of pointing out some crucial features of the modelling process, which will be specifically discussed in the various chapters which follow with direct reference to particular models.

- A mathematical model, although **approximating** the physical reality, should not hide relevant features. In particular, it should not hide nonlinear behaviors or nonlinear features of the phenomena which is modelled.

- Analysis of mathematical models essentially means solution of mathematical problems obtained by providing suitable initial and/or boundary conditions to the state equation. This type of analysis needs the development of mathematical methods that can be organized for classes of models and which may differ for each class. Mathematical methods, according to what we have said in the preceding item, should be those of nonlinear analysis. Linearity should be regarded as a particular situation.

- Generally, mathematical problems are not as mathematicians wish. In other words, real situations are not such that existence, uniqueness, and regularity of the solution can be proved. Often, mathematical problems are imposed by physical reality. In fact, it may often happen that although some information on the solution is given, some features of the model (the parameters) or of the mathematical problem (initial or boundary conditions) cannot be measured. Inverse problems are almost always ill posed. On the other hand, it is plain that the solution of inverse-type problems is of relevant importance in the construction of mathematical models.

- Physical systems sometimes show stochastic behaviors. In some situations, even if the mathematical model is of a deterministic type, the related mathematical problem may be of a stochastic type. In fact, initial or boundary conditions cannot be measured precisely and this type of information may be affected by some stochastic noise. Stochastic behaviors in mathematical models may be an unavoidable feature, and, consequently, suitable mathematical methods need to be developed in order to deal with stochastic problems.

- The modelling process may be regarded as a sort of loop that might be interrupted when there is a satisfactory agreement between simulation and observation of the phenomena.

- Modelling not only leads to a simulation of physical reality, but can also contribute to a deeper understanding of physical systems. Indeed, after the simulation, the experimental observation can be revisited and hopefully improved.

Part of the contents of a letter, Bellomo (1998), appeared on the review journal of the American Society of Mechanical Engineers is reported as it summarizes some of the concepts which have been reported above.

It is worth pointing out that modelling is a creative science, which requires observation, initiative, and invention. Modelling motivates applied mathematics which, on the other hand, needs to support modelling and contributes to address the invention along mathematically reasonable paths. Further mathematical models can often contribute to a deeper understanding of physical reality. Indeed, the construction of a mathematical model contributes to discover the organized

structures of physical systems. Moreover, the simulation can point out behaviors which have not been, or even cannot, be observed.

Then one may state that mathematical modelling constantly supports the development of technological and natural sciences by providing the essential contribution of the mathematical methods.

An additional complexity problem is related to scaling. It may happen, in the case of systems constituted by a large number of interacting elements that, although the dynamics of each element is well understood, the collective behavior of the whole system is not properly described by the sum of the dynamics of each element. The complexity source is that collective behaviors follow a dynamics totally different from that of the behavior of a few entities. It is not simply a matter of selection of the proper scale, while models should take into account the fact that in large systems, the various elements do not behave in the same way and individual behaviors can play a relevant role in the overall evolution of the whole system.

This observation introduces the concept of **complexity of living systems**, and hence the challenging problem of modeling living systems. This topic is dealt with in Chapter 4, however some preliminary observations can be anticipated for large systems of interacting individuals.

• Living systems have the ability to express specific strategies which depends on that of the other interacting individuals.

• This ability is heterogeneously distributed among individuals, while interactions are generally not additive.

• Living systems operate out of equilibrium and have the ability to extract energy from the surrounding environment for their own benefit.

Although the above remarks do not cover the whole variety of complexity features of living systems, a preliminary analysis can be referred to the example of models we have presented in this chapter.

• All models of this chapter involve, with exception of Models 1.3.5 and 1.5.2, a description of the state of the system by deterministic variables.

• All models have been derived by a causality principle, namely by a relation between "cause" and "effect". This relation is deterministic for most models besides, again, 1.3.5 and 1.5.2.

• Focusing on deterministic models, it can be observed that the causality principle is based on rigorous relations either conservation or equilibrium equations. On the other hand, the derivation of the model needs phenomenological models concerning the material behavior of the system under consideration.

• The afore–said characteristics are generally related to experiments which are valid in steady conditions, while the model is supposed to operate far from these special conditions.

This latter remark focus on one of the weakness of the modeling approach, which occurs whenever the closure of equilibrium and conservation equations is obtained by heuristic material models that are no supported by a robust theory. Due to this motivation, the definition **mathematical models** is used. On the other hand, the use of **models of mathematical**

physics can be used when conservation and/or equilibrium equations are closed by a relation derived by a theory of mathematical physics.

Very different appears to be the panorama offered by models of living systems, where the causality principle involves random variables. Moreover, the phenomenological model used to close the equilibrium and/or conservation equations may, in some cases, be stated in probability. In fact, the heterogeneous distribution of the ability to express a certain strategy requires the use of random variables and stochastic models for the interactions.

This specific characteristics and the modeling difficulty suggest to design explorative models rather than predictive ones. More precisely:

- Predictive models are supposed to depict the evolution of systems once the parameters of the model have been properly identified.

- Explorative models are supposed to depict the scenario of all conceivable evolutions corresponding to all admissible values of the parameters.

The latter class of models is very important in the case of living systems, where one may be interested to understand the behavior of the system corresponding to different interaction rules involving the entities composing the system itself.

However, the two examples that have been presented in this Section have to be considered very simple examples that need to be criticized. For instance, by the fact that interactions are linearly additive, while living systems generally undergo non-linear interactions; as an example, focusing on the vehicle traffic model, the passing probability does not depend by binary interactions only, but by the distribution of the vehicles in the whole interaction domains.

Therefore, the challenging topic we are talking about has to be treated within a well defined mathematical approach, possibly a mathematical theory, different from that widely used in this chapter. Accordingly, the modeling approach to living systems will be widely treated in the last chapter of this monograph.

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Chapter 2

Microscopic Scale Models and Ordinary Differential Equations

2.1 Introduction

This chapter deals with modeling and related mathematical problems within the framework of the microscopic observation scale. Modeling at the microscopic scale means, according to the classification of models and equations proposed in Chapter 1, deriving an evolution equation for each element constituting the system where each element is treated as a whole. Generally, the model is stated in terms of a system of ordinary differential equations.

More precisely, if m is the dimension of the state variable which defines the state of each element and n the number of elements, then the dimension of the system is $n \times m$. Equations are generally linked by the mutual interactions of the elements belonging to the system and by external actions on the elements of the system.

Microscopic modeling can be developed when the number of elements is somehow small (in some sense to be properly specified). Otherwise, when their number becomes large, the computational complexity to handle a large system of equations may involve difficulties which cannot be technically dealt with. Actually, technical difficulties do not refer to the derivation of the model, but to the computational treatment of a system of equations too large to be handled: specifically the computational time may grow exponentially with the number of equations. In this case a different way of modeling can be developed in order to reduce complexity.

This chapter deals with models and problems which do not yet generate the above type of **computational complexity**. This delicate matter cannot be hidden, being aware that **reducing complexity** is one of the challenging aspects of the science of mathematical modeling. However the real complexity problem is the modelling of nonlinear interactions rather than the approach based on assumption of linear superposition already discussed in Chapter 1.

After the above preliminaries, the contents and organization of this chapter can be described. Specifically, after this introduction:

– Section 2.2 deals with modeling methods at the microscopic scale. As we shall see, although

it is not possible to assess a unique procedure to derive a model, still some general rules can be identified. Some specific examples will show how models can be derived within the mathematical framework of ordinary differential equations.

– Section 2.3 presents a classification of ordinary differential equations, and the mathematical statement of the problems, which is obtained by linking the evolution equation to the conditions that are necessary to its solution. If these conditions are given corresponding to the initial value of the independent variable, say $t = t_0$, one has an initial-value problem, also called Cauchy problem. Otherwise, if these quantities are given at both ends of the range of the independent variable, say $t = t_0$ and $t = t_1$, one has a boundary-value problem.

– Section 2.4 deals with the representation of solutions to mathematical problems described in Section 2.3. Then an introduction to discretization methods is proposed to obtain quantitative results, that are the simulations related to the solution of the above problems. This topic is related both to initial and boundary value problems. The contents have to be regarded as an introduction to computational methods. The reader will be introduced to topics which need to be properly revisited by means of the essential contribution of the pertinent literature.

– Section 2.5 is concerned with the qualitative analysis of dynamical systems; in particular with stability definitions followed by methods to study linear and nonlinear stability.

– Section 2.6 deals with regular and singular perturbation methods developed to analyze the qualitative and quantitative behavior of solutions to initial value problems for finite models.

– Section 2.7 provides a brief introduction to the problem of bifurcation, analyzing the dependence of the equilibrium points and of their stability properties on the parameters of the model.

– Section 2.8 develops a critical analysis on the contents of this chapter focused, as already mentioned, on modelling and computational problems, looking ahead to modelling and simulation of living systems.

2.2 On the Derivation of Mathematical Models

In general, it is not reasonable to assess only one method to derive models at the microscopic scale. However some common lines can be identified. Therefore a conceivable modeling procedure will be here described and applied in the derivation of some specific models.

Let us consider the following sequential steps which may be followed for the derivation of finite mathematical models:

Step 1. Phenomenological observation of the physical system which needs to be modeled.

Step 2. Identification of the various elements composing the system and of the dependent (state) variables suitable to describe the state of each element, and hence of the whole system.

Step 3. Modeling the causes which generate the dynamics and identification of the cause-effect relationships, as well as of the conservation equations (when they exist) of quantities related to the state of the system.

Step 4. Derivation of the mathematical model, i.e. an evolution equation for the dependent variables, by exploiting the above relationships.
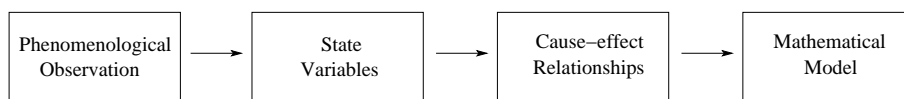

Figure 2.2.1 — Derivation of mathematical models

When the system is a mechanical one, within the framework of classical mechanics, then the derivation of the model follows methods of Newtonian and Lagrangian mechanics, as documented in the book Bellomo *et al.* (2000). The examples which follow will show how the above steps can be practically developed in the modeling systems of real world. Specifically, the first system is related to technology, the second one to economical sciences and marketing, and the third one to populations dynamics. The four aforesaid Steps 1–4 will be explicitly related to the derivation of each model.

Once the model has been derived, the analysis and the application of the model follows by stating and solving mathematical problems generated by the applications.

Example 2.2.1
Linear Electric Circuits

Consider the standard circuit with resistor R, inductance L, and capacitor C, in series, as shown in Figure 2.2.2, where it is also shown that the circuit is subject to the voltage E. The model is expected to describe the flow of the current and its derivation can be developed through the steps which follow:

Step 1. The phenomenological observation of the system indicates that it is an electric circuit: the electromotive force $E = E(t)$ may vary in time, while R, L, and C are constant parameters.

Step 2. The system is composed of one only element: ***the circuit***, the state of the system may be described either by the charge q (to be measured in Coulombs), or by the intensity of the current $i = dq/dt$ (to be measured in Ampère).

Step 3. The relationship between cause and effect can be described by Kirchoff's law (***actually a phenomenological model***) which states that the sum of the tension drops in each element equals the electromotive force $E(t)$. Moreover, it is assumed that Ohm's model is valid: the tension drop in the resistor is $V(t) = R\,i(t)$, with R constant.

Step 4. The evolution model is obtained exploiting the above relationship, which, considering that all parameters are constant, writes:

$$L\frac{di}{dt} + Ri + \frac{q}{C} = E(t)\,. \tag{2.2.1}$$

Considering that i is the derivative with respect to time of the charge q, the following second order model is derived:

$$\frac{d^2q}{dt^2} + \frac{R}{L}\frac{dq}{dt} + \frac{q}{LC} = \frac{E(t)}{L}, \tag{2.2.2}$$

which can be written as a system of first order equations using the following variables:

$$u_1 = q, \qquad u_2 = \frac{dq}{dt} = \frac{du_1}{dt},$$

so that the following system is obtained:

$$\begin{cases} \dfrac{du_1}{dt} = u_2, \\[2mm] \dfrac{du_2}{dt} = \alpha u_1 + \beta u_2 + \gamma E(t), \end{cases} \tag{2.2.3}$$

$$\alpha = -\frac{1}{LC}, \qquad \beta = -\frac{R}{L}, \qquad \gamma = \frac{1}{L}.$$

$\square$

Remark 2.2.1. *The derivation of the model (2.2.3), is obtained by particularizing the general procedure described at the beginning of this section and visualized in Fig. 2.2.1.*
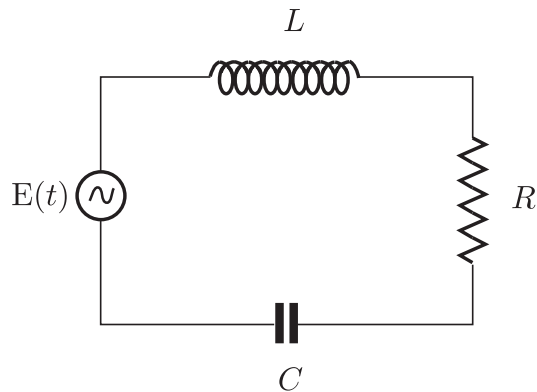

Figure 2.2.2 — Electric Circuit.

Example 2.2.2
Modeling Marketing Dynamics

Consider the interaction within an economical system constituted by potential buyers with the users of brand names in a closed marketing environment. Modeling the above system should provide the evolution in time of the numbers of the above interacting subjects. The mathematical model can be derived through the following steps:

Step 1. The system is constituted by potential buyers with the users of brand names in a closed marketing environment. Interactions modify their number.

Step 2. The state of system is supposed to be described by the number u_1 of potential buyers and the number u_2 of users of brand names.

Step 3. The relationship between cause and effect can be described by a simple phenomenological model such that u_1 grows with time at a constant rate, namely the growth is linearly depending on u_2. On the other hand such a growth is contrasted by the interaction between u_1 with u_2^p, with $p > 1$, due to saturation phenomena. Similarly u_2 grows due to the interaction between u_1 with u_2^q, with $q > 1$. On the other hand such a growth is contrasted by u_2 due to saturation of offer in the market.

Step 4. The model is obtained exploiting the above modeling of the cause and equating the cause to the effect, that is the time derivative of u_1 and u_2. The results is as follows:

$$\begin{cases} \dfrac{du_1}{dt} = \alpha - \beta u_1 u_2^p + \gamma u_2\,, \\ \dfrac{du_2}{dt} = \beta u_1 u_2^q - \delta u_2\,, \end{cases} \qquad (2.2.4)$$

where α defines the natural rate of growth of buyers, β refers to the decrease of buyers due to their contact with brand names, while brand names increase the rate of growth of buyers as ruled by the parameter γ. The parameter β is again used for their increase due to the contact with buyers, while δ refers to decay of brand names.

□

Example 2.2.3
Population Dynamics

Consider a system of n interacting populations fully isolated with respect to the outer environment. Modeling the above system means obtaining the evolution in time of the number of individuals of the above interacting populations. The mathematical model can be derived through the following steps:

Step 1. The system is fully isolated, i.e., it is assumed that there is not interaction with the outer environment. Moreover, one assumes that the state of the system is simply described by the number u_i of individuals of each ith population.

Step 2. The cause–effect relationship is assessed by two phenomenological aspects. The first aspect states that the population growth of the ith species linearly depends upon the number of the individuals belonging to the said species. A second aspect states that the interaction between individuals of different species produces a decrease proportional to the product of individuals of the interacting species.

Step 3. The mathematical model is simply obtained equating the ***cause***:

$$a_i u_i - u_i \sum_{j=1}^{n} b_{ij} u_j, \tag{2.2.5}$$

to the ***effect***:

$$\frac{du_i}{dt} = a_i u_i - u_i \sum_{j=1}^{n} b_{ij} u_j . \tag{2.2.6}$$

□

The above three simple models in Examples 2.2.1–2.2.3 show some technical differences. The first model refers to one element only, the second one to a system of two elements, while the number of elements in the third one may be arbitrarily large. All models need to be rewritten in terms of dimensionless variables after a proper selection of reference quantities as indicated in Chapter 1. The derivation of the first model is based on principles of physics, more precisely models of material behaviour of circuits subject to electrical potential. The second and third model are simply related to a phenomenological interpretation of real systems. Surely the derivation is based on naive ideas that can be critically analyzed in the last section of this chapter.

More precisely, one may observe that the first Example 2.2.1 describes the interactions between two objects, while the model 2.2.3 is concerned with the interactions among n populations. Actually, the model is meaningful if n is small. Indeed, when the number of populations becomes large, interactions between pair of individuals may be affected by the presence of a third population. In other words, the coefficients are no longer constant, but may depend on the state of the system. This is definitely an origin of complexity to be properly analyzed

2.3 Classification of Models and Mathematical Problems

Section 2.2 has shown that mathematical models can be derived at the microscopic scale in order to describe the ***time evolution*** of a finite dimensional ***state variable***: $\mathbf{u} = \mathbf{u}(t)$, where $\mathbf{u}$ is the set of dependent variables $\mathbf{u} = (u_1, \ldots, u_i, \ldots, u_n)$ defined over the domain $[t_0, t_1]$ of the independent variable t.

This section deals with the classification of microscopic models which are structured in terms of ordinary differential equations, which will be assumed to be always written in dimensionless

form. The classification refers to models where the independent variable is the time t. However, it holds for any type of independent variable and it is based on the structure of the mathematical equations.

Specifically, let us consider first systems of equations written in the commonly called **normal form**:

$$\begin{cases} \dfrac{du_1}{dt} = f_1(t, u_1, \ldots, u_n) \,, \\[2mm] \quad \vdots \\[2mm] \dfrac{du_n}{dt} = f_n(t, u_1, \ldots, u_n) \,, \end{cases} \tag{2.3.1}$$

which can be written, with obvious meaning of notation, in the compact vector form:

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(t, \mathbf{u}) \,. \tag{2.3.2}$$

Another interesting class of models is the one which refers to higher-order scalar equations:

$$\frac{d^n u}{dt^n} = f\left(t, u, \frac{du}{dt}, \ldots, \frac{d^{n-1}u}{dt^{n-1}}\right) \,. \tag{2.3.3}$$

The above equation can be rewritten in terms of a normal system of n equations in n unknowns by the change of variables:

$$u_1 = u \,, \quad u_2 = \frac{du}{dt} \,, \ldots, u_n = \frac{d^{n-1}u}{dt^{n-1}} \,, \tag{2.3.4}$$

which yields the normal form:

$$\begin{cases} \dfrac{du_1}{dt} = u_2 \,, \\[2mm] \dfrac{du_2}{dt} = u_3 \,, \\[2mm] \quad \vdots \\[2mm] \dfrac{du_n}{dt} = f(t, u_1, \ldots, u_n) \,. \end{cases} \tag{2.3.5}$$

This means, referring specifically to the class of equations represented in Eq. (2.3.1), that the following classification can be given.

Linear Models

*A system of ordinary differential equations (**the model**) is considered **linear** if it can be written as follows:*

$$
\begin{cases}
\dfrac{du_1}{dt} = a_{11}(t)u_1 + \cdots + a_{1n}(t)u_n + b_1(t)\,, \\[2mm]
\quad\vdots \\[2mm]
\dfrac{du_n}{dt} = a_{n1}(t)u_1 + \cdots + a_{nn}(t)u_n + b_n(t)\,,
\end{cases}
\tag{2.3.6}
$$

or in a compact form:

$$
\frac{d\mathbf{u}}{dt} = \mathbf{A}(t)\mathbf{u} + \mathbf{b}(t)\,,
\tag{2.3.7}
$$

where $\mathbf{A}(t)$ is the $n \times n$ matrix of the coefficients $a_{ij}(t)$, and $\mathbf{b}(t)$ is a column vector with n components.

Linear Homogeneous Models

*A linear system of ordinary differential equations (**the model**) is considered **homogeneous** if $\mathbf{b}(t) = \mathbf{0}$ or in a compact form:*

$$
\frac{d\mathbf{u}}{dt} = \mathbf{A}(t)\mathbf{u}\,.
\tag{2.3.8}
$$

Linear Models with Constant Coefficients

*A system of ordinary differential equations (**the model**) is considered **linear with constant coefficients** if the coefficients a_{ij} are constants. It can be written as follows:*

$$
\frac{d\mathbf{u}}{dt} = \mathbf{A}\mathbf{u} + \mathbf{b}(t)\,.
\tag{2.3.9}
$$

A special case is when $\mathbf{b}$ is constant. Then, is A is nonsingular, the following change of variable $\mathbf{w} = \mathbf{u} + A^{-1}\mathbf{b}$ eliminates the nonhomogeneous term.

Nonlinear Models

*A system of ordinary differential equations (**the model**) is considered **nonlinear** if the terms f_i are nonlinear functions of the dependent variables $\mathbf{u}$.*

Nonlinearly Weakly Perturbed Models

*A system of ordinary differential equations (**the model**) is considered **weakly perturbed semilinear** if it can be written in the form:*

$$\frac{d\mathbf{u}}{dt} = \mathbf{A}(t)\mathbf{u} + \mathbf{b}(t) + \varepsilon\, \mathbf{f}(t, \mathbf{u})\,, \qquad (2.3.10)$$

where ε is a small, dimensionless parameter.

A further aspect which plays an important role in modeling is the presence of time.

Autonomous Models

*A system of ordinary differential equations (**the model**) is considered **autonomous** if the time t does not explicitly appear as an argument of $\mathbf{f}$. Otherwise, the model is called **nonautonomous**.*

For instance, in Eq. (2.3.9) $\mathbf{A}$ and $\mathbf{b}$ are, respectively, a constant matrix and a constant vector, so the system is autonomous. On the other hand, mathematical models presenting time dependent forcing terms are nonautonomous.

Remark 2.3.2. *Linear homogeneous systems can be written in the following form:*

$$\frac{d\mathbf{u}}{dt} = \mathcal{L}(\mathbf{u})\,, \qquad (2.3.11)$$

where $\mathcal{L}(\mathbf{u})$ is a linear operator, i.e.

$$\mathcal{L}(\mathbf{u}_1 + \mathbf{u}_2) = \mathcal{L}(\mathbf{u}_1) + \mathcal{L}(\mathbf{u}_2)\,, \quad \mathcal{L}(\lambda \mathbf{u}) = \lambda \mathcal{L}(\mathbf{u})\,, \qquad (2.3.12)$$

where λ is a real constant. On the other hand, nonlinear systems can be written as follow:

$$\frac{d\mathbf{u}}{dt} = \mathcal{N}(\mathbf{u})\,, \qquad (2.3.13)$$

where $\mathcal{N}$ does not satisfy condition (2.3.12).

In some very general cases models may have even a structure of the type of the type:

$$f\left(t, u, \frac{du}{dt}, \cdots, \frac{d^n u}{dt^n}\right) = 0\,. \qquad (2.3.14)$$

In this case, writing the model in normal form as indicated in Eq. (2.3.1) may be hard or even impossible. Actually, the above very particular cases are not dealt with in these Lecture Notes.

Let us now consider mathematical problems which are generated by the analysis of real systems. These problems are stated by joining the evolution equation with the conditions necessary for its solution. Conditions for the solutions of problems are called **initial** and **limit conditions** which may be defined as follows:

Initial and Limit Conditions

*Consider Eq. (2.3.1) defined in the time interval $[t_0, t_1]$; we call the **initial condition** for each component of* **u**, *the value:*

$$u_i(t_0) = u_{i0} \tag{2.3.15}$$

*of the variable u_i at $t = t_0$, and similarly the **limit condition** the value:*

$$u_j(t_1) = u_{j1} \tag{2.3.16}$$

of the variable u_j at the time $t = t_1$.

Initial conditions for all components of **u** define the state of the system before the evolution starts, while limit conditions define constraint on the final configuration that is assumed by the system.

Linking the evolution equation to initial and/or limit conditions generates the following mathematical problems:

Initial-value problem

*The **initial-value problem** for Eq. (2.3.1) is obtained by coupling the system of n evolution equations with n **initial conditions** u_{i0}, for $i = 1, \ldots, n$:*

$$\begin{cases} \dfrac{d\mathbf{u}}{dt} = \mathbf{f}(t, \mathbf{u}), \\ \mathbf{u}(t_0) = \mathbf{u}_0. \end{cases} \tag{2.3.17}$$
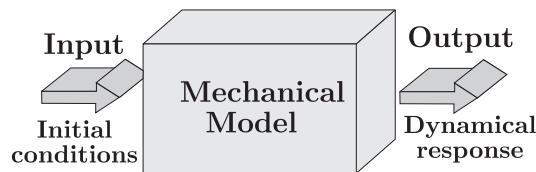
Figure 2.3.1 — Input–output box for a homogeneous system

One may look at the initial-value problem as presented by the input–output system shown in Figure 2.3.1. The output is the **dynamical response**, while the **mechanical model** is contained in the box. If the model is subject to an external field, the block representation also includes the term **b** as one of the inputs, as shown in Figure 2.3.2, while the mechanical model is still contained in the box. The forcing term is related to the physical situation characterizing the interactions between the inner and outer system.
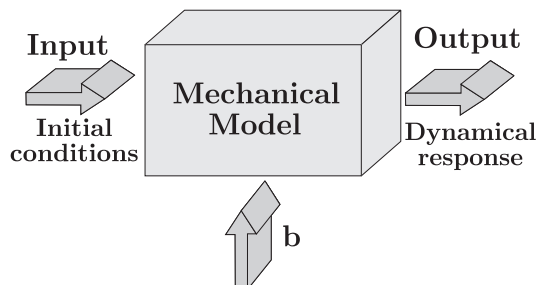
Figure 2.3.2 — Input–output box for a nonhomogeneous system

It should be noted that a system of n ordinary differential equations needs n initial conditions – one per state variable – in order to be transformed into an initial-value problem. If some of the initial conditions are replaced with limit conditions, then one has a boundary-value problem. In this case, it is not necessary to have a condition per state variable. Indeed, the problem can be stated with two types of conditions, namely both initial and limit conditions on a component, and no condition at all on the other one. This situation is described in the following definition:

Boundary-value problem

*The **boundary-value problem** for Eqs. (2.3.1) is obtained by linking the system of n evolution equations to $p < n$ **initial conditions**:*

$$u_i(t_0) = u_{i0}, \quad i = 1, \ldots, p, \tag{2.3.18}$$

*each associated with a different component, and to $(n - p)$ **limit conditions**:*

$$u_i(t_1) = u_{i1}, \quad i = p + 1, \ldots, n, \tag{2.3.19}$$

each associated with a different component.

The above conditions can be replaced by linear or nonlinear combinations of the boundary conditions.

The formal application of the above concepts to the statement of problems for some of the models described in Section 2.2 is dealt with in the following examples.

Example 2.3.1
Initial Value Problems for Marketing Models

Consider the mathematical model described through Example 2.2.2. The initial value problem is obtained linking the values that the variables u_1 and u_2 attain at the initial time $t = t_0$. The

problems is as follows:

$$\begin{cases} \dfrac{du_1}{dt} = \alpha - \beta u_1 u_2^p + \gamma u_2 \,, \\[2mm] \dfrac{du_2}{dt} = \beta u_1 u_2^q - \delta u_2 \,, \\[2mm] u_1(t_0) = u_{10} \,, \\[2mm] u_2(t_0) = u_{20} \,, \end{cases} \qquad (2.3.20)$$

where u_{10} and u_{20} are given constants.

$\square$

Example 2.3.2
Boundary Value Problems for a Population Model

Consider the mathematical model described through Example 2.2.3 for a two population dynamics. A boundary value problem is obtained for example linking the values that the variable u_1 attain at the initial time $t = t_0$ and the one that u_2 attain at the final time $t = t_1$. The problem is as follows:

$$\begin{cases} \dfrac{du_1}{dt} = a_1 u_1 - u_1(b_{11}u_1 + b_{12}u_2) \,, \\[2mm] \dfrac{du_2}{dt} = a_2 u_2 - u_2(b_{21}u_1 + b_{22}u_2) \,, \\[2mm] u_1(t_0) = u_{10} \,, \\[2mm] u_2(t_1) = u_{21} \,. \end{cases} \qquad (2.3.21)$$

$\square$

2.4 Solution Schemes and Time Discretization

Section 2.3 has shown in that once a model has been properly derived, its practical application to the analysis of the behavior of real system needs the statement of a mathematical problem and the related technical solution. It follows that mathematical methods for ordinary differential equations should be developed to obtain quantitative simulations.

The development of analytic methods does not generally give sufficiently operative tools to deal with mathematical problems. In fact, the presence of nonlinearity in the model often (or almost always) requires the development of computational schemes and possibly scientific software for the application of solution algorithms.

Several books are available in the literature which deal with analytic and/or computational methods. For instance, and among others, one may consider the book Marasco and Romano

(2001), into which, after the definition of the proper analytic background concerning existence of solutions, stability properties, bifurcation analysis, various computational schemes are developed with the aid of the Software *Mathematica*©. A similar line is followed in the previously cited book Bellomo *et al.* (2000), which is mainly oriented on the analysis of models of classical mechanics. The interested reader is addressed to the above literature to obtain a relatively more complete background on analytic and computational methods.

This section provides a concise description of solution schemes by analytic and discretization methods. Completeness is not claimed, the aim being simply to show how it is possible to obtain quantitative results from simulation of a large variety of class of problems. In details, this section is organized through four subsections which deal with the following topics:

  i) existence of solutions to initial value problems;

 ii) analytic methods for linear initial value problems;

iii) discretization schemes for initial value problems;

iv) boundary value problems.

2.4.1 Existence of solutions for initial value problems

This subsection deals with qualitative analysis related to the solution of the initial-value problems for ordinary differential equations. Referring to the above class of problems, the following definitions can be given:

> **Well-posedness**
>
> *A problem is **well formulated** if the evolution equation is associated with the correct number of initial (or boundary) conditions for its solution, while a problem is **well posed** if the solution exists, it is unique and depends continuously on the initial data.*

The main purpose of a model related to a certain physical system is to predict, for a certain time interval, the behavior of the system starting from the knowledge of the state at the initial time t_0. The predictions of the model are then obtained by solving the initial-value problem. To do that, there are some basic requirements that a problem should satisfy:

  i) The solution should exist, at least for the period of time desired;

 ii) The solution should be unique;

iii) The solution should depend continuously on the initial data and on the parameters of the model, so that if a small error is made in describing the present state, one should expect the effect of this error to be small in the future.

As already stated, if these requirements are satisfied, then the ***initial-value problem*** is said to be ***well posed***.

Consider a norm in $\mathbb{R}^n$, which might be, for instance, the Euclidean norm:

$$\|\mathbf{u}\| = \left(\sum_{i=1}^{n} u_i^2 \right)^{\frac{1}{2}} , \qquad (2.4.1)$$

and give the following definition:

> **Lipschitz condition**
>
> *A vector function* $\mathbf{f}(t, \mathbf{u})$ *satisfies a **Lipschitz condition** in a region* $\mathcal{D}$ *of the* $(t, \mathbf{u})$-*space if there exists a constant* L *(called **Lipschitz constant**), such that, for any* $(t, \mathbf{u})$ *and* $(t, \mathbf{v})$ *in* $\mathcal{D}$ *one has:*
>
> $$\left\| \mathbf{f}(t, \mathbf{u}) - \mathbf{f}(t, \mathbf{v}) \right\| \leq L \left\| \mathbf{u} - \mathbf{v} \right\|. \tag{2.4.2}$$
>
> *where both terms on the left-hand side of (2.4.2) are referred to the same instant of time.*

The Lipschitz condition is a property related both to continuity and differentiability. Indeed, it can be proved that if $\mathbf{f}(t, \mathbf{u})$ is defined in a bounded, closed, and convex domain $\mathcal{D}$, and if the partial derivatives of $\mathbf{f}$ with respect to u_i exist with:

$$\max_{i,j=1,\dots,n} \sup_{(t,\mathbf{u}) \in \mathcal{D}} \left| \frac{\partial f_i}{\partial u_j} \right| \leq M, \tag{2.4.3}$$

then $\mathbf{f}$ satisfies a Lipschitz condition in $\mathcal{D}$ with a Lipschitz constant equal to M. We recall that a domain is convex if any segment joining two points of the domain lies entirely within the domain.

Of course, if $\mathbf{f}(t, \mathbf{u})$ satisfies a Lipschitz condition in $\mathcal{D}$, $\mathbf{f}$ is a continuous function of $\mathbf{u}$ in $\mathcal{D}$ for each fixed t. The opposite is not true: for instance:

$$f(u) = \sqrt[3]{u^2}$$

is continuous, however it does not satisfies the Lipschitz condition in any region containing the origin. On the other hand, if $\mathbf{f}(t, \mathbf{u})$ is differentiable to respect to $\mathbf{u}$, for all times, then it satisfies the Lipschitz condition, but the opposite it is not true, as it is shown by $|u|$ that satisfies the Lipschitz condition with constant $L = 1$ though it is not differentiable in $u = 0$.

Functions like:

$$f(u) = u^q \quad \text{with} \quad q > 1, \qquad \text{or} \qquad f(u) = \cosh u,$$

do not satisfy the Lipschitz condition in $\mathbb{R}$. In fact, roughly speaking, their derivative grows without bound as u goes to infinity. However, they satisfy the Lipschitz condition in any closed bounded interval with Lipschitz constant equal to the maximum of the absolute value of the derivative in the interval.

Let us now consider, after the above preliminary definitions, the qualitative analysis of the initial-value problem with initial time denoted by t_0. Existence and uniqueness of solutions is stated by the following two theorems:

Theorem 2.1 Existence

If $\mathbf{f}(t, \mathbf{u})$ is continuous in the rectangle:

$$\mathcal{R} = \left\{ (t, \mathbf{u}) : \|\mathbf{u} - \mathbf{u}_0\| \leq K, \ |t - t_0| \leq T \right\}, \tag{2.4.4}$$

then there exists **at least one solution** to the initial-value problem (2.3.17) and it is of class C^1 for $|t - t_0| \leq \widehat{T}$, where:

$$\widehat{T} = \min\left\{ T, \frac{K}{M} \right\} \qquad \text{and} \quad M = \max_{(t, \mathbf{u}) \in \mathcal{R}} \|\mathbf{f}(t, \mathbf{u})\|.$$

Theorem 2.2 Uniqueness

If, in addition to the continuity condition of Theorem 2.1, the function $\mathbf{f}$ satisfies a Lipschitz condition in $\mathcal{R}$, then the solution $\mathbf{u}(t)$ to the initial-value problem (2.3.17) is **unique**, and:

$$\|\mathbf{u}(t) - \mathbf{u}_0\| \leq M\widehat{T}. \tag{2.4.5}$$

Notice that the Lipschitz condition is not needed to assure the existence of a solution of the initial-value problem. Instead, it is essential in the uniqueness proof. Actually, Theorem 2.1 can be slightly improved, mainly by specializing the proofs to particular cases. For instance, existence results can be obtained for $\mathbf{f}(t, \mathbf{u})$ with a limited number of finite discontinuities.

Consider now the problem of the **continuous dependence on the initial data**, and let $\widehat{\mathbf{u}}$ and $\widetilde{\mathbf{u}}$ be the two solutions of the two initial-value problem (2.3.17) with initial data $\mathbf{u}(t_0) = \widehat{\mathbf{u}}_0$ and $\mathbf{u}(t_0) = \widetilde{\mathbf{u}}_0$, respectively.

Theorem 2.3 Continuous dependence on the initial data

If $\mathbf{f}$ is continuous and satisfies the Lipschitz condition, then the following inequality holds:

$$\left\| \widehat{\mathbf{u}}(t) - \widetilde{\mathbf{u}}(t) \right\| \leq \left\| \widehat{\mathbf{u}}_0 - \widetilde{\mathbf{u}}_0 \right\| e^{L|t - t_0|}, \tag{2.4.6}$$

where L is the Lipschitz constant.

Finally, referring to the analysis of the **continuous dependence on** $\mathbf{f}$, consider for $t \in [t_0, t_0 + T]$ the initial-value problems:

$$\begin{cases} \dfrac{d\mathbf{u}}{dt} = \mathbf{f}(t, \mathbf{u}), \\ \mathbf{u}(t_0) = \mathbf{u}_0, \end{cases} \qquad \text{and} \qquad \begin{cases} \dfrac{d\mathbf{u}}{dt} = \mathbf{f}^*(t, \mathbf{u}), \\ \mathbf{u}(t_0) = \mathbf{u}_0^*, \end{cases} \tag{2.4.7}$$

with $\mathbf{f}$ and $\mathbf{f}^*$ defined and continuous in a common domain $\mathcal{D}$.

Theorem 2.4   Continuous dependence on f

If one of $\mathbf{f}$ or $\mathbf{f}^*$ satisfies a Lipschitz condition with constant L and if:

$$\left\|\mathbf{f}(t,\mathbf{u})-\mathbf{f}^*(t,\mathbf{u})\right\| \leq \varepsilon, \qquad \forall\,(t,\mathbf{u}) \in \mathcal{D}, \tag{2.4.8}$$

then

$$\left\|\mathbf{u}(t)-\mathbf{u}^*(t)\right\| \leq \left\|\mathbf{u}_0-\mathbf{u}_0^*\right\|e^{L|t-t_0|} + \frac{\varepsilon}{L}\left[e^{L|t-t_0|}-1\right], \tag{2.4.9}$$

where $\mathbf{u}(t)$ and $\mathbf{u}^*(t)$ are the solutions of the two initial-value problems defined in (2.4.7).

Although the above analysis answers the questions posed at the beginning of this section and can be applied to most of the initial-value problems occurring in nature, an important question still remains unanswered: how large is the domain of the solution? The existence results shown above assure existence and uniqueness of the solution which may, however, lead to useless estimates on the existence interval.

Of course, the domain might be larger than the estimate given by the theorems, possibly extending to all $t \geq t_0$. Then one needs criteria to determine the largest possible domain of existence. This question gives rise to the class of what is known as the ***extension theorems***. Namely, extensions of the solution can be developed if one can prove that the norm of the solution does not grow too fast. This type of analysis is often based on a deep understanding of the qualitative properties of the system. For instance boundness properties can be recovered by a qualitative analysis of energy conservation. Of course, one needs to prove that the *a priori* estimates hold true in the same function space where the local existence theorem has been stated. This type of analysis can be recovered in the classical literature on ordinary differential equations, see for example Pontriaguine (1975).

2.4.2 Analytic methods for linear initial value problems

In general, ***analytic solutions*** can be sought for in the case of ***linear systems*** of ordinary differential equations. The qualitative analysis of linear systems is widely dealt with in the literature and can be approached in several ways. Some general results can be summarized here:

Remark 2.4.1. *Any linear system:*

$$\frac{d\mathbf{u}}{dt} = \mathbf{A}(t)\mathbf{u} + \mathbf{b}(t), \tag{2.4.10}$$

*with continuous coefficients on a time interval $[0,T]$ satisfies the **Lipschitz condition** with*

$$L = \sum_{i,j=1}^{n} \max_{t \in I} |A_{ij}(t)|. \tag{2.4.11}$$

Remark 2.4.2. *The initial-value problem:*

$$
\begin{cases}
\dfrac{d\mathbf{u}}{dt} = \mathbf{A}(t)\mathbf{u} + \mathbf{b}(t)\,, \\[2mm]
\mathbf{u}(t_0) = \mathbf{u}_0\,,
\end{cases}
\tag{2.4.12}
$$

with $A_{ij}(t)$ and $b_i(t)$ defined and continuous for $|t-t_0| \leq T$, has a unique solution for $|t-t_0| \leq T$, by Theorems 2.1–2.2.

Remark 2.4.3. *If $\mathbf{u}_1(t), \ldots, \mathbf{u}_m(t)$ are m solutions of the homogeneous linear system:*

$$
\frac{d\mathbf{u}}{dt} = \mathbf{A}(t)\mathbf{u}\,, \qquad \mathbf{u} \in \mathbb{R}^{\mathrm{n}}\,,
\tag{2.4.13}
$$

then any linear combination:

$$
\sum_{i=1}^{m} C_i \mathbf{u}_i(t)\,, \quad C_1, \ldots, C_m \in \mathbb{R}
\tag{2.4.14}
$$

is still a solution of (2.4.13).

Theorem 2.5   Solutions of the Linear Homogeneous Models

There exist n linearly independent solutions $\mathbf{u}_1, \ldots, \mathbf{u}_n$ of (2.4.13) such that any solution of (2.4.13) can be written as follows:

$$
\mathbf{u}(t) = \sum_{i=1}^{n} \widehat{C}_i \mathbf{u}_i(t)\,,
\tag{2.4.15}
$$

for suitable $\widehat{C}_1, \ldots, \widehat{C}_n \in \mathbb{R}$.

Remark 2.4.4. *The initial value problem:*

$$
\begin{cases}
\dfrac{d\mathbf{u}}{dt} = \mathbf{A}(t)\mathbf{u}\,, \\[2mm]
\mathbf{u}(t_0) = \mathbf{u}_0\,,
\end{cases}
\tag{2.4.16}
$$

is solved by imposing the n initial conditions to $\mathbf{u}(t)$, given by (2.4.15), to find the values of the constants $\widehat{C}_1, \ldots, \widehat{C}_n$.

A set of independent solutions for the homogeneous problem is called a ***fundamental set*** and it can be ordered into a matrix:

$$
\mathbf{U}(t) = \begin{pmatrix} u_{11}(t) & \cdots & u_{1n}(t) \\ \vdots & \ddots & \vdots \\ u_{n1}(t) & \cdots & u_{nn}(t) \end{pmatrix}
\tag{2.4.17}
$$

called the **fundamental matrix**.

The above results can be exploited to obtain also analytic solutions of the nonhomogeneous linear Eq. (2.4.10):

> **Theorem 2.6   Solutions of the Linear Models**
>
> *Any solution of Eq.(2.4.10) can be written as follows:*
>
> $$\mathbf{u}(t) = \sum_{i=1}^{n} C_i \mathbf{u}_i(t) + \widetilde{\mathbf{u}}(t) \,, \tag{2.4.18}$$
>
> *for suitable coefficients $C_1, \ldots, C_n \in \mathbb{R}$, where $\{\mathbf{u}_1(t), \ldots, \mathbf{u}_n(t)\}$ is a fundamental set for the homogeneous system (2.4.13) associated to (2.4.10), and $\widetilde{\mathbf{u}}$ is a solution of Eq. (2.4.10).*

Summarizing the results stated in the above Theorems, the solution of a linear initial value problem (2.4.12) is obtained according to the following steps:

Step 1. *Find a fundamental set $\{\mathbf{u}_1(t), \ldots, \mathbf{u}_n(t)\}$ for the homogeneous system (2.4.13) associated to (2.4.10).*

Step 2. *Find a solution $\widetilde{\mathbf{u}}$ of the nonhomogeneous system (2.4.10). This step sometimes can be made by inspection, otherwise one can use the rule which determines $\widetilde{\mathbf{u}}(t)$ as one of the following functions:*

$$\widetilde{\mathbf{u}}(t) = \mathbf{U}(t) \int \mathbf{U}^{-1}(t)\mathbf{b}(t) \, dt \,, \tag{2.4.19}$$

where $\mathbf{U}$ is the fundamental matrix defined by the functions obtained in Step 1, which amounts to choosing a constant of integration.

Step 3. *Impose the n initial conditions to (2.4.18) to find the values of the coefficients $C_1, \ldots, C_n$.*

In the case of systems of ordinary differential equations with constant coefficients:

$$\frac{d\mathbf{u}}{dt} = \mathbf{A}\mathbf{u} \,, \qquad \mathbf{u} \in \mathbb{R}^n \,, \tag{2.4.20}$$

it is possible to give a general procedure to complete Step 1, and Step 2 can be developed in a simplified way. In fact, one can look for solutions in the form:

$$\mathbf{u}(t) = \mathbf{v}e^{\lambda t} \,. \tag{2.4.21}$$

Substituting (2.4.21) into (2.4.20) indicates that λ and $\mathbf{v}$ have to satisfy:

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = \mathbf{0} \,. \tag{2.4.22}$$

Hence, they have to be an eigenvalue and the corresponding eigenvector of the matrix $\mathbf{A}$. Detailed calculations differ technically according to the fact that the number of distinct eigenvalues differs from n or is the same. In particular

• If $\mathbf{A}$ has n linearly independent eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$ corresponding to the eigenvalues $\lambda_1, \ldots, \lambda_n$ (which need not all be distinct and may be complex), then the solution of (2.4.20) is:

$$\mathbf{u} = C_1 \mathbf{v}_1 e^{\lambda_1 t} + \cdots + C_n \mathbf{v}_n e^{\lambda_n t}. \tag{2.4.23}$$

A complex conjugate pair of eigenvalues $\lambda_r \pm i\lambda_i$ and eigenvectors $\mathbf{v}_r \pm i\mathbf{v}_i$ gives rise to a solution:

$$\begin{aligned}\mathbf{u} &= (C_r + iC_i)(\mathbf{v}_r + i\mathbf{v}_i)e^{(\lambda_r + i\lambda_i)t} + (C_r - iC_i)(\mathbf{v}_r - i\mathbf{v}_i)e^{(\lambda_r - i\lambda_i)t} \\ &= 2e^{\lambda_r t}\Big[\big(C_r \mathbf{v}_r - C_i \mathbf{v}_i\big)\cos(\lambda_i t) - \big(C_r \mathbf{v}_i + C_i \mathbf{v}_r\big)\sin(\lambda_i t)\Big]. \end{aligned} \tag{2.4.24}$$

This matter has to be dealt with differently if there are eigenvalues with multiplicity $r > 1$ and $p < r$ corresponding eigenvectors. Without entering into details, we consider just the following particular case:

• If $\mathbf{A}$ has $n - 2$ distinct eigenvalues $\lambda_1, \ldots, \lambda_{n-2}$ with corresponding distinct eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_{n-2}$ and a double eigenvalue $\lambda_{n-1} = \lambda_n = \lambda$ corresponding to a single eigenvector $\mathbf{v}$, the solution of (2.4.20) is as follows:

$$\mathbf{u} = C_1 \mathbf{v}_1 e^{\lambda_1 t} + \cdots + C_{n-2} \mathbf{v}_{n-2} e^{\lambda_{n-2} t} + \Big[C_{n-1}\mathbf{v} + C_n(\mathbf{w} + \mathbf{v}t)\Big]e^{\lambda t}, \tag{2.4.25}$$

where $\mathbf{w}$ is a solution of $(\mathbf{A} - \lambda \mathbf{I})\mathbf{w} = \mathbf{v}$.

The case of a single equation of order n:

$$a_n \frac{d^n u}{dt^n} + \cdots + a_1 \frac{du}{dt} + a_0 u = 0 \tag{2.4.26}$$

is somewhat simpler since the procedure can be reduced to the solution of what is commonly called the ***characteristic equation***:

$$a_n \lambda^n + \cdots + a_1 \lambda + a_0 = 0. \tag{2.4.27}$$

A real root λ corresponds to the solution $(c_0 + \cdots + c_\mu t^\mu)e^{\lambda t}$, where μ is the multiplicity of λ. A complex conjugate pair, $\lambda^+ = \lambda_r + i\lambda_i$, and $\lambda^- = \lambda_r - i\lambda_i$, corresponds to the solution:

$$e^{\lambda_r t}\Big[(c_0 + \ldots + c_\mu t^\mu)\cos\lambda_i t + (d_0 + \ldots + d_\mu t^\mu)\sin\lambda_i t\Big], \tag{2.4.28}$$

where again μ is the multiplicity of λ^+.

2.4.3 Discretization schemes for initial value problems

Generally, mathematical models, as we have seen in various examples, are nonlinear. In this case, the analysis of mathematical problems needs more sophisticated analytic methods and explicit solutions are almost never obtained, while computational schemes have to be applied. The above schemes are all based on the concept of discretizing the time variable $t \in [t_0, T]$ into a suitable set:

$$I_t = \{t_0, \ldots, t_i, \ldots, t_n = T\}, \tag{2.4.29}$$

and by approximating the solution in the points of the discretization by suitable algorithms.

This section provides a brief survey to deal with the above discretization scheme. The analysis is in two steps. We first introduce the concepts of **accuracy** and **stability**.

In order to understand these concepts, consider the simplest conceivable method for solving initial-value problems, the forward Euler method. If one knows the state variable at time t_i and wants to compute its value at time $t_{i+1} = t_i + h$, the simplest idea consists in approximating the solution of:

$$\begin{cases} \dfrac{d\mathbf{u}}{dt} = \mathbf{f}(t, \mathbf{u}), \\[2mm] \mathbf{u}(t_i) = \mathbf{u}_i. \end{cases} \tag{2.4.30}$$

with:

$$\mathbf{u}_{i+1} = \mathbf{u}_i + h\mathbf{f}(t_i, \mathbf{u}_i). \tag{2.4.31}$$

Since:

$$\mathbf{f}\big(t_i, \mathbf{u}(t_i)\big) = \frac{d\mathbf{u}}{dt}(t_i), \tag{2.4.32}$$

the above discretization corresponds to a Taylor expansion of the solution u stopped at first order, which corresponds somewhat to following the direction of the tangent to the solution in t_i, as shown in a scalar case in Figure 2.4.1.
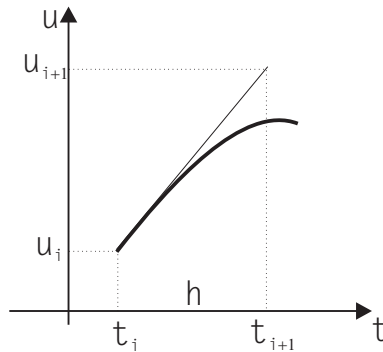

Figure 2.4.1 — Representation of forward Euler method

Truncation Error

*The **truncation error** T_{err} is defined as the norm of the difference between the solution to the differential equation and the numerical solution divided by the time step used in the numerical scheme.*

In the case of forward Euler method it can be proved, under suitable regularity assumptions, that for each component:

$$T_{\mathrm{err}} \cong -\frac{h}{2}\frac{d^2 u}{dt^2}(\xi)\,, \qquad \xi \in (t_i, t_{i+1})\,, \tag{2.4.33}$$

where ξ changes from component to component.

Accuracy

*If the truncation error goes like h^p, the **method is $\mathbf{p}^{th}$ order**, which means that halving the step divides the error by 2^p. This is what is generally meant by **accuracy of the method**.*

From (2.4.33), for the forward Euler method the error goes like h and one has a first order method.

Another important requirement of a numerical scheme is that the time step has to be chosen so that the scheme is ***absolutely stable***:

Absolute Stability

*A numerical scheme is **absolutely stable** in a point ah of the complex plane if a sequence $\{u_i\}$ generated by the method applied to the model:*

$$\frac{du}{dt} = au\,, \tag{2.4.34}$$

with time step $\Delta t = h$ is bounded for $i \to +\infty$.

Stability Region

*The **stability region** is the set of points ah in the complex plane for which the method is absolutely stable*

It can be proved that each scheme is characterized by a stability region, which can be used to determine a condition on the time step to be used in the integration. The procedure to be used is the following:

Step 1. Starting from a nonlinear model, consider its linearized form:

$$\frac{d\mathbf{u}}{dt} = \mathbf{Au}\,, \tag{2.4.35}$$

obtained for instance by linearization about the initial condition;

Step 2. Compute the eigenvalues $\lambda_1, \ldots, \lambda_n$ of $\mathbf{A}$, the so-called spectrum of the linearized model;

Step 3. Choose, if possible, a not too restrictive time step h such that $h\lambda_1$, $\ldots$, $h\lambda_n$ all belong to the stability region.

Therefore, the numerical errors are not amplified as the integration is continued. If, instead, there are some eigenvalues which remain outside the stability region, then one must be aware that the numerical errors grow exponentially in time. The literature on computational methods reports about a large variety of algorithms to obtain simulations of finite models. The interested reader is addressed to Chapter 3 of the book Bellomo and Preziosi (1995) as well as to Marasco and Romano (2001) for computational schemes.

Consider, as an example of algorithm, the ***Runge–Kutta methods*** which are very popular for their adaptability and versatility and work quite well for all nonstiff problems. They are obtained by evaluating the function f at different values of t and u, and by suitably combining of these values. In this way it is possible to obtain methods of any order of accuracy. For instance, one has:

$$2^{\text{nd}} \text{ order}: \quad \mathbf{u}_{i+1} = \mathbf{u}_i + \frac{h}{2}\left(\mathbf{K}_1 + \mathbf{K}_2\right), \tag{2.4.36}$$

where

$$\mathbf{K}_1 = \mathbf{f}(t_i, \mathbf{u}_i), \qquad \mathbf{K}_2 = \mathbf{f}(t_i + h, \mathbf{u}_i + h\mathbf{K}_1). \tag{2.4.37}$$

$$3^{\text{rd}} \text{ order}: \quad \mathbf{u}_{i+1} = \mathbf{u}_i + \frac{h}{6}\left(\mathbf{K}_1 + 4\mathbf{K}_2 + \mathbf{K}_3\right), \tag{2.4.38}$$

where

$$\begin{aligned} \mathbf{K}_1 &= \mathbf{f}(t_i, \mathbf{u}_i), \\ \mathbf{K}_2 &= \mathbf{f}\left(t_i + \frac{h}{2}, \mathbf{u}_i + \frac{h}{2}\mathbf{K}_1\right), \\ \mathbf{K}_3 &= \mathbf{f}\left(t_i + h, \mathbf{u}_i + h(2\mathbf{K}_2 - \mathbf{K}_1)\right). \end{aligned} \tag{2.4.39}$$

$$4^{\text{th}} \text{ order}: \quad \mathbf{u}_{i+1} = \mathbf{u}_i + \frac{h}{6}\left(\mathbf{K}_1 + 2\mathbf{K}_2 + 2\mathbf{K}_3 + \mathbf{K}_4\right), \tag{2.4.40}$$

where

$$\begin{aligned} \mathbf{K}_1 &= \mathbf{f}(t_i, \mathbf{u}_i), \\ \mathbf{K}_2 &= \mathbf{f}\left(t_i + \frac{h}{2}, \mathbf{u}_i + \frac{h}{2}\mathbf{K}_1\right), \\ \mathbf{K}_3 &= \mathbf{f}\left(t_i + \frac{h}{2}, \mathbf{u}_i + \frac{h}{2}\mathbf{K}_2\right), \\ \mathbf{K}_4 &= \mathbf{f}(t_i + h, \mathbf{u}_i + h\mathbf{K}_3). \end{aligned} \tag{2.4.41}$$

Recalling that the initial-value problem with initial condition $\mathbf{u}(t_i) = \mathbf{u}_i$ can be written in integral form as:

$$\mathbf{u}(t) = \mathbf{u}_i + \int_{t_i}^{t} \mathbf{f}\big(s, \mathbf{u}(s)\big)\, ds\,, \tag{2.4.42}$$

and, in particular,

$$\mathbf{u}(t_{i+1}) = \mathbf{u}_{t_i} + \int_{t_i}^{t_{i+1}} \mathbf{f}\big(s, \mathbf{u}(s)\big)\, ds\,, \tag{2.4.43}$$

it can be observed that both the third-order and the fourth-order methods are closely related to Simpson's rule applied to the integrals in (2.4.43).

The stability regions of the second-order method has an ellipsoidal shape, while that of the third-order and fourth-order methods are bean-like shaped.

Third-order and fourth-order Runge–Kutta methods are recommended in dealing with problems for which the spectrum is not available, since they include both a part of the imaginary axis and a part of the negative real axis. The disadvantage of these schemes is that several evaluations of $\mathbf{f}$ have to be performed per time step and therefore if the computation of $\mathbf{f}$ is very heavy, this method may demand an excessive amount of labor per step and becomes inconvenient.

Runge–Kutta methods have the property of being self-starting as well as adaptive. In other words, the time step can be changed at any moment according to an estimate of the local error. Unfortunately, it is not trivial to get the above estimate of time step. In this case, to be practical, the time step has then to be decreased if the difference between the two values (over h) is larger than a specified maximum tolerance and can be increased if this difference is smaller than the minimum required tolerance. Of course, this checking is time consuming.

2.4.4 On boundary value problems

Boundary-value problems for ordinary differential equations with time as independent variable often arise in several applications. For example when some of the initial conditions at $t = t_0$ cannot be measured and are replaced by the corresponding conditions at a certain control time, say $t = t_1$, where their identification is possible.

Finding a solution to boundary-value problems is not an easy task. We remember that initial-value problems generally have unique solutions, while some boundary-value problems may have more than one solution and others have no solutions at all, as it will be shown in the Example 2.4.1 in what follows.

An existence theorem may be formulated for linear boundary-value problems. Here, we will refer to a linear second order problem:

$$\begin{cases} \dfrac{d^2u}{dt^2} + a_1(t)\dfrac{du}{dt} + a_0(t)u = b(t)\,, \\[2mm] u(t_0) = u_0\,, \\[2mm] u(t_1) = u_1\,, \end{cases} \tag{2.4.44}$$

and consider the following theorem:

Theorem 2.7   Existence and uniqueness

If a_0, a_1, and b are continuous in $[t_0, t_1]$ and if

$$
t_1 - t_0 < \begin{cases} \dfrac{2}{A_1} & \text{if } a_0(t) = 0 \,, \\[2ex] 2\dfrac{\sqrt{A_1^2 + 2A_0} - A_1}{A_0} & \text{otherwise} \,, \end{cases}
\tag{2.4.45}
$$

where

$$
|a_0(t)| \leq A_0 \;\; \text{and} \;\; |a_1(t)| \leq A_1 \qquad \forall t \in [t_0, t_1] \,,
$$

then the boundary-value problem (2.4.44) has a unique solution in $[t_0, t_1]$.

Remark 2.4.5. *When the existence of the solution of a linear boundary value problem is assured (for example from Theorem 2.7), we can apply to the problem the results of Theorems 2.5–2.6. Then, imposing the initial and/or boundary conditions we get the solution of the problem.*

In order to clarify the importance of the existence and uniqueness issues related to boundary-value problems, consider the following example.

$$\text{\emph{Example 2.4.1}}$$
$$\text{\emph{Nonuniqueness and Buckling of a Rod}}$$

Consider a simple mass-spring system governed by the ordinary differential equation:

$$
\frac{d^2 u}{dt^2} + \Omega^2 u = 0 \,,
\tag{2.4.46}
$$

where $\Omega^2 = k/m$, which has solution:

$$
u(t) = C_1 \cos(\Omega\, t) + C_2 \sin(\Omega\, t) \,.
\tag{2.4.47}
$$

If we join to (2.4.46) the initial conditions:

$$
u(0) = u_0 \qquad \text{and} \qquad \frac{du}{dt}(0) = u_0' \,,
\tag{2.4.48}
$$

the unique solution is:

$$
u(t) = u_0 \cos(\Omega t) + \frac{u_0'}{\Omega} \sin(\Omega t) \,.
\tag{2.4.49}
$$

In a similar way, if we join to (2.4.46) the boundary conditions:

$$
u(0) = u_0 \qquad \text{and} \qquad u(T) = u_T \,,
\tag{2.4.50}
$$

with $T \neq h\pi/\Omega$, $h \in \mathbf{N}$, we again have a unique solution:

$$u(t) = u_0 \cos(\Omega t) + \frac{u_T - u_0 \cos(\Omega T)}{\sin(\Omega T)} \sin(\Omega t) \ . \tag{2.4.51}$$

If $T = h\pi/\Omega$, the boundary-value problem has no solution at all if $u_T \neq (-1)^h u_0$, and infinitely many solutions given by:

$$u(t) = u_0 \cos(\Omega t) + C \sin(\Omega t), \quad \forall C \in \mathbb{R}, \tag{2.4.52}$$

if $u_T = (-1)^h u_0$.

The existence theorem considered above assures existence and uniqueness only if:

$$T < \frac{2\sqrt{2}}{\Omega} < \frac{\pi}{\Omega} \ . \tag{2.4.53}$$

Using the following argument this result can be used to explain the buckling of a rod. Consider a rod of length T subject at its ends to a compressive load F, as shown in Figure 2.4.2. The linear theory of elasticity tells us that for small deformations the angle of deflection u of the rod can be found by solving (2.4.46) with $\Omega^2 = F/(EI)$, where E is Young's modulus of elasticity for the rod, and I is the moment of inertia of the cross section of the rod about its axis.
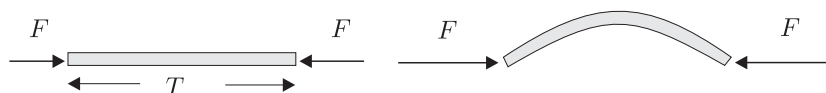
Figure 2.4.2 — Buckling of a rod: (a) small loads, (b) large loads

The previous discussion can then be reprocessed in the following terms: if $T < \pi/\Omega$, that is if $F < EI\pi^2/T^2$, then there is no deflection, but as soon as F reaches the critical compressive load (first buckling load) $F = EI\pi^2/T^2$, the solution is not unique and no longer small, which also indicates a failure of the linear theory of elasticity to model the situation.

$\square$

2.5 Stability Methods

As already mentioned, it is possible to give a general procedure to obtain analytic solutions only for some classes of linear differential equations or for very special nonlinear problems. On the other hand, it is impossible in most cases to find analytic solutions. It is then desirable to have at least some knowledge on the qualitative behavior of the solution.

In details, this Section is organized in three subsection which follows this brief introduction. The first subsection proposes some preliminary definitions, while the next two subsections explain suitable methods for the analysis of the stability of equilibrium configurations, respectively the linear stability method the first subsection, and the nonlinear stability method the second one.

2.5.1 Stability Definitions

In view of the study of the equilibrium configurations and their stability of a mathematical model, we introduce the following definition:

Equilibrium points

Consider the autonomous system of ordinary differential equations:

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u}) \, . \tag{2.5.1}$$

The states $\mathbf{u}_e$ such that:

$$\mathbf{f}(\mathbf{u}_e) = \mathbf{0} \tag{2.5.2}$$

*are called the **equilibrium points**. If $\mathbf{u}(t_0) = \mathbf{u}_e$, then $\mathbf{u}(t) = \mathbf{u}_e$ for all times.*

It is trivial to verify that if an equilibrium point is occupied initially, it is maintained for all times.

The next problem is to decide whether an initially perturbed system gradually returns back to the equilibrium point, or at least remains next to it, or wanders away. The following definitions are given:

Stability and instability of equilibrium points

*The equilibrium state $\mathbf{u}_e$ is said to be **stable** if for any $\varepsilon > 0$ it is possible to find a $\delta(\varepsilon) > 0$ such that for any initial condition $\mathbf{u}(t_0)$ with:*

$$\left\| \mathbf{u}(0) - \mathbf{u}_e \right\| < \delta(\varepsilon) \, , \tag{2.5.3}$$

one has that:

$$\left\| \mathbf{u}(t) - \mathbf{u}_e \right\| < \varepsilon \qquad \forall \, t \geq t_0 \, . \tag{2.5.4}$$

*An equilibrium state that is not stable is called **unstable**.*

Asymptotic stability and basin of attraction

*A stable equilibrium point $\mathbf{u}_e$ is also **asymptotically stable** if there is a neighborhood $\mathcal{D}_e$ of $\mathbf{u}_e$ such that for $\mathbf{u}(t_0) \in \mathcal{D}_e$, one has:*

$$\lim_{t \to +\infty} \left\| \mathbf{u}(t) - \mathbf{u}_e \right\| = 0 \,. \tag{2.5.5}$$

*The largest possible $\mathcal{D}_e$ is called the **basin of attraction** of $\mathbf{u}_e$ and is denoted in the following by $\mathcal{B}_e$.*

The definition of stability has a local meaning. Indeed, if we want that the system remains, within a given tolerance, near $\mathbf{u}_e$, the initial condition has to be sufficiently close to $\mathbf{u}_e$. In general an equilibrium position can be stable to small perturbations, but unstable to large ones.

Conditional stability and global stability

*Consider an asymptotically stable equilibrium point. If it is stable with respect to small perturbations but unstable with respect to large ones, then the basin of attraction $\mathcal{B}_e$ is not the entire space and only the solutions starting in $\mathcal{B}_e$ will tend toward $\mathbf{u}_e$. In this case $\mathbf{u}_e$ is said to be **conditionally stable**, otherwise $\mathbf{u}_e$ is said to be **globally stable**.*

2.5.2 Linear Stability Methods

The aim of this subsection is to provide suitable methods for linear stability analysis of equilibrium points. The simplest approach to establish the stability properties of an equilibrium configuration is to investigate what happens if the perturbation is very small. The stability condition we will provide is often referred to as the *linear stability criterion*.

Consider then the autonomous system (2.5.1) and the expansion of $\mathbf{f}$ in a Taylor series about the equilibrium state, which can be performed under suitable regularity assumptions on $\mathbf{f}$. In this way it is possible to approximate each component of $f_i(\mathbf{u})$, $i = 1, \ldots, n$ as follows:

$$f_i(\mathbf{u}) \approx f_i(\mathbf{u}_e) + (\mathbf{u} - \mathbf{u}_e) \cdot \nabla f_i(\mathbf{u}_e) + o\Big(|\mathbf{u} - \mathbf{u}_e|\Big) \,, \tag{2.5.6}$$

where by the definition of equilibrium point $f_i(\mathbf{u}_e) = 0$. Therefore for infinitesimal perturbations $\mathbf{v} = \mathbf{u} - \mathbf{u}_e$ about the equilibrium state, one can neglect the other terms in the expansion, and the differential system (2.5.1) can be approximated by its linearized form:

$$\frac{d\mathbf{v}}{dt} = \mathbf{J}(\mathbf{u}_e)\mathbf{v} \,, \tag{2.5.7}$$

where $\mathbf{J}$ is the Jacobian matrix of the vector $\mathbf{f}$:

$$\mathbf{J} = \begin{pmatrix} \dfrac{\partial f_1}{\partial u_1} & \dfrac{\partial f_1}{\partial u_2} & \cdots & \dfrac{\partial f_1}{\partial u_n} \\[2ex] \dfrac{\partial f_2}{\partial u_1} & \dfrac{\partial f_2}{\partial u_2} & \cdots & \dfrac{\partial f_2}{\partial u_n} \\[2ex] \vdots & \vdots & \ddots & \vdots \\[2ex] \dfrac{\partial f_n}{\partial u_1} & \dfrac{\partial f_n}{\partial u_2} & \cdots & \dfrac{\partial f_n}{\partial u_n} \end{pmatrix}. \tag{2.5.8}$$

Equation (2.5.7) is a linear differential system with constant coefficients which can be solved using the analytic methods presented in Section 2.4.

It is possible to relate these reasoning on the linearized system (2.5.7) to the behavior of the nonlinear system via the following classical ***linearized stability criterion***.

> ***Theorem 2.8   Linear stability***
>
> *If $\mathbf{f}(\mathbf{u})$ is twice continuously differentiable, denoting by λ_i the eigenvalues of the Jacobian matrix evaluated at the equilibrium state and by $\Re e(\lambda_i)$ the real part of λ_i, one has:*
>
> *If $\forall\, i = 1, \ldots, n$ $\Re e(\lambda_i) < 0$, then $\mathbf{u}_e$ is **asymptotically stable**;*
>
> *If $\exists\, \widehat{\imath}$ such that $\Re e(\lambda_{\widehat{\imath}}) > 0$, then $\mathbf{u}_e$ is **unstable**.*

It is crucial to remark that this theorem guarantees the existence of a ***sufficiently small*** neighborhood $\mathcal{I}_e$ of $\mathbf{u}_e$ such that if $\mathbf{u}(t_0) \in \mathcal{B}_e$, then $\mathbf{u}(t)$ tends to $\mathbf{u}_e$, but does not give an algorithm for the actual computation of the basin of attraction $\mathcal{D}_e$. For this reason, this criterion is also named ***stability with respect to infinitesimal perturbations***. This is certainly a limit to the utility of the above theorem for the applications. However, it is useful for instability analysis. Indeed, if $\mathbf{u}_e$ is linearly unstable, i.e., unstable with respect to infinitesimal perturbations, then it is also unstable to larger perturbations.

If $\mathbf{u}_e$ is asymptotically stable, then (2.5.7) can be solved to describe the evolution of the system for suitably small initial values.

The above concepts can be specialized in the case of two-dimensional dynamic systems such that the Jacobian defined in (2.5.8) is a 2×2 square matrix. In this case some particular dynamic responses can be classified and their qualitative behavior can be visualized. In particular, we consider the following two cases:

• If λ_1 and λ_2 are both real eigenvalues, then, if $\lambda_1 \neq \lambda_2$ the solution of (2.5.7) can be written as Eq. (2.4.23), which reduces to:

$$\mathbf{v}(t) = C_1\mathbf{v}_1 e^{\lambda_1 t} + C_2\mathbf{v}_2 e^{\lambda_2 t}, \tag{2.5.9}$$

where C_1 and C_2 are integration constants, and $\mathbf{v}_1$ and $\mathbf{v}_2$ are the eigenvectors of $\mathbf{J}$.
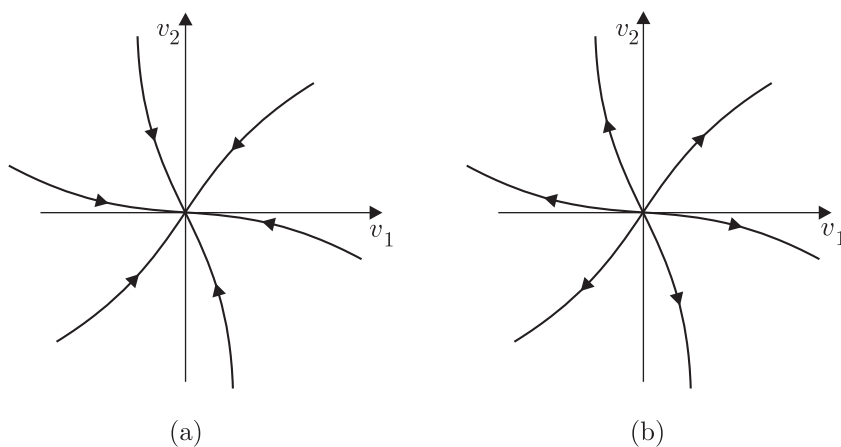
Figure 2.5.1 — Qualitative behavior of the dynamic response: (a) stable, (b) unstable node.

In particular, if λ_1 and λ_2 are both negative, one has:

$$\lim_{t \to +\infty} \mathbf{v}(t) = \mathbf{0}, \qquad (2.5.10)$$

and this equilibrium point is called a **stable node**. On the other hand, if one of the eigenvalue is positive, it follows that:

$$\lim_{t \to +\infty} \mathbf{v}(t) = +\infty. \qquad (2.5.11)$$

The equilibrium point is called an **unstable node** if both eigenvalues are positive and a **saddle point** otherwise. In this latter case, two of the trajectories meet at the equilibrium point and two depart from it. They are therefore called **stable and unstable manifolds**.
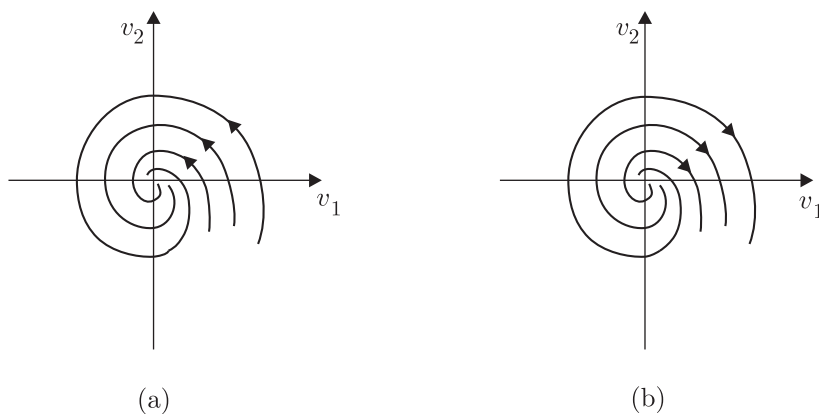
Figure 2.5.2 — Qualitative behavior of the dynamic response: (a) stable and (b) unstable focus.

• If the eigenvalues are complex conjugate, i.e., $\lambda_1 = \lambda + i\omega$, $\lambda_2 = \lambda - i\omega$, the solution to the

initial-value problem (2.5.7) can be written as in Eq. (2.4.24) by a linear combination of sine and cosine functions.

In particular, if:

$$\lambda = \Re e(\lambda_1) = \Re e(\lambda_2) < 0 \quad \Rightarrow \quad \lim_{t \to +\infty} \mathbf{v}(t) = \mathbf{0} \,, \tag{2.5.12}$$

the equilibrium point is called a **stable focus**. If, instead,

$$\lambda = \Re e(\lambda_1) = \Re e(\lambda_2) > 0 \quad \Rightarrow \quad \lim_{t \to +\infty} |\mathbf{v}(t)| = +\infty \,, \tag{2.5.13}$$

the equilibrium point is called an **unstable focus**. Finally, if:

$$\lambda = \Re e(\lambda_1) = \Re e(\lambda_2) = 0 \,,$$

then $\mathbf{v}(t)$ stays bounded and the equilibrium state is a **center point**.

The qualitative behavior of the solution in the case of stable and unstable node is represented in Figure 2.5.1. The qualitative behavior of the solution in the case of stable and unstable focus is represented in Figure 2.5.2.

(a)   (b)
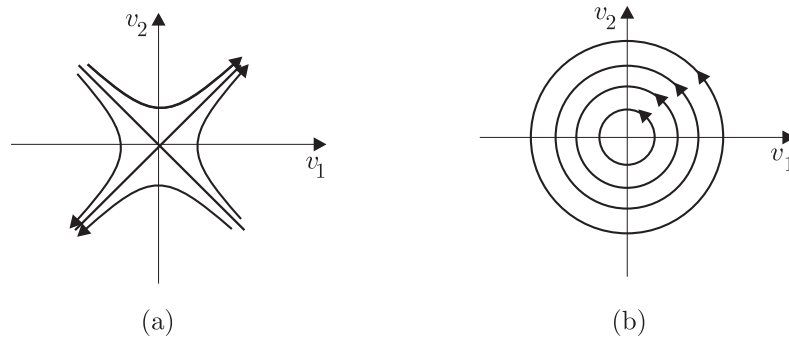
Figure 2.5.3 — Qualitative behavior of the dynamic response: (a) saddle and (b) center point.

Finally, the qualitative behavior of the solution in the case of saddle and center point is represented in Figure 2.5.3.

If $\lambda_1 = \lambda_2$, the discussion gives the same results though (2.5.9) cannot be the solution of (2.5.7) as shown in (2.4.23).

Note that for $n = 2$ the eigenvalues of $\mathbf{J}$ are:

$$\lambda = \frac{\operatorname{tr} \mathbf{J}}{2} \pm \sqrt{\frac{(\operatorname{tr} \mathbf{J})^2}{4} - \det \mathbf{J}} \,, \tag{2.5.14}$$

where $\operatorname{tr} \mathbf{J} = J_{11} + J_{22}$, and have both negative real part if and only if:

$$\operatorname{tr} \mathbf{J} < 0 \qquad \text{and} \qquad \det \mathbf{J} > 0 \,. \tag{2.5.15}$$

Example 2.5.1
Stability for the van der Pol Model

As an example, consider the van der Pol model which can for instance model the behavior of some nonlinear electric circuits. The mathematical model can be written as follows:

$$\begin{cases} \dfrac{di}{dt} = v\,, \\[2mm] \dfrac{dv}{dt} = (\alpha - \beta i^2)v - \gamma i\,, \end{cases} \tag{2.5.16}$$

and is characterized by a unique equilibrium given by:

$$\begin{cases} v = 0\,, \\[2mm] (\alpha - \beta i^2)v + \gamma i = 0\,, \end{cases} \tag{2.5.17}$$

that is $i = v = 0$, which, according to what has just been stated, is linearly stable if α is negative, as the Jacobian:

$$\mathbf{J}(i = v = 0) = \begin{pmatrix} 0 & 1 \\ -\gamma & \alpha \end{pmatrix} \tag{2.5.18}$$

has always positive determinant and trace equal to α. Hence, the equilibrium point is stable if $\alpha < 0$. More in details, the eigenvalues of the Jacobian are:

$$\lambda = \frac{1}{2}\left[\alpha \pm \sqrt{\alpha^2 - 4\gamma}\right]\,, \tag{2.5.19}$$

which are complex conjugate if $|\alpha| < 2\sqrt{\gamma}$, and real if $|\alpha| \geq 2\sqrt{\gamma}$.

The stability results can be summarized in the following table:

α	eigenvalues	stability result
$\alpha \leq -2\sqrt{\gamma}$	real and negative	stable node
$-2\sqrt{\gamma} < \alpha < 0$	complex with $\Re e(\lambda) < 0$	stable focus
$\alpha = 0$	purely imaginary $(\pm i\sqrt{\gamma})$	center point
$0 < \alpha < 2\sqrt{\gamma}$	complex with $\Re e(\lambda) > 0$	unstable focus
$\alpha \geq 2\sqrt{\gamma}$	real and positive	unstable node

Figure 2.5.4 — Stability analysis for the van der Pol Model

□

2.5.3 Nonlinear Stability

The linear stability criterion guarantees stability with respect to indefinitely small disturbances. To obtain this result one has to study the linear system (2.5.7), which is an approximation of the real model. In order to obtain more information on nonlinear stability criteria by only using the right-hand side of the ordinary differential equation, Liapunov suggested a method which for this reason is usually called **Liapunov direct method**. For those who are not familiar with stability theory, the method consists in finding a function, called **Liapunov function**, which essentially plays the role of a **generalized energy** for the system. If this "energy" decreases as the system evolves, i.e., if the system is **dissipative**, then the system will tend to a stable configuration.

Bearing this in mind, we introduce the following concept:

Liapunov function

*Let $\mathbf{u}_e$ be an isolated equilibrium of the system of equation $\dfrac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u})$ in some open neighborhood $\mathcal{D}_e$ of $\mathbf{u}_e$. A function $V = V(\mathbf{u})$ is called a **Liapunov function** if it satisfies the following properties:*

i) It is continuous in $\mathcal{D}_e$ and differentiable in $\mathcal{D}_e - \{\mathbf{u}_e\}$;

ii) It has a local minimum in $\mathbf{u}_e$, i.e., for instance:

$$V(\mathbf{u}_e) = 0\,, \qquad V(\mathbf{u}) > 0 \qquad \text{for} \ \ \mathbf{u} \in \mathcal{D}'_e - \{\mathbf{u}_e\}$$

with $\mathcal{D}'_e$ open neighborhood of $\mathbf{u}_e$;

iii) It is a nonincreasing function of time over any solution $\mathbf{u}(t)$ with initial condition $\mathbf{u}(t_0) = \mathbf{u}_0 \in \mathcal{D}_e - \{\mathbf{u}_e\}$, i.e. $\forall\, t \geq t_0$:

$$\frac{dV}{dt}\big(\mathbf{u}(t)\big) = \sum_{i=1}^{n} \frac{\partial V}{\partial u_i}\frac{du_i}{dt} = \sum_{i=1}^{n} \frac{\partial V}{\partial u_i} f_i\big(\mathbf{u}(t)\big) \leq 0\,. \tag{2.5.20}$$

Theorem 2.9   Liapunov stability

If there exists a Liapunov function V in a neighborhood $\mathcal{D}_e$ of the isolated equilibrium state $\mathbf{u}_e$, then $\mathbf{u}_e$ is stable. Furthermore, if $\dfrac{dV}{dt}\big(\mathbf{u}(t)\big) < 0$, then $\mathbf{u}_e$ is also asymptotically stable.

It is important to remark that the condition $\dfrac{dV}{dt}\big(\mathbf{u}(t)\big) < 0$ means that V decreases as the system evolves. This implies that the trajectory will remain in the region delimited by the level curve $V(\mathbf{u}) = V(\mathbf{u}_0)$.

It is hard to say, in general, how to proceed to identify the best Liapunov function. For

instance, in the case of systems of two equations, let consider the quadratic function:

$$V = av_1^2 + 2bv_1v_2 + v_2^2 \qquad (2.5.21)$$

with $a > b^2$, that is always nonnegative. Then one has to check that the sign of:

$$\frac{1}{2}\frac{dV}{dt} = \big(av_1 + bv_2\big)f_1(v_1, v_2) + \big(bv_1 + v_2\big)f_2(v_1, v_2) \qquad (2.5.22)$$

be negative in some region near $v_1 = v_2 = 0$ for some values of a and b with $a > b^2$.

Another method is to look for V as a quadratic form $V = \mathbf{v} \cdot \mathbf{A}\mathbf{v}$ with $\mathbf{A}$ such that:

$$\mathbf{J}^T\mathbf{A} + \mathbf{A}\mathbf{J} = -\mathbf{I}, \qquad (2.5.23)$$

where $\mathbf{J}$ is the Jacobian of f in $\mathbf{v} = \mathbf{0}$, and $\mathbf{I}$ is the identity matrix.

Liapunov Theorem 2.9 is partially inverted by the following theorem:

Theorem 2.10   Chetayev theorem

Let $\mathbf{u}_e$ be an isolated equilibrium of $d\mathbf{u}/dt = \mathbf{f}(\mathbf{u})$ in some open set $\mathcal{D}$. If there exists a differentiable function $V = V(\mathbf{u})$ and an open set $\mathcal{D}_+$ such that

i) $\mathbf{u}_e$ belongs to the border $\partial\mathcal{D}_+$ of $\mathcal{D}_+$,

ii) $V(\mathbf{u}) > 0$ in $\mathcal{D}_+$ and $V(\mathbf{u}) = 0$ on $\partial\mathcal{D}_+$,

iii) $\dfrac{dV}{dt} > 0$ in $\mathcal{D}_+$,

then $\mathbf{u}_e$ is unstable.

Example 2.5.2
Stability through Liapunov Method

Consider the system:

$$\begin{cases} \dfrac{du_1}{dt} = -u_1 + u_2\,, \\[2mm] \dfrac{du_2}{dt} = u_2 + 2u_1u_2\,, \end{cases} \qquad (2.5.24)$$

which has $u_1 = u_2 = 0$ and $u_1 = u_2 = -1/2$ as equilibrium points. In order to check the nonlinear stability of $u_1 = u_2 = -1/2$, it is useful to introduce the perturbation (v_1, v_2) defined by:

$$u_1 = -\frac{1}{2} + v_1\,, \qquad u_2 = -\frac{1}{2} + v_2\,. \qquad (2.5.25)$$

Eq. (2.5.24) then rewrites in terms of the new variables as:

$$\begin{cases} \dfrac{dv_1}{dt} = -v_1 + v_2\,, \\[2mm] \dfrac{dv_2}{dt} = -v_1 + 2v_1v_2\,. \end{cases} \qquad (2.5.26)$$

Consider the function:

$$V = v_1^2 - v_1 v_2 + \frac{3}{2} v_2^2 \,, \qquad (2.5.27)$$

which is positive definite as can be written as $V = \mathbf{v} \cdot (\mathbf{A}\mathbf{v})$, where $\mathbf{v} = (v_1, v_2)$ and

$$\mathbf{A} = \begin{pmatrix} 1 & -\dfrac{1}{2} \\[2mm] -\dfrac{1}{2} & \dfrac{3}{2} \end{pmatrix} \qquad (2.5.28)$$

has both positive eigenvalues.

The computation of dV/dt yields:

$$\frac{dV}{dt} = (2v_1 - v_2)\frac{dv_1}{dt} + (3v_2 - v_1)\frac{dv_2}{dt} = -v_1^2 - v_2^2 + 6v_1 v_2^2 - 2v_1^2 v_2 \,. \qquad (2.5.29)$$

Rewriting $-v_1^2 - v_2^2 + 6v_1 v_2^2 - 2v_1^2 v_2 \le 0$ as follows:

$$(2v_2 + 1)v_1^2 - 6v_1 v_2^2 + v_2^2 \ge 0 \,, \qquad (2.5.30)$$

the equality is solved by:

$$v_1 = \frac{3v_2^2 \pm \sqrt{v_2^2(9v_2^2 - 2v_2 - 1)}}{2v_2 + 1} \,. \qquad (2.5.31)$$

If $9v_2^2 - 2v_2 - 1 \le 0$, that is, if

$$v_2 \in I = \left[\frac{1 - \sqrt{10}}{9} \,, \; \frac{1 + \sqrt{10}}{9} \right] \,,$$

then (2.5.30) is always satisfied, as in I, $2v_2 + 1 > 0$.

$\square$

2.6 Regular and Singular Perturbation Methods

As we have already seen, mathematical models must always be written in terms of suitable dimensionless variables. This technical manipulation may generate dimensionless numbers which are small with respect to unity, while the independent and dependent variables are of the order of unity. Almost always, these parameters have a well defined physical meaning which should be related to the solution of mathematical problems (or vice versa).

This section provides a brief introduction to regular and singular perturbation methods by means of simple examples where the dependent variable is a scalar or a two dimension vector.

We first define a **_perturbed_** model. Let ε be a positive number which is small with respect to unity.

Regularly Perturbed Model

A finite mathematical model:

$$\begin{cases} \dfrac{du}{dt} = f(t, u, \varepsilon) \,, \\[2mm] u(t_0, \varepsilon) = u_0(\varepsilon) \,. \end{cases} \qquad (2.6.1)$$

*is called **regularly perturbed** if $f(t, u, \varepsilon)$ and $u_0(\varepsilon)$ depend smoothly on their arguments.*

Singularly Perturbed Model

*A finite mathematical model is called **singularly perturbed** if it can be written as*

$$\begin{cases} \varepsilon \dfrac{du}{dt} = f(t, u) \,, \\[2mm] u(t_0, \varepsilon) = u_0(\varepsilon) \,. \end{cases} \qquad (2.6.2)$$

The above definitions are given for a scalar problem. Their generalization to systems of equations requires technical additional calculations..

As it is shown in the examples which follow, the parameter ε (in a regularly perturbed problem) is linked to the presence in the model of nearly negligible physical phenomena, while in a singularly perturbed problem the parameter ε is generally related to the scaling and to the dimensional analysis of the variables.

Different methods have to be developed for each of the above classes of models, as it will be shown in the next subsections. The starting point is the idea of looking for an asymptotic expansion, in the sense of Poincaré, for $\varepsilon \to 0$, uniformly valid in an interval $[t_0, T]$, for the solution $u(t, \varepsilon)$ of the perturbed problem, and we write:

$$u(t, \varepsilon) \sim \sum_{i=0}^{\infty} u_i(t)\varepsilon^i \qquad \text{as} \qquad \varepsilon \to 0 \,. \qquad (2.6.3)$$

This means that there exists a positive constant ε_0 and that $\forall N \geq 0$, there exist functions $\{u_i(t)\}_{i=0}^{N}$ defined in $[t_0, T]$, and a positive constant K_N such that:

$$\left| \frac{u(t, \varepsilon) - \sum_{i=0}^{N} u_i(t)\varepsilon^i}{\varepsilon^{N+1}} \right| < K_N, \qquad (2.6.4)$$

for all $\varepsilon \in (0, \varepsilon_0)$ and for all $t \in [t_0, T]$.

Using the Landau symbol "O", condition (2.6.4) can be written:

$$u(t, \varepsilon) = \sum_{i=0}^{N} u_i(t)\varepsilon^i + O(\varepsilon^{N+1}) \qquad \text{as} \qquad \varepsilon \to 0 \,, \qquad (2.6.5)$$

uniformly valid for $t \in [t_0, T]$. The series on the right-hand side of (2.6.3) is called asymptotically convergent, uniformly in $[t_0, T]$. The concepts of convergent series and asymptotically convergent series are quite different: we refer to De Jager and Furu (1996) for a discussion about convergence versus asymptotic convergence.

Starting from the above preliminaries it is shown in the next subsection how to deal with the relatively simpler case of regular perturbations. Subsequently the case of singular perturbed problems is considered.

2.6.1 Regular perturbation method for initial value problems

Let us consider the regularly perturbed problem (2.6.1) and let us define as limiting problem associated to (2.6.1) the initial value problem obtained from (2.6.1) for $\varepsilon = 0$:

$$\begin{cases} \dfrac{du^{(0)}}{dt} = f(t, u^{(0)}, 0) \,, \\ u^{(0)}(t_0, 0) = u_0(0) \,. \end{cases} \tag{2.6.6}$$

Due to the smoothness of $f(t, u, \varepsilon)$ and $u_0(\varepsilon)$ with respect to their arguments, we espect that the solution $u(t, \varepsilon)$ of (2.6.1) depends smoothly on t and ε and that it tends to the solution $u^{(0)}(t)$ of the limiting problem (2.6.6), as $\varepsilon \to 0$, uniformly with respect to $t \in [t_0, T]$.

Following De Jager and Furu (1996), let us assume that $f(t, u, \varepsilon)$, defined on $\mathbb{R}^2 \times [0, 1]$, has the following expansion:

$$f(t, u, \varepsilon) \sim \sum_{i=0}^{\infty} f^{(i)}(t, u)\varepsilon^i \qquad \text{as} \qquad \varepsilon \to 0 \,, \tag{2.6.7}$$

uniformly valid in any bounded domain of $\mathbb{R}^2$, with the functions $f^{(i)}(t, u)$ infinitely differentiable in $\mathbb{R}^2$, and assume that:

$$u_0(\varepsilon) \sim \sum_{i=0}^{\infty} u_{0i}\varepsilon^i \,. \tag{2.6.8}$$

Then, let us look for an asymptotic expansion for the solution of problem (2.6.1):

$$u(t, \varepsilon) \sim \sum_{i=0}^{\infty} u^{(i)}(t)\varepsilon^i \,, \tag{2.6.9}$$

along the following steps:

Step 1. Substituting (2.6.9) in (2.6.7), yields:

$$f(t, u(t, \varepsilon), \varepsilon) \sim \sum_{i=0}^{\infty} \varepsilon^i \, f^{(i)}\Big(t, \sum_{j=0}^{\infty} u^{(j)}(t)\varepsilon^j\Big)$$

$$\sim \sum_{i=0}^{\infty} \varepsilon^i \left\{ f^{(i)}(t, u^{(0)}(t)) + \frac{\partial f^{(i)}}{\partial u}(t, u^{(0)}(t)) \sum_{j=1}^{\infty} u^{(j)}(t)\varepsilon^j \right.$$

$$+ \frac{1}{2} \frac{\partial^2 f^{(i)}}{\partial u^2}(t, u^{(0)}(t)) \Big(\sum_{j=1}^{\infty} u^{(j)}(t)\varepsilon^j \Big)^2 + \cdots \Big\}$$

$$= f^{(0)}(t, u^{(0)}(t)) + \varepsilon \Big\{ \frac{\partial f^{(0)}}{\partial u}(t, u^{(0)}(t))u^{(1)}(t)$$

$$+ f^{(1)}(t, u^{(0)}(t)) \Big\} + \varepsilon^2 \Big\{ \frac{\partial f^{(0)}}{\partial u}(t, u^{(0)}(t))u^{(2)}(t)$$

$$+ \frac{1}{2} \frac{\partial^2 f^{(0)}}{\partial u^2}(t, u^{(0)}(t))(u^{(1)}(t))^2 + \frac{\partial f^{(1)}}{\partial u}(t, u^{(0)}(t))u^{(1)}(t)$$

$$+ f^{(2)}(t, u^{(0)}(t)) \Big\} + \cdots + \varepsilon^p \Big\{ \frac{\partial f^{(0)}}{\partial u}(t, u^{(0)}(t))u^{(p)}(t)$$

$$+ \tilde{f}^{(p)}(t, u^{(0)}(t), u^{(1)}(t), \cdots, u^{(p-1)}(t)) \Big\} + \cdots, \qquad (2.6.10)$$

with $\tilde{f}^{(p)}$ are known functions depending only on $(t, u^{(0)}, u^{(1)}, \cdots, u^{(p-1)})$.

Step 2. Consider from Step 1, that:

$$f(t, u(t, \varepsilon), \varepsilon) \sim f^{(0)}(t, u^{(0)}(t)) + \sum_{i=1}^{\infty} \varepsilon^i \Big\{ \frac{\partial f^{(0)}}{\partial u}(t, u^{(0)}(t))u^{(i)}(t)$$

$$+ \tilde{f}^{(i)}(t, u^{(0)}(t), u^{(1)}(t), \cdots, u^{(i-1)}(t)) \Big\}, \qquad (2.6.11)$$

then substituting (2.6.11), (2.6.9) and (2.6.8) into the corresponding terms of problem (2.6.1), and equating the same powers of ε, the following systems are obtained:

$$\begin{cases} \dfrac{du^{(0)}}{dt} = f^{(0)}(t, u^{(0)}), \\ u^{(0)}(t_0) = u_{00}, \end{cases} \qquad (2.6.12)$$

and

$$\begin{cases} \dfrac{du^{(i)}}{dt} = \dfrac{\partial f^{(0)}}{\partial u}(t, u^{(0)}) u^{(i)} + \tilde{f}^{(i-1)}(t, u^{(0)}, u^{(1)} \cdots, u^{(i-1)}), \\ u^{(i)}(t_0) = u_{0i}, \end{cases} \qquad (2.6.13)$$

for $i = 1, 2, \ldots$.

Step 3. Applying to problem (2.6.12) the existence and uniqueness Theorems 2.1-2.2, we get the existence of a unique solution $u^{(0)}(t)$ of (2.6.12), for $t \in [t_0, T]$. Recalling that $f^{(0)}(t, u)$ is infinitely differentiable, the solution $u^{(0)}$ is C^{∞}. Moreover, referring to subsection 2.4.2, the solutions of the linear differential systems (2.6.13) in the same interval $[t_0, T]$ is obtained.

Step 4. The procedure has to be completed showing that the formal expansion (2.6.9) for $u(t, \varepsilon)$, where the terms $u^{(i)}(t)$ are the solutions of systems (2.6.12) and (2.6.13) obtained in

Step 3, is an asymptotic expansion for $u(t, \varepsilon)$. This means that, writing $\forall N \geq 0$,

$$u(t, \varepsilon) = \sum_{i=0}^{N} u^{(i)}(t)\varepsilon^i + R_N(t, \varepsilon), \qquad (2.6.14)$$

it has to be proved that:

$$R_N(t, \varepsilon) = O(\varepsilon^{N+1}), \qquad (2.6.15)$$

uniformly in $t \in [t_0, T]$. The reader is addressed to O'Malley (1991) or De Jager and Furu (1996) for the details of this proof.

Remark 2.6.1. *The precedure described in Step 1 - Step 4 refers to the scalar problem (2.6.1). In the general case of a system of equations, the method of looking for an asymptotic expansion for the solution of the system can also be applied, as it is shown in the following example from Humi and Miller (1988).*

<div align="center">*Example 2.6.1*</div>

Consider the system:

$$\begin{cases} \dfrac{du}{dt} = -2u + v + \varepsilon v^2, \\[2mm] \dfrac{dv}{dt} = u - 2v + \varepsilon u^2, \\[2mm] u(0) = v(0) = 1, \end{cases} \qquad (2.6.16)$$

and the perturbation expansions for u and v:

$$u(t, \varepsilon) \sim \sum_{i=0}^{\infty} u^{(i)}(t)\varepsilon^i, \qquad v(t, \varepsilon) \sim \sum_{i=0}^{\infty} v^{(i)}(t)\varepsilon^i. \qquad (2.6.17)$$

Appling the perturbation method outlined above, we obtain at order $i = 0$ and $i = 1$, respectively:

$$\begin{cases} \dfrac{du^{(0)}}{dt} = -2u^{(0)} + v^{(0)}, \\[2mm] \dfrac{dv^{(0)}}{dt} = u^{(0)} - 2v^{(0)}, \\[2mm] u^{(0)}(0) = v^{(0)}(0) = 1, \end{cases} \qquad (2.6.18)$$

and

$$\begin{cases} \dfrac{du^{(1)}}{dt} = -2u^{(1)} + v^{(1)} + (v^{(0)})^2, \\[2mm] \dfrac{dv^{(1)}}{dt} = u^{(1)} - 2v^{(1)} + (u^{(0)})^2, \\[2mm] u^{(1)}(0) = v^{(1)}(0) = 0. \end{cases} \qquad (2.6.19)$$

We may observe that (2.6.16) is symmetric in u, v, as well as (2.6.18) and (2.6.19) are symmetric in $u^{(0)}, v^{(0)}$ and $u^{(1)}, v^{(1)}$ respectively. Solving the linear systems (2.6.18) and (2.6.19) yields:

$$u^{(0)}(t) = v^{(0)}(t) = e^{-t}, \qquad u^{(1)}(t) = v^{(1)}(t) = e^{-t} - e^{-2t}, \tag{2.6.20}$$

that gives as solution of (2.6.16):

$$u(t, \varepsilon) = v(t, \varepsilon) = e^{-t} + \varepsilon(e^{-t} - e^{-2t}) + O(\varepsilon^2). \tag{2.6.21}$$

□

Example 2.6.2
Duffing's Equation - Part I

Let consider the following system related to the motion of a mass attached to a nonlinear spring (hard spring):

$$\begin{cases} \dfrac{d^2 u}{dt^2} + u + \varepsilon u^3 = 0, \\ u(0) = a, \quad \dfrac{du}{dt}\bigg|_{t=0} = 0, \end{cases} \tag{2.6.22}$$

where $\varepsilon \in (0, 1)$, which can be considered as a regular perturbation of

$$\begin{cases} \dfrac{d^2 u}{dt^2} + u = 0, \\ u(0) = a, \quad \dfrac{du}{dt}\bigg|_{t=0} = 0. \end{cases} \tag{2.6.23}$$

Problem (2.6.22) is equivalent to the following two-dimensional first order system:

$$\begin{cases} \dfrac{du}{dt} = v, \\ \dfrac{dv}{dt} = -u - \varepsilon u^3, \\ u(0) = a, \quad v(0) = 0. \end{cases} \tag{2.6.24}$$

The power series expansion method gives at order $i = 0$ and $i = 1$ the following systems:

$$\begin{cases} \dfrac{d^2 u^{(0)}}{dt^2} + u^{(0)} = 0, \\ u^{(0)}(0) = a, \quad \dfrac{du^{(0)}}{dt}\bigg|_{t=0} = 0, \end{cases} \tag{2.6.25}$$

and

$$\begin{cases} \dfrac{d^2 u^{(1)}}{dt^2} + u^{(1)} = -(u^{(0)})^3 \,, \\[2mm] u^{(1)}(0) = 0 \,, \quad \dfrac{du^{(1)}}{dt}\bigg|_{t=0} = 0 \,, \end{cases} \tag{2.6.26}$$

where (2.6.25) is solved by $u^{(0)}(t) = a\cos t$, so that system (2.6.26) for $u^{(1)}$ can be written as follows:

$$\begin{cases} \dfrac{d^2 u^{(1)}}{dt^2} + u^{(1)} = -a^3\left(\dfrac{1}{4}\cos 3t + \dfrac{3}{4}\cos t\right), \\[2mm] u^{(1)}(0) = 0 \,, \quad \dfrac{du^{(1)}}{dt}\bigg|_{t=0} = 0 \,. \end{cases} \tag{2.6.27}$$

Its solution is:

$$u^{(1)}(t) = a^3\left[\dfrac{1}{32}\left(\cos 3t - \cos t\right) - \dfrac{3}{8}t\sin t\right], \tag{2.6.28}$$

so that the solution of (2.6.22) can be written as follows:

$$u(t,\varepsilon) = a\cos t + \varepsilon a^3\left[\dfrac{1}{32}\left(\cos 3t - \cos t\right) - \dfrac{3}{8}t\sin t\right] + O(\varepsilon^2)\,, \tag{2.6.29}$$

uniformly in any bounded interval $0 < t < T$.

$\square$

Remark 2.6.2. *It is interesting to remark that we do not get any answer to the question of how big can be the deviation of the solution of problem (2.6.1) from the solution of problem (2.6.6) on a large time interval. The following simple examples show that this deviation may even be not small.*

Example 2.6.3

Let consider the scalar system, from Mishchenko and Rozov (1980),

$$\begin{cases} \dfrac{du}{dt} = (u + \varepsilon)^2 \,, \\[2mm] u(0) = 0 \,, \end{cases} \tag{2.6.30}$$

that for $\varepsilon = 0$ becomes:

$$\begin{cases} \dfrac{du}{dt} = u^2 \,, \\[2mm] u(0) = 0 \,. \end{cases} \tag{2.6.31}$$

The solution of (2.6.31) is $u(t) = 0$, $\forall t \in [0, \infty)$, while the solution of (2.6.30) is $u(t,\varepsilon) = \dfrac{\varepsilon}{1 - \varepsilon t} - \varepsilon$ and it is defined only for $t \in [0, 1/\varepsilon)$.

$\square$

<div align="center">

Example 2.6.4
Lindstedt-Poincaré Algorithms

</div>

Coming back to Example 2.6.2, we see that expression (2.6.29) is a reasonable approximation of the solution for bounded time intervals but not for $t \in [0, \infty)$. In fact due to the term $-(3/8)\, t\, \sin t$ in (2.6.29), when $t = O(1/\varepsilon)$ the second term of the expansion is no longer $O(\varepsilon)$ and when $t = O(1/\varepsilon^2)$ the second term blows up.

Let us notice here that the term $-(3/8)\, t\, \sin t$ in (2.6.29) is due to the presence of the term $-(3/4)a^3 \cos t$ in (2.6.27) (the so–called **resonance** effect). On the other hand, (2.6.22) has only bounded (and periodic) solutions, as it describes a conservative system with the energy integral:

$$\left(\frac{du}{dt}\right)^2 + u^2 + \frac{\varepsilon}{2}u^4 = a^2 + \frac{\varepsilon}{2}a^4\,, \tag{2.6.32}$$

which implies u and du/dt are bounded for $t \in [0, \infty)$.

This suggests to use a different expansion of the solution in which unbounded terms do not appear: a possible approach is the Lindstedt-Poincaré algorithm.

Let s be a new variable defined as follows:

$$t = s\,\omega(\varepsilon)\,, \tag{2.6.33}$$

where

$$\omega(\varepsilon) = 1 + \varepsilon\omega_1 + \varepsilon^2\omega_2 + \cdots\,. \tag{2.6.34}$$

System (2.6.22) can now be written in the unknown $u(s) = u(t(s))$ as:

$$\begin{cases} \dfrac{d^2u}{ds^2} + (1 + \varepsilon\omega_1 + \varepsilon^2\omega_2 + \cdots)^2(u + \varepsilon u^3) = 0\,, \\[3mm] u(0) = a\,, \quad \dfrac{du}{ds}\bigg|_{s=0} = 0\,. \end{cases} \tag{2.6.35}$$

The above procedure can be applied to this problem looking for an asymptotic power series expansions for the solution of the type:

$$u(s, \varepsilon) \sim \sum_{i=0}^{\infty} u^{(i)}(s)\varepsilon^i\,. \tag{2.6.36}$$

The power series expansion method gives, respectively to the order $i = 0, 1, 2$, the following systems:

$$\begin{cases} \dfrac{d^2u^{(0)}}{ds^2} + u^{(0)} = 0\,, \\[3mm] u^{(0)}(0) = a\,, \quad \dfrac{du^{(0)}}{ds}\bigg|_{s=0} = 0\,, \end{cases} \tag{2.6.37}$$

$$
\begin{cases}
\dfrac{d^2u^{(1)}}{ds^2} + u^{(1)} = -(u^{(0)})^3 - 2\omega_1 u^{(0)}\,, \\[2mm]
u^{(1)}(0) = 0\,, \quad \dfrac{du^{(1)}}{ds}\bigg|_{s=0} = 0\,,
\end{cases}
\tag{2.6.38}
$$

$$
\begin{cases}
\dfrac{d^2u^{(2)}}{dt^2} + u^{(2)} = -3(u^{(0)})^2 u^{(1)} - 2\omega_1(u^{(1)} + (u^{(0)})^3) \\[2mm]
\qquad\qquad - (\omega_1{}^2 + 2\omega_2)u^{(0)}\,, \\[2mm]
u^{(2)}(0) = 0\,, \quad \dfrac{du^{(2)}}{ds}\bigg|_{s=0} = 0\,.
\end{cases}
\tag{2.6.39}
$$

The solution of (2.6.37) is $u^{(0)}(s) = a\,\cos s$, so that system (2.6.38) for $u^{(1)}$ can be rewritten as follows:

$$
\begin{cases}
\dfrac{d^2u^{(1)}}{ds^2} + u^{(1)} = -\dfrac{1}{4}a^3\cos(3s) - \Big(\dfrac{3}{4}a^2 + 2\omega_1\Big)a\cos s\,, \\[2mm]
u^{(1)}(0) = 0\,, \quad \dfrac{du^{(1)}}{ds}\bigg|_{s=0} = 0\,,
\end{cases}
\tag{2.6.40}
$$

so that, we can choose ω_1 such that:

$$
\frac{3}{4}a^2 + 2\omega_1 = 0\,,
\tag{2.6.41}
$$

in order to avoid the resonance effect. Therefore, the following bounded solution of (2.6.37) is obtained:

$$
u^{(1)}(s) = \frac{1}{32}a^3\left(\cos 3s - \cos s\right).
\tag{2.6.42}
$$

Consequently,

$$
u(s,\varepsilon) = a\,\cos s + \frac{1}{32}a^3\left(\cos 3s - \cos s\right)\varepsilon + O(\varepsilon^2)\,,
\tag{2.6.43}
$$

that is uniformly valid in any finite s interval, with the coordinate s given by:

$$
s = t\,\omega(\varepsilon)^{-1} = t\left(1 - \frac{3}{8}a^2\varepsilon + \cdots\right)^{-1}.
\tag{2.6.44}
$$

Finally the solution of (2.6.22) can be written as follows:

$$
u(t,\varepsilon) = a\cos(\Omega t) + \frac{\varepsilon}{32}a^3(\cos(3\Omega t) - \cos(\Omega t)) + O(\varepsilon^2)\,,
\tag{2.6.45}
$$

where

$$
\Omega = \omega(\varepsilon)^{-1} = \left(1 - \frac{3}{8}a^2\varepsilon + \cdots\right)^{-1} = 1 + \frac{3}{8}a^2\varepsilon + O(\varepsilon^2)\,.
\tag{2.6.46}
$$

$\square$

2.6.2 Singularly perturbed problems

As we have seen in the preceding subsection, in the case of regularly perturbed problem (2.6.1), the solution depends on the parameter ε in such a way that the solution $u(t, \varepsilon)$ converges, as $\varepsilon \to 0$, to the solution $u^{(0)}(t)$ of the limiting problem (2.6.6), uniformly with respect to $t \in [t_0, T]$. On the other hand, in the case of the **singularly** perturbed problem (2.6.2), the convergence $u(t, \varepsilon) \to u^{(0)}(t)$ generally fails. Let us introduce some basic notions and definitions through the following examples.

<hr>

Example 2.6.5

Initial Layer Effect - First Order Problem

Let us consider the problem:

$$\begin{cases} \varepsilon \dfrac{du}{dt} + u = 1 \,, \\ u(0) = u_0 \,, \end{cases} \tag{2.6.47}$$

which has the unique solution:

$$u(t, \varepsilon) = 1 + (u_0 - 1)e^{-\frac{t}{\varepsilon}} \,, \quad \forall \, t > 0 \,. \tag{2.6.48}$$

Assuming $\varepsilon > 0$ and $u_0 \neq 1$ yields:

$$\lim_{\varepsilon \to 0^+} u(t, \varepsilon) = 1 \quad \text{for} \quad t > 0 \,, \quad u(0, \varepsilon) = u_0 \,, \tag{2.6.49}$$

that proves that the convergence of $u(t, \varepsilon)$ to 1, for $\varepsilon \to 0^+$, is not uniform in any right-neighbourhood of $t = 0$.

$\square$

Remark 2.6.3. *The solution (2.6.48) of system (2.6.47) is the sum of two terms: the first one, the* **outer or bulk solution***, is an asymptotic solution of the differential equation for $t > 0$, and the second one,* **the initial layer solution***, is a function of what is called* **stretched time variable***:*

$$\tau = \frac{t}{\varepsilon} \,. \tag{2.6.50}$$

As $\tau \to +\infty$, the initial layer solution is decreasing to zero. The stretched time can be considered as a rescaling parameter which magnifies the region of non-uniform convergence.

<hr>

Example 2.6.6

Initial Layer Effect - Second Order Problem

Let us now consider the following nonlinear second order boundary value problem:

$$\begin{cases} \varepsilon \dfrac{d^2 u}{dt^2} = \left(\dfrac{du}{dt}\right)^2 \,, \\ u(0) = 1 \,, \quad u(1) = 0 \,, \end{cases} \tag{2.6.51}$$

which is solved by:

$$u(t, \varepsilon) = -\varepsilon \log\left(t + e^{-\frac{1}{\varepsilon}}(1 - t)\right), \quad \text{for} \quad t \in [0, 1] \quad \text{and} \quad \varepsilon > 0. \tag{2.6.52}$$

As in the preceding example, we have:

$$\lim_{\varepsilon \to 0^+} u(t, \varepsilon) = 0, \quad u(0, \varepsilon) = 1, \tag{2.6.53}$$

which shows that the convergence $u(t, \varepsilon) \to 0$ for $\varepsilon \to 0$ is uniform to respect to t on each closed subinterval of $(0, 1]$, but not in $[0, 1]$.

□

Different solution techniques can be applied to solve and to overcome the problem of non-uniform convergence both for singularly perturbed initial value problems and for singularly perturbed boundary value problems. Here we limit ourselves to show in the following example of singularly perturbed boundary value problem how an asymptotic expansion technique can be applied.

Example 2.6.8
Friedrichs' Problem

Consider the following second order linear boundary value problem:

$$\begin{cases} \varepsilon \dfrac{d^2 u}{dt^2} + \dfrac{du}{dt} + u = 0, \\[2mm] u(0) = a, \quad u(1) = b, \end{cases} \tag{2.6.54}$$

for $t \in [0, 1]$ and $\varepsilon \in (0, 1)$, whose exact solution is:

$$u(t, \varepsilon) = \frac{(ae^{s_2} - b)e^{s_1 t} + (b - ae^{s_1})e^{s_2 t}}{e^{s_2} - e^{s_1}}, \tag{2.6.55}$$

with $s_{1,2} = \dfrac{-1 \pm \sqrt{1 - 4\varepsilon}}{2\varepsilon}$.

Assume now that we don't know the exact solution and we want to try to determine an asymptotic form of the solution of (2.6.54) writing:

$$u(t, \varepsilon) = U(t, \varepsilon) + \tilde{u}(\tau, \varepsilon), \tag{2.6.56}$$

where $\tau = \dfrac{t}{\varepsilon}$.

Referring to the definitions stated in Remark 2.6.3, $U(t, \varepsilon)$ represents the outer solution and $\tilde{u}(\tau, \varepsilon)$ the initial layer solution. Let us assume that the following power series expansion holds:

$$U(t, \varepsilon) \sim \sum_{i=0}^{\infty} U^{(i)}(t)\varepsilon^i, \quad \tilde{u}(\tau, \varepsilon) \sim \sum_{i=0}^{\infty} \tilde{u}^{(i)}(\tau)\varepsilon^i. \tag{2.6.57}$$

and assume that $\tilde{u}^{(i)}$ and its derivatives tend to zero as $\tau \to +\infty$, providing the desired result that the correction term $\tilde{u}$ has only a significant value in a neighbourhood of $t = 0$. The outer solution U has to solve:

$$\begin{cases} \varepsilon \dfrac{d^2 U}{dt^2} + \dfrac{dU}{dt} + U = 0 \,, \\[2mm] U(1, \varepsilon) = b \,. \end{cases} \tag{2.6.58}$$

The expansion gives the following first order linear problems defined inductively:

$$\frac{dU^{(0)}}{dt} + U^{(0)} = 0 \,, \quad U^{(0)}(1) = b \,, \tag{2.6.59}$$

$$\frac{dU^{(i)}}{dt} + U^{(i)} = -\frac{d^2 U^{(i-1)}}{dt^2} \,, \quad U^{(i)}(1) = 0 \quad i = 1, 2, \dots \,. \tag{2.6.60}$$

Solving the related problems gives:

$$U(t, \varepsilon) = b e^{1-t} + \varepsilon b (1 - t) e^{1-t} + O(\varepsilon^2) \,, \tag{2.6.61}$$

which is asymptotically valid for $t \in (0, 1]$. For $t = 0$ we have:

$$U(0, \varepsilon) = be + \varepsilon be + O(\varepsilon^2) \neq a \,, \tag{2.6.62}$$

which shows that for taking into account the initial condition, the initial layer correction $\tilde{u}$ must be considered. The problem for $\tilde{u}$ is the following linear homogeneous one:

$$\frac{d^2 \tilde{u}}{d\tau^2} + \frac{d\tilde{u}}{d\tau} + \varepsilon \tilde{u} = 0 \,, \quad \tilde{u}(0, \varepsilon) = a - U(0, \varepsilon) \,. \tag{2.6.63}$$

The expansion for $\tilde{u}$ gives at order $i = 0$:

$$\frac{d\tilde{u}^{(0)}}{d\tau} + \tilde{u}^{(0)} = 0 \,, \quad \tilde{u}^{(0)}(0) = a - U^{(0)}(0) = a - be \,. \tag{2.6.64}$$

which is solved by:

$$u^{(0)}(\tau) = (a - be) \, e^{-\tau} \,. \tag{2.6.65}$$

So we have shown that Problem (2.6.54) has the following unique asymptotic solution:

$$u(t, \varepsilon) = U^{(0)}(t) + \tilde{u}^{(0)}\left(\frac{t}{\varepsilon}\right) + O(\varepsilon) = b \, e^{1-t} + (a - be) \, e^{-\frac{t}{\varepsilon}} + O(\varepsilon) \,. \tag{2.6.66}$$

It is worth stressing that $u(0, \varepsilon) = a$, and for $\varepsilon > 0$ we have $u(1, \varepsilon) = b + (a - be) \, e^{-\frac{1}{\varepsilon}}$ and $u(1, \varepsilon) \to b$ as $\varepsilon \to 0^+$.

□

The algorithm shown in Example 2.6.8 can also be applied to the initial value problem for an autonomous system of differential equations in the form:

$$\begin{cases} \varepsilon \dfrac{du}{dt} = f(u, v)\,, \\[2mm] \dfrac{dv}{dt} = g(u, v)\,, \\[2mm] u(0) = \mu(\varepsilon)\,, \qquad v(0) = \eta(\varepsilon)\,, \end{cases} \tag{2.6.67}$$

where u and v can be scalar or vector functions of t, and the dimensions of u and v can be different.

Implementing such an algorithm from a numerical point of view, as reported in Mika and Palczewski (1991), means to solve a number of equations equal to the order of approximation plus one. In this paper, the authors propose a different algorithm which involves only one differential equation for a single function. This algorithm is here briefly illustrated in the following example, while the reader is addressed to the original paper for the details.

Example 2.6.9
Mika and Palczewski's Algorithm

Consider the boundary value problem:

$$\begin{cases} \varepsilon \dfrac{d^2 u}{dt^2} + \dfrac{du}{dt} + u^2 = 0\,, \\[2mm] u(0) = \eta\,, \quad \left. \dfrac{du}{dt} \right|_{t=0} = \mu\,, \end{cases} \tag{2.6.68}$$

which corresponds to the system:

$$\begin{cases} \varepsilon \dfrac{du_1}{dt} = -u_1 - u_2{}^2\,, \\[2mm] \dfrac{du_2}{dt} = u_1 \\[2mm] u_1(0) = \mu\,, \quad u_2(0) = \eta\,. \end{cases} \tag{2.6.69}$$

The algorithm leads, as first order approximation, to solve the following system:

$$\begin{cases} \varepsilon \dfrac{dw}{dt} = -w^2 - 2\varepsilon w^2\,, \\[2mm] w(0) = \eta + \varepsilon(\mu + \eta^2)\,, \end{cases} \tag{2.6.70}$$

and it is possible to prove that the accuracy obtained in this new algorithm is similar to that for the first order standard algorithm and much better than the zero order standard algorithm.

$\square$

2.7 Bifurcation and Chaotic Motions

This section focus on how the equilibrium configurations of a dynamical system usually depend on the parameters which characterize the model. In particular, it may occur that as one of the parameters crosses a critical value, the solution will tend toward another equilibrium configuration. The aim of this Section is to give some hints for the study of the bifurcation of a dynamical system without claiming any completeness on the treatment of the subject. For a detailed treatment of the subject, refer for instance to the book Bellomo *et al.* (2000).

Consider a mathematical model described by a scalar autonomous ordinary differential equation depending on a parameter α:

$$\frac{du}{dt} = f(u; \alpha) \, . \tag{2.7.1}$$

The equilibrium configurations are determined by solving the algebraic equation:

$$f(u; \alpha) = 0 \, . \tag{2.7.2}$$

This equation is usually nonlinear and for each value of α it can be solved by a certain number of values of u, or possibly by no value at all. The number of solutions of (2.7.2) cannot be determined *a priori* and generally changes with α. As will be shown later in this section, the values of α for which the number of solutions of (2.7.2) changes are particularly important in the stability analysis.

Then, one can represent by dots in the (u, α)-plane, the solutions of (2.7.2) obtained for each fixed value of α. If α varies continuously, the solution of (2.7.2) defines a certain number of curves, each of which can be locally described by an equation $u = u_e(\alpha)$, implicitly defined by (2.7.2), i.e., such that $f(u_e(\alpha); \alpha) = 0$.

If one is able to determine the stability property of each equilibrium configuration, then this piece of information can also be reported on the diagrams using the following classical convention:

- Stable equilibrium configurations are identified by a heavy solid line;

- Unstable equilibrium configurations are identified by a dashed line.

The figures obtained by drawing these curves are called ***stability diagrams***, (or bifurcation diagrams, branching diagrams, response diagrams), and each of the curves appearing in the diagram is called a ***branch***.

The generalization of the above considerations, given for the scalar case, to systems of equations is technical.

The following definitions are recalled:

Branch points

*The values $\big(\alpha, \mathbf{u}_e(\alpha)\big)$ where the number of equilibrium solutions changes are called **branch points**.*

Bifurcation points

*An equilibrium solution **bifurcates** from another at $\alpha = \alpha_b$ if there are two distinct branches $\hat{\mathbf{u}}_e(\alpha)$ and $\check{\mathbf{u}}_e(\alpha)$ continuous in α, such that $\hat{\mathbf{u}}_e(\alpha_b) = \check{\mathbf{u}}_e(\alpha_b)$. The common value $\big(\alpha_b, \hat{\mathbf{u}}_e(\alpha_b)\big) = \big(\alpha_b, \check{\mathbf{u}}_e(\alpha_b)\big)$ in the $(\alpha, \mathbf{u})$-space is called a **bifurcation point**.*

Not all branch points are, however, bifurcation points. That is, not all changes in the number of equilibrium solutions are due to the intersection of curves in the stability diagram. Bifurcation points can be further classified, e.g. pitchfork bifurcation, supercritical, subcritical and transcritical bifurcations and Hopf bifurcations, referring again to the book Bellomo *et al.* (2000) for details. The following definitions can be reported:

Pitchfork bifurcation

*If one of the two branches intersecting at the bifurcation point $(\alpha_b, \mathbf{u}_b)$ is one sided (i.e., defined only for $\alpha \geq \alpha_b$ or for $\alpha \leq \alpha_b$), then the bifurcation is of the **pitchfork** type.*

Supercritical and subcritical bifurcations

*A pitchfork bifurcation is defined as being **supercritical** if the one-sided branch is stable and is otherwise **subcritical**.*

Transcritical bifurcations

*A bifurcation is **transcritical** if on both sides of the bifurcation point there are locally two equilibrium solutions.*

In many applications it may happen that, still departing from an unstable configuration, the system will neither go to another stationary configuration nor wander away, but will start oscillating approaching a periodic orbit. The oscillations described here are also referred to in mechanics as ***self-sustained oscillations***, to distinguish them from those which are due to oscillatory forcing terms. One can then state the following definition:

Limit cycle

*An **orbit** $\mathbf{u}(t)$ tends to a closed curve Γ called the **limit cycle** if there exists a **period** $T > 0$ such that the sequence of points $\mathbf{u}(t + nT)$ tends to a point of Γ as the integer n goes to infinity.*

*A **cycle** Γ is asymptotically stable if there exists a neighborhood $\mathcal{U}_\Gamma$ of Γ such that if $\mathbf{u}(0) \in \mathcal{U}_\Gamma$, then $\mathbf{u}(t)$ tends to Γ.*

The relevance of limit cycles is basically related to the problem of how time-periodic behaviors may arise from the bifurcation of a steady state. This is an interesting problem in the case of systems of equations, i.e. in the case of dimension more than one. In fact, for a scalar problem (2.7.1), it is impossible to have a nonconstant periodic solution.

The behavior of a dynamical system may change, according to the value assumed by a parameter α and the solution will tend to a time periodic orbit, as a critical value α_b is crossed. In this case, the bifurcation is called the **Hopf bifurcation**.

The identification of self-sustained oscillations is far more difficult than that of equilibrium points. As a consequence, recognizing the existence of a Hopf bifurcation can be a hard task. In this respect, the following theorem, known as the **Hopf Theorem**, is often very helpful.

Theorem 2.11 Hopf Theorem

Focussing on the dependence of the equilibrium configuration $\mathbf{u}_e$ on a parameter α, let us assume that there is a critical value α_b, such that $\mathbf{u}_e(\alpha)$ is asymptotically stable for $\alpha < \alpha_b$ and unstable for $\alpha > \alpha_b$. If for $\alpha = \alpha_b$ the Jacobian $\mathbf{J}$ of $\mathbf{f}$ has a simple pair of purely imaginary eigenvalues:

$$\lambda(\alpha_b) = \pm i\Omega \,, \tag{2.7.3a}$$

and all the other eigenvalues have a negative real part and, furthermore, for α close to α_b:

$$\lambda(\alpha) = \mu(\alpha) \pm i\omega(\alpha) \,, \qquad \text{with} \qquad \frac{d\mu}{d\alpha}(\alpha = \alpha_b) > 0 \,. \tag{2.7.3b}$$

Therefore for α sufficiently near the critical value α_b, there exists a limit cycle with initial period:

$$T = \frac{2\pi}{\Omega} \,. \tag{2.7.3c}$$

If, in addition, the equilibrium configuration $\mathbf{u}(\alpha = \alpha_b)$ is locally asymptotically stable, then the limit cycle is stable.

The theorem above uses again the eigenvalues of the Jacobian and the knowledge of the stability properties which are not too hard to verify. In particular, it pays attention to what happens to the first eigenvalue which will have positive real part as the bifurcation value is crossed.

We already know that at criticality. i.e. for α equal to the critical value α_b, the real part of an eigenvalue or of a pair of eigenvalues vanishes and becomes positive as the bifurcation value is passed by, while that of the others is negative. The theorem states that if also the imaginary part vanishes, i.e., the eigenvalue is zero, then the bifurcation involves stationary configurations. If, instead, there is a pair of purely imaginary eigenvalues, then the bifurcation involves self-sustained oscillations. This situation is represented in Figure 2.7.1. In particular, in Figure 2.7.1b a pair of eigenvalues of $\mathbf{J}$ crosses the imaginary axis from left to right away from the origin as α, increasing from stable values to unstable ones, crosses criticality.

Generally, the Hopf theorem does not tell whether a stable (supercritical) limit cycle exists for $\alpha > \alpha_b$ or an unstable (subcritical) limit cycle exists for $\alpha < \alpha_b$, inside of which all orbits spiral toward $\mathbf{u}_e$ and outside of which the orbits diverge. In order to know whether the limit cycle is
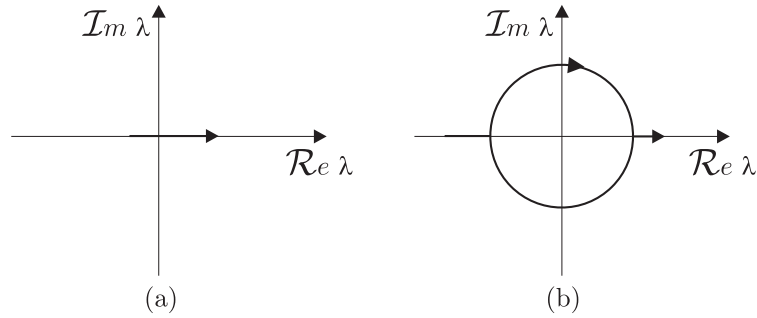
Figure 2.7.1 — Behavior of the critical eigenvalues as α increases from stable values to unstable ones in the case of (a) stationary bifurcation and (b) Hopf bifurcation.

stable or unstable, it must be proved that $\mathbf{u}_e$ is locally asymptotically stable at criticality. This information can be achieved by using the Liapunov method. In fact, linear stability criteria are useless because at criticality the eigenvalues are purely imaginary. This precludes any conclusion on the character of the nonlinear system. This second part is, however, certainly not simple.

These concepts are now applied to the following example.

_____ ***Example 2.7.1*** _____
Limit Cycle for the van der Pol Model

Consider the van der Pol equation already encountered in Example 2.5.1:

$$\frac{d^2u}{dt^2} - (\alpha - \beta u^2)\frac{du}{dt} + u = 0\,, \tag{2.7.4}$$

with $\beta > 0$ and, without loss of generality, $\gamma = 1$.

The only equilibrium configuration is $u = 0$, which is asymptotically stable for $\alpha < 0$ and unstable for $\alpha > 0$. In fact, the eigenvalues of the Jacobian are:

$$\lambda = \frac{\alpha \pm \sqrt{\alpha^2 - 4}}{2}\,.$$

Therefore, near the origin $\mu = \Re e(\lambda) = \alpha/2$. Furthermore, at criticality,

$$\lambda(\alpha = 0) = \pm i \neq 0 \qquad \text{and} \qquad \frac{d\mu}{d\alpha}(\alpha = 0) = \frac{1}{2} > 0\,.$$

From Hopf theorem, then, there exists a limit cycle. To establish if the limit cycle is subcritical (unstable) or supercritical (stable), one has to verify that $u = 0$ is locally asymptotically stable for $\alpha = 0$.

By using $V = u^2 + \left(\dfrac{du}{dt}\right)^2$ as a Liapunov function, one can compute for $\alpha = 0$,

$$\frac{dV}{dt} = -\beta u^2 \left(\frac{du}{dt}\right)^2 , \qquad (2.7.5)$$

which is always negative for non-trivial solutions.

$\square$

2.8 Critical Analysis

An introduction to mathematical modelling at the microscopic scale has been given in this chapter focusing on models stated in terms of ordinary differential equations. It has been shown that the analysis of nonlinear systems needs to be approached using both analytic and computational schemes. Analytic methods can provide existence results and some information on the qualitative behavior of the solution, for instance stability properties, asymptotic behavior, bifurcations, while computational schemes integrate the information by visualizing and completing what found by analytic methods.

Generally, none of the two approaches, namely analytic and computational, is sufficient to deliver a complete information, while a sinergetic use can be successful in providing a picture, as complete as possible of the solution patterns. Simulations, based on computational schemes, have to be focussed on completing, and possible enlarging, what is delivered (and not delivered) by the analytic qualitative analysis.

Let us analyze some modeling and complexity issues related to the contents of this chapter. Finite models, i.e. at the microscopic scale, consider each system as a whole. It is worth reasoning about some implications of the above approximation of physical reality. In fact, this approximation can be, in some cases, not acceptable when the number of elements constituting the overall system under consideration is large, namely the number of ordinary differential equations to be dealt with is too high for the qualitative analysis, as well as for computational treatment.

Moreover, let us critically consider that all models we have seen in this chapter need parameters related to the material behavior of the system under consideration. For instance, elasticity characteristics of spring, coefficients of competitive and/or cooperative models, and so on. Generally, these parameters are measured by empirical data obtained near equilibrium, while their values are needed to describe the evolution of the system far from equilibrium.

Finally, let us observe that most of the models presented in this chapter belong to the inert matter. Therefore they do not take into account the ability of living systems to extract energy from the outer environment and live out of equilibrium. Moreover, the deterministic causality principles, which are valid for models of the inert matter, should be replaced by relations where the effect is related to the cause only in some probabilistic sense.

This aspect is even more difficult to treat in the case of large systems where, as in most living systems, interactions are not linearly additive. This chapter has skipped over all aforesaid problems which will be treated later in Chapter 4, by mathematical tools that appear to be appropriate to take into account all topics outlined in this section.

Chapter 3

Macroscopic Scale Models
and Partial Differential Equations

3.1 Introduction

This chapter deals with the derivation and analysis of mathematical models derived at the macroscopic scale. These models, according to the definitions given in Chapter 1, provide a description of real systems by suitable evolution equations for locally averaged quantities which can be called **macroscopic observable quantities**. Of course, all physical systems are constituted by several interacting elements. However, the local averaging is an acceptable approximation when a small volume, in terms to be still precisely defined, contains a sufficiently large number of elements.

The above approximation can be called **continuous matter assumption**, which states that given two points belonging to the system, however close each other, some matter is included between these points. A typical example is the flow of fluid particles regarded as a continuum system. Rather than modelling the dynamics of each single particle and then averaging to obtain gross quantities such as mass density and linear momentum, the macroscopic approach provides directly, as we shall see, the evolution in time and space of the above macroscopic quantities. This approach was already analyzed in Chapter 1, where a few introductory examples have also been proposed. Therefore we simply recall that the derivation of equations in continuum physics has been a fundamental chapter in the history of mathematical physics and, in general, in the history of sciences.

Models of continuum physics, e.g. fluid dynamics, elasticity, electromagnetism fields, have been derived at the macroscopic scale under the continuum matter approximation, and are nowadays the fundamental background of the mathematical models of natural, applied, and technological sciences. Moreover, the derivation of several models in technology takes advantage of the above fundamental models of mathematical physics.

As we have already seen in Chapter 1, **macroscopic models** are characterized by a state variable $\mathbf{u}$ which depends on time and space. In general this dependence is continuous and one

can write

$$\mathbf{u} = \mathbf{u}(t, \mathbf{x}) : \quad [0, T] \times \mathcal{D} \longmapsto \mathbb{R}^n \,, \tag{3.1.1}$$

where $\mathcal{D} \subseteq \mathbb{R}^3$ is the domain of the space variable and $\mathbf{u}$ is an n-dimensional vector. Mathematical models are generally stated in terms of a system of partial differential equations for the variable $\mathbf{u}$.

If the state variable is a scalar and the space variable is in dimension one, then one simply has

$$u = u(t, x) : \quad [0, T] \times [a, b] \longmapsto \mathbb{R} \,. \tag{3.1.2}$$

In this case the model is a scalar partial differential equation.

Static continuous models are such that the dependence on time drops and the state variable is

$$\mathbf{u} = \mathbf{u}(\mathbf{x}) : \quad \mathcal{D} \longmapsto \mathbb{R}^n \,. \tag{3.1.3}$$

The organization of this chapter is somehow analogous to the one of the previous one. After the above introduction, the contents are organized as follows:

– Section 3.2 deals first with the description of some general modelling methods; then, these methods are will be applied to the derivation of some elementary models of mathematical physics related to simple phenomena, such as wave propagation, thermal diffusion.

– Section 3.3 analyzes the contents of the preceding section and deals with a classification of models and equations. This means looking at the mathematical structure of the models to provide a classification based on common properties of the said equations. As we shall see, the classification, based on mathematical properties, can be related to different classes of physical phenomena described by the model.

– Section 3.4 deals, on the basis of the above classification, with the statement of mathematical problems. The above classification is finalized to the correct statement of mathematical problems technically related to the development of mathematical methods. The mathematical formulation of problems is, as we shall see, preliminary to their solution and to the development of simulations.

– Section 3.5 deals with an introduction to analytic methods for linear problems. It is only a brief introduction considering that these Lecture Notes are mainly devoted to nonlinear models and problems, a relatively deeper insight can be obtained by the pertinent literature which will be given in what follows.

– Section 3.6 deals with the discretization of continuous models into a discrete number of finite models. Using this method, one obtains a set of models which approximate the continuous one by a system of ordinary differential equations related to the evolution of each finite element.

– Section 3.7 proposes a critical analysis mainly focused on the selection of the macroscopic scale to represent the system.

It is worth mentioning that this chapter does not aim to provide a complete presentation of the large variety of models of mathematical physics. The aim is to deal with methodological aspects which may contribute to address the reader to mathematical modelling as a science. The examples of models proposed in this chapter have to be regarded as relatively simple ones proposed as a mathematical description of simple phenomena.

3.2 Modelling Methods and Applications

This section deals with the analysis of the methodological aspects of the mathematical modelling of continuous systems, which will be then applied to the study of a number of physical systems chosen as suitable examples.

As usual, the derivation of a mathematical model suitable to describe a certain physical system requires a preliminary phenomenological observation both of the physical system and of its connection with the outer environment. Then, the modelling procedure can be developed along the following steps:

1: Selection of the state variable which describes, by the model, the real system: this variable can be called *state variable*;

2: Modelling of the *interactions* between the inner system under consideration and the outer environment;

3: Assessment of the equilibrium, conservation, and/or balance equations, related to the above defined state variable, including the action of the outer environment to the inner system.

4: Modelling the material behavior of the system by means of phenomenological models, which will be called *constitutive or material models*;

5: Derivation, using the equations dealt with in Steps 3 and 4, of a mathematical model. Such model consists of a suitable set of equations describing in time and space the evolution of the state variable.

The above scheme does not claim to cover all conceivable types of modelling procedures. However, various examples are proposed to the reader to achieve a general understanding of the above methodology and of its generalization.

Then, once the mathematical model has been designed, the usual procedure for its analysis can be organized: formulation of mathematical problems by a proper statement of initial and boundary conditions, qualitative analysis, solution of mathematical problems, and validation of the model.

As mentioned in Step 3, several methodological approaches can be followed toward the derivation of a certain model, while a common feature of the analysis developed in what follows is that we consider a real system represented with reference to a certain fixed, generally inertial, frame.

Moreover, models are derived under the assumption that the matter is continuous. This is certainly an approximation, since intermolecular distances are always positive quantities. On

the other hand, when these distances are sufficiently small with respect to the characteristic dimensions of the body, the continuum hypothesis becomes reasonable and can be regarded as an acceptable simplification. If this hypothesis is no longer applicable, for instance for a rarefied gas, then mathematical models have to be derived at a molecular scale, as we shall see in the next chapter.

Some examples of models and of the related modelling techniques will be now given in what follows.

Example 3.2.1
Modelling the Vibration of an Elastic String

Let us consider, with reference to Fig. 3.2.1, an elastic string fixed at both its extrema. The modelling procedure for the dynamics of the system can be based upon the following assumptions:

- The string is held in A and B by a strong tension directed along the string. This implies that gravity can be neglected, and that consequently the string takes at equilibrium a straight configuration, identified by the axis with unit vector $\mathbf{i}$.

- The string is subjected to small displacements from the equilibrium configuration.

- The motion of the string is localized on a plane, identified by the unit vectors $\mathbf{i}$ and $\mathbf{j}$ and every point of the string moves along $\mathbf{j}$, namely perpendicularly to the equilibrium state.

- The state variable is the perpendicular displacement

$$u = u(t,x) : \quad [0,T] \times [0,\ell] \longmapsto \mathbb{R}, \tag{3.2.1}$$

where the independent variables are time t and location x along the string.

- A fluid-dynamic drag is exerted on the string by the outer environment. A phenomenological model of the force acting upon the string element Δx is as follows

$$\mathbf{F} = -h \left| \frac{\partial u}{\partial t} \right|^n \frac{\partial u}{\partial t} \Delta x \, \mathbf{j}, \tag{3.2.2}$$

where h and c are suitable constant quantities, and $n \geq 0$.

- A constant internal tension $T(x) = T_0$ can be assumed in the framework of linear elasticity, related to the initial stretching of the string, while small deformations do not modify the internal tension.

Referring then to Fig. 3.2.1, if θ is the slope of the string, then the component of the tension along $\mathbf{j}$ acting over the element Δx of the string is

$$\Delta T = T_0 \sin \theta(x + \Delta x) - T_0 \sin \theta(x). \tag{3.2.3}$$
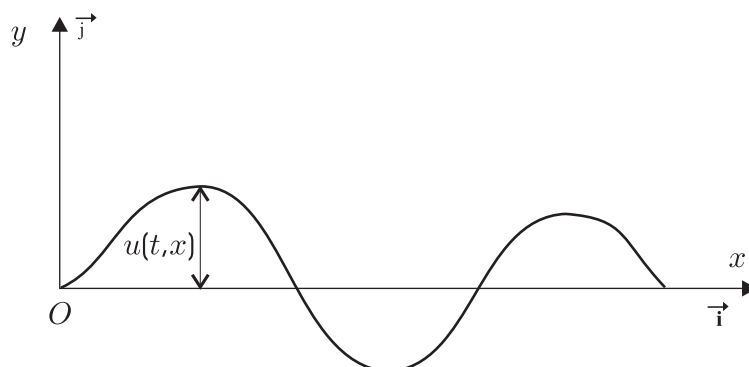
Figure 3.2.1 — Representation of a vibrating string.

Considering that for small deformations one has:

$$\sin\theta \cong \frac{\Delta u}{\sqrt{\Delta u^2 + \Delta x^2}} \cong \frac{\Delta u}{\Delta x} \cong \frac{\partial u}{\partial x}\,, \tag{3.2.4}$$

then the approximation

$$\Delta T \cong T_0\left[\frac{\partial u}{\partial x}(x+\Delta x) - \frac{\partial u}{\partial x}(x)\right] \cong T_0\Delta x \frac{\partial^2 u}{\partial x^2}(x) \tag{3.2.5}$$

is obtained.

Therefore, the element Δx is subject to the following actions:

- $T_0 \dfrac{\partial^2 u}{\partial x^2}\Delta x$ is the action of the internal tension;

- $-\rho \dfrac{\partial^2 u}{\partial t^2}\Delta x$ is the inertial force;

- $-h \left|\dfrac{\partial u}{\partial t}\right|^p \dfrac{\partial u}{\partial t}\Delta x$ is the fluid-dynamic drag.

In the material reference frame, these forces set the system in equilibrium (Newton's mechanical model or, more properly, d'Alembert's principle). The application of the equilibrium equation yields the following continuous dynamic model

$$\frac{\partial^2 u}{\partial t^2} = c^2\frac{\partial^2 u}{\partial x^2} - k^2\left|\frac{\partial u}{\partial t}\right|^p \frac{\partial u}{\partial t}\,, \tag{3.2.6}$$

where $c = \sqrt{T_0/\rho}$, and $k = \sqrt{h/\rho}$.

$\square$

Remark 3.2.1. *The model is derived under the assumption of small deformations of the string. Hence its validity is limited to the case of small vibrations. If the model is used to describe large deformations, then unreliable descriptions follow.*

Remark 3.2.2. *The above model is nonlinear. Neglecting the fluid dynamic drag leads to the following linear model:*

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}\,. \tag{3.2.7}$$

The model is linear also if $p = 0$

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} - k^2 \frac{\partial u}{\partial t}\,. \tag{3.2.8}$$

Example 3.2.2
Linear Temperature Diffusion Model

Consider a linear diffusion model homogeneous in the space. The assumptions which generate the model are the following:

- The physical quantity which defines the state of the system is the temperature in the body:

$$u = u(t, x, y, z) : \quad [0, T] \times \mathbb{R}^3 \to \mathbb{R}_+.$$

- The mass per unit volume of the medium is assumed to be constant, as well as the heat capacity of the medium.
- The diffusion of temperature in a certain direction is described by a phenomenological model which states that the said velocity is directly proportional to the directional derivative of u in the above direction.

The evolution model, i.e. the evolution equation for u, can be obtained equating the net heat flux in a control volume to the increase of heat capacity:

$$\frac{\partial u}{\partial t} = k \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) u = k\,\Delta u\,, \tag{3.2.9}$$

which is linear and where k is the diffusion coefficient.

$\square$

Example 3.2.3
Equilibrium Temperature Profiles Model

Consider a linear diffusion phenomena homogeneous in the space according to Example 3.2.2. The temperature profiles can be obtained by Model 3.2.2 simply assuming that the temperature does not change in time. The following model is obtained:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) u = \Delta u = 0\,, \tag{3.2.10}$$

which is also known as **Laplace equation**.

□

Remark 3.2.3. *Nonlinear models are obtained if the diffusion coefficient depends on the temperature. This applies to both Models 3.2.2 and 3.2.3.*

<div align="center">

Example 3.2.4

Hydrodynamic Models
</div>

Consider a description of the fluid such that the state variable $\mathbf{u}$ is simply defined by density ρ, and velocity $\mathbf{v}$, regarded as functions of time and space. The derivation of the model is based on mass and momentum conservation equations. The velocity $\mathbf{v}$ is a three dimensional vector:

$$\mathbf{v} = v_x\,\mathbf{i} + v_y\,\mathbf{j} + v_z\,\mathbf{k}\,. \tag{3.2.11}$$

Therefore, the model needs four scalar components related to the variable:

$$\mathbf{u} = \{\rho\,, v_x\,, v_y\,, v_z\}\,. \tag{3.2.12}$$

Referring to **mass conservation**, we consider an arbitrary volume Ω in the space occupied by the fluid and let Σ be the regular surface containing Ω. By definition, the mass contained in Ω is

$$M = \int_\Omega \rho(t,x,y,z)\,dx\,dy\,dz\,, \tag{3.2.13}$$

while the mass flow through Ω is given by

$$G = -\int_\Omega \rho(t,x,y,z)\mathbf{v}(t,x,y,z)\mathbf{n}\,d\Omega\,, \tag{3.2.14}$$

where $d\Omega$ is the elementary surface and $\mathbf{n}$ is the unit vector orthogonal to the surface conventionally directed towards the outer region.

Gauss Theorem allows to transform the surface integral into a volume integral by replacing the function to be integrated by its divergence

$$G = -\int_\Omega \nabla_\mathbf{x}(\rho\mathbf{v})(t,x,y,z)\,dx\,dy\,dz\,, \tag{3.2.15}$$

where

$$\nabla_\mathbf{x} = \frac{\partial}{\partial x}\,\mathbf{i} + \frac{\partial}{\partial y}\,\mathbf{j} + \frac{\partial}{\partial \mathbf{z}}\,\mathbf{k}\,. \tag{3.2.16}$$

The time evolution of the mass in the control volume Ω equals the mass flux given by (3.2.14) through Ω. Due to the arbitrary choice of Ω, the conservation equation can be written in differential terms as follows:

$$\frac{\partial \rho}{\partial t} + \nabla_\mathbf{x}(\rho\mathbf{v}) = 0\,, \tag{3.2.17}$$

which, in the one dimensional case, $\rho = \rho(t, x)$, writes

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v_x) = 0 \,. \tag{3.2.18}$$

Mass conservation equation (3.2.17) also writes as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial y}(\rho v_y) + \frac{\partial}{\partial z}(\rho v_z) = 0 \,, \tag{3.2.19}$$

where $\rho = \rho(t, x, y, z)$, and $\mathbf{v} = \mathbf{v}(t, x, y, z)$.

Similarly one can deal with **conservation of momentum**:

$$\mathbf{Q} = \mathbf{Q}(t, x, y, z), \qquad \mathbf{Q} =: \rho \mathbf{v} \,, \tag{3.2.20}$$

for a system subject to an external field which may depend on the density and velocity of the flow: $\mathbf{F} = \mathbf{F}(t, x, y, z, \rho, \mathbf{v})$, referred to the unit mass at the time t in the point (x, y, z).

The integral conservation relation writes

$$\frac{\partial}{\partial t} \int_{\Omega} \rho \mathbf{v} \, dx \, dy \, dz + \int_{\Omega} \nabla_{\mathbf{x}} \left((\rho \mathbf{v}) \cdot \mathbf{v} \right) dx \, dy \, dz = \int_{\Omega} \rho \mathbf{F}(t, \cdot) \, dx \, dy \, dz \,. \tag{3.2.21}$$

The application of Gauss theorem yields the differential model

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla_{\mathbf{x}} \left((\rho \mathbf{v}) \cdot \mathbf{v} \right) = \rho \mathbf{F}(t, x, y, z, \rho, \mathbf{v}) \,, \tag{3.2.22}$$

which, in the one dimensional case, writes

$$\frac{\partial}{\partial t}(\rho v_x) + \frac{\partial}{\partial x} \left((\rho v_x) v_x \right) = \rho F_x(t, x, \rho, \mathbf{v}) \,. \tag{3.2.23}$$

Model (3.2.22) generates three scalar evolution equation which can be explicitly written as follows:

$$\begin{cases} \dfrac{\partial}{\partial t}(\rho v_x) + \rho v_x \nabla_{\mathbf{x}} \mathbf{v} + v_x \nabla_{\mathbf{x}}(\rho \mathbf{v}) = \rho F_x(t, x, y, z, \rho, \mathbf{v}) \,, \\[2mm] \dfrac{\partial}{\partial t}(\rho v_y) + \rho v_y \nabla_{\mathbf{x}} \mathbf{v} + v_y \nabla_{\mathbf{x}}(\rho \mathbf{v}) = \rho F_y(t, x, y, z, \rho, \mathbf{v}) \,, \\[2mm] \dfrac{\partial}{\partial t}(\rho v_z) + \rho v_z \nabla_{\mathbf{x}} \mathbf{v} + v_z \nabla_{\mathbf{x}}(\rho \mathbf{v}) = \rho F_z(t, x, y, z, \rho, \mathbf{v}) \,. \end{cases} \tag{3.2.24}$$

System (3.2.24) coupled with (3.2.18) gives the evolution model. However additional microscopic modelling is needed to define the term $\mathbf{F}$ generated by the external applied field and by the internal viscous forces. A simple example of model is given in what follows.

$\square$

Example 3.2.5
A One-dimensional Hydrodynamic Model

Consider, with reference to Model 3.2.4, the one-dimensional flow of a fluid in a duct, and let x be the coordinate of the axis of the duct. Moreover, assume that the variation of density and velocity in the direction orthogonal to the axis can be neglected. In this case the expressions of mass and linear momentum conservation equations simplify as follows:

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \dfrac{\partial}{\partial x}(\rho v) = 0 \,, \\ \dfrac{\partial v}{\partial t} + v \dfrac{\partial v}{\partial x} = F(\rho, v) \,. \end{cases} \tag{3.2.25}$$

The above equation can generate a self-consistent model if the action F, namely the force acting on the volume element, can be properly modelled. One can distinguish two kind of forces: those acting on the entire volume from outside, e.g. gravity, and those generated by the **pressure** of the liquid present in the near volume elements pushing our volume element through the sections separating them. The former are generally called **body forces** and can be written as $F_b = A f \, dx$, where f is the force per unit volume. The latter are generally called **contact forces** and give rise to a net force

$$F_c = A[-P(t, x+dx) + P(t, x)] = -\frac{\partial P}{\partial x}(t, x) A dx \,. \tag{3.2.26}$$

Therefore, momentum balance writes

$$\rho \left(\frac{\partial v}{\partial t} + 2v \frac{\partial v}{\partial x} \right) = f - \frac{\partial P}{\partial x} \,. \tag{3.2.27}$$

Equation (3.2.27) needs a phenomenological description of the dependence of the body and contact forces on the state variables ρ and v. For instance, if the duct is vertical and only gravity acts on the fluid, one can show that $f = \rho g$. On the other hand, the phenomenological law for the pressure P involves the identification of a constitutive relation which states how the fluid responds to deformations (in this case compression). It is found, for instance, that certain gases, called polytropic gases, satisfy the following constitutive law:

$$P = \alpha \rho^\gamma \,, \quad \gamma > 1, \tag{3.2.28}$$

which yields the following self-consistent hydrodynamic model

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \dfrac{\partial}{\partial x}(\rho v) = 0 \,, \\ \dfrac{\partial v}{\partial t} + 2v \dfrac{\partial v}{\partial x} = -\alpha \gamma \rho^{\gamma-2} \dfrac{\partial \rho}{\partial x} + g \,. \end{cases} \tag{3.2.29}$$

$\square$

Remark 3.2.4. *In some cases of unsteady flow conditions, it is used a constitutive law which holds true at equilibrium. This is certainly an approximation of physical reality and the example gives an idea of the difficulty of mathematical modelling.*

Wave phenomena can be described by higher order equations to include the modelling of solitary waves. This is the case of the celebrated Korteweg-deVries model.

<div align="center">

Example 3.2.6

Korteweg-deVries - Solitary wave models

</div>

Solitary wave phenomena can be described by a model derived in 1895 by Korteweg and de Vries. This model describes the evolution of the long water waves in a channel of rectangular cross-section and is characterized by an appropriate balance between nonlinearity and dispersion. The model arises in several fields of fluid mechanics, such as water waves, internal gravity waves in stratified fluids, and waves in rotating atmosphere and can be regarded as one of the relevant paradigms of the nonlinear waves and soliton solutions.

In details consider the following evolution equation mixing transport and third order backward diffusion:

$$\frac{\partial u}{\partial t} + u^m \frac{\partial u}{\partial x} + \mu \frac{\partial^3 u}{\partial x^3} = 0 \,, \qquad (3.2.30)$$

where u defines the wave depth.

It is useful stressing, in view of development of simulation methods, reporting some analytic solutions which may be compared with computational ones. Specifically, the solution for a single soliton is

$$u(x,t) = \left[A \operatorname{sech}^2(\kappa x - \omega t - x_0) \right]^{1/m} \,, \qquad (3.2.31)$$

where κ and ω are free parameters and

$$A = 2 \frac{\mu \kappa^2}{m^2} (m+1)(m+2) \qquad \omega = \frac{4\mu \kappa^3}{m^2} \,. \qquad (3.2.32)$$

The model has an infinite number of conserved densities that, integrated over the whole range of the space domain, are independent of time. The first five invariant quantities are

$$I_1 = \int_{-\infty}^{+\infty} u \, dx \,, \qquad (3.2.33)$$

$$I_2 = \int_{-\infty}^{+\infty} \frac{1}{2} u^2 \, dx \,, \qquad (3.2.34)$$

$$I_3 = \int_{-\infty}^{+\infty} \left[u^3 + \frac{1}{2} \left(\frac{\partial u}{\partial x} \right)^2 \right] dx \,, \qquad (3.2.35)$$

$$I_4 = \int_{-\infty}^{+\infty} \left[5u^4 + 10u \left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial^2 u}{\partial x^2} \right)^2 \right] dx \,, \qquad (3.2.36)$$

and

$$I_5 = \int_{-\infty}^{+\infty} \left[21u^5 + 105u^2 \left(\frac{\partial u}{\partial x} \right)^2 + 21u \left(\frac{\partial^2 u}{\partial x^2} \right)^2 + \left(\frac{\partial^3 u}{\partial x^3} \right)^2 \right] dx \,, \qquad (3.2.37)$$

where the first three conservation equations correspond to mass, momentum, and energy, respectively, of the wave. These equations can be used to test the application of computational schemes.

$\square$

The last model of this section focus on vehicular dynamics, already introduced in Section 1.5 of Chapter One, according to the conservation of mass equation, which writes

$$\frac{\partial u}{\partial t} + \frac{\partial (uv)}{\partial x} = 0 \,, \qquad (3.2.38)$$

where u is the dimensionless number density of vehicles, namely the real density divided by the maximal value reached in bumper-to-bumper conditions, and v is the dimensionless mean velocity, that is the real mean velocity divided by the maximal one, for instance that obtained by speed limits.

The modeling approach takes advantage of the so called **fundamental diagram** which reports, in **steady uniform conditions**, the flux $q = uv$ versus the density $u \in [0, 1]$. A typical model, which approximates empirical data, is the following

$$q = u \, v = u \, (1 - u), \qquad v = 1 - u \,, \qquad (3.2.39)$$

which is valid for a large variety of one–lane road. This phenomenological model is used to derive a traffic dynamics model although more refined interpretation of physical reality can be proposed. Still it is consistent with the tutorial reasonings presented in the following.

Example 3.2.7
Macroscopic Vehicular Model

First order models of vehicular traffic can be obtained by closing the mass conservation (3.2.38) by phenomenological model linking the velocity v to the local density conditions. It is suggested in De Angelis (1999) that this relation can be offered by using in the expression of v the perceived density w, rather than the real one, modeled as follows:

$$w = u \left[1 + \varepsilon \, (1 - u) \frac{\partial u}{\partial x} \right] . \qquad (3.2.40)$$

Therefore, using $q = u(1 - w)$ yields

$$\frac{\partial u}{\partial t} + (1 - 2u)\frac{\partial u}{\partial x} = \varepsilon \, u^2 \, (1 - u) \frac{\partial^2 u}{\partial x^2} + \varepsilon \, (2u - 3u^2) \left(\frac{\partial u}{\partial x} \right)^2 , \qquad (3.2.41)$$

Remark 3.2.5. *Model 3.2.39 is a non-linear transport diffusion equation that can be written as follows:*

$$\frac{\partial u}{\partial t} + c(u)\frac{\partial u}{\partial x} = \varepsilon\,\frac{\partial}{\partial x}\left[k(u)\,\frac{\partial u}{\partial x}\right], \qquad (3.2.42)$$

where $c(u) = (1 - 2u)$ is the density dependent transport velocity, and $k(u) = u^2(1 - u)$ is the density dependent diffusion term.

Remark 3.2.6. *The phenomenological model 3.2.38 basically states that the perceived density w is higher/lower in the presence of postive/negative density gradients. Moreover, this effect depends on $(1 - u)$, namely it increases with decreasing density.*

□

3.3 Classification of Models and Equations

Once a mathematical model has been derived, its application can be developed in view of the qualitative and computational analysis of mathematical problems generated by its application to real world analysis. As we have seen in the examples given in Section 3.2, the governing equations appears to be relatively more complex than those encountered for discrete systems. Dealing with the statement of mathematical problems requires, actually it is even necessary, dealing with a detailed analysis of the qualitative properties of the models.

Indeed the statement of the problems and the qualitative behavior of the solutions depends on the properties of the models which can be classified according to their mathematical structure. The application of computational schemes also needs to be related to the above properties. This topic is dealt with in this section devoted to the classification of mathematical equations on the basis of some structural properties of the equations themselves.

As we have seen, a large variety of macroscopic models can be written in terms of partial differential equations. This section deals with the qualitative analysis of a large class of first and second order equations, related to the models we have seen in Section 3.2. Considering that the variety of this type of equations is extremely broad, completeness is not claimed.

Bearing all above in mind, consider the following class of second-order partial differential equation in two dependent variables:

$$\sum_{i,j=1}^{n} A_{ij}(\mathbf{x})\frac{\partial^2 u}{\partial x_i \partial x_j} = F\left(\mathbf{x}; u, \frac{\partial u}{\partial x_1}, \dots, \frac{\partial u}{\partial x_n}\right), \qquad (3.3.1)$$

where $\mathbf{x}$ includes time and space variables.

Consider the eigenvalues of the matrix $\mathbf{A}$ that appear as coefficients of the second-order derivatives ($\mathbf{A}$ is symmetric and therefore its eigenvalues are real). Then, the following classification

can be proposed:

$$
\left.\begin{array}{lll}
\forall i & \lambda_i \neq 0 & \exists! \lambda_i > 0 \\
\forall i & \lambda_i \neq 0 & \exists! \lambda_i < 0
\end{array}\right\} \implies \text{hyperbolic},
$$

$$
\left.\begin{array}{c}
\det \mathbf{A} = 0 \\
(\text{or equivalently} \ \ \exists \lambda_i = 0)
\end{array}\right\} \implies \text{parabolic},
$$

$$
\left.\begin{array}{ll}
\forall i & \lambda_i > 0 \\
\forall i & \lambda_i < 0
\end{array}\right\} \implies \text{elliptic}.
$$

Analogous classification can be developed for first order models, such as those we have seen with reference to hydrodynamic models. Specifically, consider quasi-linear systems of n first-order partial differential equations in two independent variables:

$$
\sum_{j=1}^{n} A_{ij}(\mathbf{x}, \mathbf{u}) \frac{\partial u_j}{\partial t} + \sum_{j=1}^{n} B_{ij}(\mathbf{x}, \mathbf{u}) \frac{\partial u_j}{\partial x} = f_i(\mathbf{x}, \mathbf{u}), \quad i = 1, \ldots, n, \tag{3.3.2}
$$

which can be written also in vector form

$$
\mathbf{A}(\mathbf{x}, \mathbf{u}) \frac{\partial \mathbf{u}}{\partial t} + \mathbf{B}(\mathbf{x}, \mathbf{u}) \frac{\partial \mathbf{u}}{\partial x} = \mathbf{f}(\mathbf{x}, \mathbf{u}). \tag{3.3.3}
$$

If the dependence on $\mathbf{u}$ drops in A_{ij} and B_{ij}, then the system is said to be **_almost linear_**. If it drops also in f_i, then the system of partial differential equations is **_linear_**.

Under the assumption that $\mathbf{A}$ is nonsingular, the classification is based on the calculations of the roots of the eigenvalue problem

$$
P_n(\lambda) = \det(\mathbf{B} - \lambda \mathbf{A}) = 0, \tag{3.3.4}
$$

and on the number of independent eigenvectors satisfying

$$
(\mathbf{B}^T - \lambda \mathbf{A}^T) \mathbf{v} = \mathbf{O}. \tag{3.3.5}
$$

It reads as follows:

- If $P_n(\lambda)$ has n real distinct zeros $\implies$ hyperbolic;
- If $P_n(\lambda)$ has n real zeros at least one of which is repeated and n independent eigenvectors $\implies$ hyperbolic;
- If $P_n(\lambda)$ has n real zeros at least one of which is repeated and fewer than n independent eigenvectors $\implies$ parabolic;
- If $P_n(\lambda)$ has no real zeros $\implies$ elliptic.

This classification, which does not cover all possibilities due to the assumptions on the Matrices $\mathbf{A}$ and $\mathbf{B}$, is however useful to deal with a large variety of models. For instance, it can

be verified that the equation

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = f(t, x; u), \qquad c > 0, \tag{3.3.6}$$

is hyperbolic.

As a particular case of Eq. (3.3.1), consider the following class of equations:

$$A(t, x)\frac{\partial^2 u}{\partial t^2} + 2B(t, x)\frac{\partial^2 u}{\partial t \partial x} + C(t, x)\frac{\partial^2 u}{\partial x^2} = F\left(t, x; u, \frac{\partial u}{\partial t}, \frac{\partial u}{\partial x}\right). \tag{3.3.7}$$

Applying the above rules yields:

$$\begin{aligned} B^2 - AC > 0 &\implies \text{hyperbolic,} \\ B^2 - AC = 0 &\implies \text{parabolic,} \\ B^2 - AC < 0 &\implies \text{elliptic.} \end{aligned} \tag{3.3.8}$$

Considering that A, B, and C are functions of t and x, then the type of equation depends upon the local values of the coefficients. In this case the model may change of type. For instance, the abstract model

$$\frac{\partial^2 u}{\partial t^2} + C(t, x)\frac{\partial^2 u}{\partial x^2} = F\left(t, x; u, \frac{\partial u}{\partial t}, \frac{\partial u}{\partial x}\right), \tag{3.3.9}$$

which is such that $A = 1$ and $B = 0$. Therefore $B^2 - AC = -C(t, x)$, then the equation is elliptic, parabolic, or hyperbolic according to the sign of C. In particular, it is elliptic, hyperbolic, or parabolic when, respectively, C is positive, negative, or equal to zero.

The above classification can be applied to the following specific examples:

Example 3.3.1
Hyperbolic, parabolic, and elliptic

Referring to the models presented in Section 3.2, the following properties holds true:

- Model 3.2.1 (vibrating string) is hyperbolic.

- Model 3.2.2 (diffusion phenomena) is parabolic.

- Model 3.2.3 (Laplace's equation) is elliptic.

□

Example 3.3.2
Ferrari and Tricomi Model

A model, which changes of type, was proposed by Ferrari and Tricomi, to describe the space evolution of the velocity potential, in the velocity space, for inviscid flow around the sonic line for transonic flow around thin airfoils. The model is as follows:

$$\frac{\partial^2 u}{\partial x^2} + y\frac{\partial^2 u}{\partial y^2} = 0 \,, \tag{3.3.13}$$

which is elliptic for $y > 0$, which corresponds to subsonic flow, parabolic for $y = 0$, which corresponds to the sonic line, and hyperbolic for $y < 0$, which corresponds to supersonic flow.

$\square$

It can be shown that the **qualitative behavior of the solutions** depends on the above qualitative properties of the model related to the above classification. Referring to the specialized literature, e.g. Dautray and Lions (1990), the following examples are given:

• Parabolic equations are evolution equations that describe diffusion-like phenomena. In general, the solution of a parabolic problem is smooth with respect to both space and time even if the initial data are not continuous. In other words, parabolic systems have a **smoothing action** so that singularities do not develop, nor can be maintained. Moreover, even if the initial data have compact support, at any $t > 0$ the initial condition is felt everywhere. This is usually indicated by saying that parabolic systems have an **infinite speed of propagation**.

• Elliptic equations describe systems in the equilibrium or steady state. They can be seen as equations describing, for instance, the final state reached by a physical system described by a parabolic equation after the transient term has died out.

• Hyperbolic equations are evolution equations that describe wave-like phenomena. The solution of an hyperbolic initial-value problem cannot be smoother than the initial data. On the other hand, it can actually develop, as time goes by, singularities even from smooth initial data, which then characterize the whole evolution and are propagated along special curves called **characteristics**. In particular, if the solution has initially a compact support, then such a support expands with a finite **speed of propagation** of the effect modelled by the hyperbolic equation.

The above qualitative properties will be analyzed with reference to the examples which follow:

Example 3.3.3
Initial Value Problem for the Linear Transport Model

Consider the linear transport model:

$$\mathcal{L}u = \left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right)u \,, \qquad c > 0 \,, \tag{3.3.14}$$

linked to the initial condition: $u(t = 0, x) = e^{-x^2}$. Then the solution is $u(t, x) = e^{-(x-ct)^2}$, which travels unchanged to the right with speed equal to c.

□

<div align="center">

Example 3.3.4

Initial Value Problem for the Linear Diffusion Model

</div>

Consider the linear diffusion model:

$$\mathcal{L}u = \left(\frac{\partial}{\partial t} - h \frac{\partial^2}{\partial x^2} \right) u, \qquad h > 0, \tag{3.3.15}$$

linked to the initial condition given in Example 3.3.3. Then the solution is

$$u(t, x) = \frac{1}{\sqrt{1 + 4ht}} e^{-\dfrac{x^2}{1 + 4ht}}, \tag{3.3.16}$$

which shows how the bell shape of the initial condition is preserved, but it broadens out; the maximum is always at $x = 0$, but it decreases with time.

□

<div align="center">

Example 3.3.5

Initial Value Problem for the Linear Wave Model

</div>

Consider the linear wave model:

$$\mathcal{L}u = \left(\frac{\partial^2}{\partial t^2} - c^2 \frac{\partial^2}{\partial x^2} \right) u, \tag{3.3.17}$$

linked to the same above initial condition in Example 3.3.3 and to an additional condition stating that the initial speed is equal to zero

$$\frac{\partial u}{\partial t}(t = 0, x) = 0. \tag{3.3.18}$$

Then, the solution is as follows:

$$u(t, x) = \frac{1}{2} \left[e^{-(x-ct)^2} + e^{-(x+ct)^2} \right], \tag{3.3.19}$$

which shows that the initial the bell shaped condition is split in two and both parts travel with speed c, one to the left and the other to the right.

□

Remark 3.3.1. *If the solution to the initial value problem related to the above models is developed for initial conditions with compact support:* $u(t = 0, x) = 0$ *for* $x \notin [a, b]$, *and* $u(t = 0, x) = u_{in}(x) > 0$ *for* $x \in [a, b]$, *then the support at time t is:*
- $[a + ct, b + ct]$ *for the transport model;*
- $[a - ct, b - ct] \cup [a + ct, b + ct]$ *for the wave propagation problem;*
- $\mathbb{R}$ *for the diffusion problem;*

Remark 3.3.2. *It can be observed that the solution to the transport model remains constant on the lines* $x = x_0 + ct$. *Similarly, the solution to the wave equation is made up of two terms: the first remains constant on the lines* $x = x_0 + ct$, *the second on the lines* $x = x_0 - ct$. *From this observation it should be clear that these are peculiar curves in the* (t, x)-*plane which deserve to be named. They are, in fact, called* ***characteristics*** *and, as we shall see, are very important both from the physical and the mathematical point of view.*

To understand the concept of characteristic, consider the three-dimensional transport equation

$$\frac{\partial u}{\partial t} + \mathbf{c}(t, \mathbf{x}) \cdot \nabla u = f(t, \mathbf{x}; u), \qquad \mathbf{x} \in \mathcal{D} \subseteq \mathbb{R}^3. \tag{3.3.20}$$

This equation is called a transport equation, since the state variable is sort of transported by the convection current $\mathbf{c}(t, \mathbf{x})$. In fact, if we consider the curves $\mathbf{x}(t)$ defined by

$$\frac{d\mathbf{x}}{dt} = \mathbf{c}(t, \mathbf{x}), \tag{3.3.21}$$

and evaluate u on them we have that its temporal evolution is given by

$$\frac{d}{dt}u(t, \mathbf{x}(t)) = \frac{\partial u}{\partial t} + \nabla u \cdot \frac{d\mathbf{x}}{dt}. \tag{3.3.22}$$

Recalling Eq. (3.3.20), yields

$$\frac{d}{dt}u(t, \mathbf{x}(t)) = f\Big(t, \mathbf{x}(t); u\big(t, \mathbf{x}(t)\big)\Big). \tag{3.3.23}$$

The line

$$\begin{cases} \dfrac{d\mathbf{x}}{dt} = \mathbf{c}(t, \mathbf{x}), \\ \mathbf{x}(\hat{t}) = \widehat{\mathbf{x}}, \end{cases} \tag{3.3.24}$$

is the so-called ***characteristic*** through $(\hat{t}, \widehat{\mathbf{x}})$.

The evolution of the solution on it is then given by

$$\begin{cases} \dfrac{d}{dt}u\big(t, \mathbf{x}(t)\big) = f\Big(t, \mathbf{x}(t); u\big(t, \mathbf{x}(t)\big)\Big) \\ u(\hat{t}, \widehat{\mathbf{x}}) = \widehat{u}, \end{cases} \tag{3.3.25}$$

where $\widehat{u}$ is the value of u in $(\hat{t}, \widehat{\mathbf{x}})$.

Thus we have reduced the solution of a first-order **partial** differential equation to the solution of two coupled first-order **ordinary** differential equations.

Example 3.3.6
Characteristic lines

The characteristics of the equation

$$\frac{\partial u}{\partial t} + (\alpha x + \beta t + \gamma)\frac{\partial u}{\partial x} = 0 \qquad (3.3.26)$$

can be found by solving the ordinary differential equation

$$\frac{dx}{dt} = \alpha x + \beta t + \gamma\,, \qquad (3.3.27)$$

the solution of which is

$$x(t) = \begin{cases} Ce^{\alpha t} - \dfrac{\alpha\gamma + \beta}{\alpha^2} - \dfrac{\beta}{\alpha}t\,, & \text{if } \alpha \neq 0 \\[3mm] C + \gamma t + \dfrac{\beta}{2}t^2\,, & \text{if } \alpha = 0\,, \end{cases} \qquad (3.3.28)$$

where C is an integration constant. Hence the characteristic through the point $(\hat{t}, \widehat{x})$ is

$$x(t) = \widehat{x}e^{\alpha(t-\hat{t})} + \frac{\alpha\gamma + \beta}{\alpha^2}\big(e^{\alpha(t-\hat{t})} - 1\big) + \frac{\beta}{\alpha}\big(\hat{t}e^{\alpha(t-\hat{t})} - t\big)\,, \qquad (3.3.29)$$

if $\alpha \neq 0$, and

$$x(t) = \widehat{x} + \gamma(t - \hat{t}) + \frac{\beta}{2}(t^2 - \hat{t}^2)\,, \qquad (3.3.30)$$

if $\alpha = 0$. Then the state variable remains constant along the characteristics.

□

3.4 Mathematical Formulation of Problems

This section deals with the mathematical formulation of problems related to models stated in terms of partial differential equations. A line similar to that of Chapter 2 will be followed: after having verified the consistency of a mathematical model, the formulation of mathematical problems is stated adding to the evolution equation the conditions necessary to find quantitative solutions. Possibly, before dealing with the search of solutions, the well position of the mathematical problem should be verified.

The analysis developed in two steps: first we refer to scalar models in one space dimension and then various generalizations are dealt with. Let us consider the class of models involving dimensionless scaled independent and dependent variables:

$$u = u(t, x): \quad [0, 1] \times [0, 1] \to [0, 1],$$ (3.4.1)

stated in terms of partial differential equations which can be written, in normal form, as follows:

$$\frac{\partial u}{\partial t} = f\left(t, x; u, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}\right).$$ (3.4.2)

Relatively more general cases can be technically developed starting from the indications given for the above class of models. For instance higher order problems as well as problems in unbounded domain, and so on.

Remark 3.4.1. *Actually the range of the dependent variable cannot be stated precisely without solving the equation. Therefore, only the physics can contribute to identify the smallest and largest value of the dependent variable. Therefore, (3.4.1) can be interpreted by saying that u is of the order of unity.*

Remark 3.4.2. *(Statement of problems) If both time and space derivatives appear in the mathematical model, then both initial and boundary conditions usually have to be assigned. The relative mathematical problem is then called an **initial-boundary-value problem**. If, instead, the mathematical model is static, i.e., time independent, then initial conditions are not needed. In this case, the mathematical problem is defined as a **boundary-value problem**.*

Bearing all above in mind, some mathematical problems, in **one space dimension**, will be stated in what follows.

Problem (Dirichlet) 3.4.1. *The **Dirichlet** initial-boundary value problem for Eq. (3.4.2) is stated with initial condition*

$$u(0, x) = \varphi(x), \qquad \forall\, x \in [0, 1],$$ (3.4.3)

and Dirichlet boundary conditions

$$u(t, 0) = \alpha(t), \quad \text{and} \quad u(t, 1) = \beta(t), \qquad \forall\, t \in [0, 1],$$ (3.4.4)

where φ is a given function of space, while α and β are given continuous functions of time.

Problem (Neumann) 3.4.2. *The **Neumann** initial-boundary value problem for Eq. (3.4.2) is stated with initial condition (3.4.3) and Neumann boundary conditions*

$$\frac{\partial u}{\partial x}(t, 0) = \gamma(t) \qquad \text{and} \qquad \frac{\partial u}{\partial x}(t, 1) = \delta(t), \qquad \forall\, t \in [0, 1],$$ (3.4.5)

where γ and δ are given continuous functions of time.

Problem (Mixed) 3.4.3. *The **mixed** initial-boundary value problem for Eq. (3.4.2) is stated with initial condition (3.4.3), to Dirichlet boundary conditions on one side, and Neumann boundary conditions on the other one:*

$$u(t,0) = \alpha(t) \qquad and \qquad \frac{\partial u}{\partial x}(t,1) = \delta(t), \qquad \forall\, t \in [0,1], \qquad (3.4.6)$$

or viceversa

$$\frac{\partial u}{\partial x}(t,0) = \gamma(t) \qquad and \qquad u(t,1) = \beta(t), \qquad \forall\, t \in [0,1]. \qquad (3.4.7)$$

Problem (Robin) 3.4.4. *The **Robin** initial-boundary value problem for Eq. (3.4.2) is stated with initial condition (3.4.3), to the boundary conditions defined as a linear combination of Dirichlet and Neumann boundary conditions, say*

$$c_1(t)\alpha(t) + c_2(t)\gamma(t) = u_a(t) \quad and \quad c_3(t)\beta(t) + c_4(t)\delta(t) = u_b(t), \qquad (3.4.8)$$

where $c_{1,2,3,4}$ and $u_{a,b}$ are given functions of time $\forall\, t \in [0,1]$.

In general one may have problems with nonlinear boundary conditions:

Problem (Nonlinear boundary value) 3.4.5. *The initial-boundary value problem for Eq. (3.4.2) with nonlinear boundary conditions is stated with initial condition (3.4.3), to the boundary conditions defined as a nonlinear combination of Dirichlet and Neumann boundary conditions, say*

$$g_1(\alpha(t), \gamma(t)) = b_a(t) \qquad and \qquad g_2(\beta(t), \delta(t)) = b_b(t), \qquad (3.4.9)$$

$\forall\, t \in [0,1]$, *where $b_{a,b}$ are given functions of time, and $g_{1,2}$ are suitable functions of their arguments.*

Remark 3.4.3. *(**Sufficient initial and boundary conditions**) The above statement of problems has been obtained linking to the evolution equations a number of information on the behavior of the state variable on the boundary of the independent variable equal to the highest order of the partial derivative with respect to the said variable.*

Remark 3.4.4. *(**Problems in unbounded domains**) Some problems refer to systems in a half-space $x \in [0,\infty)$, or in the whole space $x \in \mathbb{R}$. In this case boundary conditions have to be stated as above, at the boundaries $x = 0$ and $x \to \infty$, or for $x \to -\infty$ and $x \to \infty$. Asymptotic behavior can be stated letting the time variable to infinity.*

Example 3.4.1
Mathematical Problems for the Linear Wave Model

Consider the linear wave model

$$\mathcal{L}u = \left(\frac{\partial^2}{\partial t^2} - c^2 \frac{\partial^2}{\partial x^2} \right) u = 0 \,, \tag{3.4.10}$$

which can be written as a system of two first order equations:

$$\begin{cases} \dfrac{\partial u}{\partial t} = v \,, \\[2mm] \dfrac{\partial v}{\partial t} = \dfrac{\partial^2 u}{\partial x^2} \,. \end{cases} \tag{3.4.11}$$

Then, according to Remark 3.4.3, the first equation needs only an initial condition for the variable u, while the second one an initial condition for the variable v and two boundary conditions for the variable u.

$\square$

Bearing in mind the above definition of statement of problems, the following general definition can be given:

> **Well-formulated problems**
>
> *If the model is implemented with enough initial and boundary conditions to find a solution, then the relative mathematical problem is said to be **well-formulated.***

Well-posedness is not an immediate consequence of the statement of problems. It has to be proven by a specific qualitative analysis. The above analysis needs a deep knowledge of the theory of partial differential equations, which is not object of the aims of these Lecture Notes mainly addressed to modelling aspects.

The interested reader is addressed to the specialized literature, e.g Lions and Magenes (1968), and Dautray and Lions (1990), to recover the above knowledge. On the other hand, a few examples are given in this section simply with the aim of show how the above reasonings can be properly developed. Before dealing with this topic we will show how the statement of problems can be generalized to model in several space variables.

Consider first scalar models involving the whole set of space variables, say $\mathbf{x} = \{x_1, x_2, x_3\}$.

Specifically, consider the case of models which can be written as follows:

$$\frac{\partial u}{\partial t} = f\left(t, \mathbf{x}, \frac{\partial u}{\partial x_1}, \dots, \frac{\partial^2 u}{\partial x_1^2}, \frac{\partial^2 u}{\partial x_2^2}, \dots, \frac{\partial^2 u}{\partial x_1 \partial x_2}, \dots \right) \,, \tag{3.4.12}$$

where u is the dependent variable

$$u = u(t, \mathbf{x}) : \quad [0,1] \times D \to \mathbb{R} \,, \tag{3.4.13}$$

where the boundary of the domain of $D \subseteq \mathbb{R}^3$ of the space variables is denoted by ∂D. The statement of some related mathematical problems is as follows:

Problem (Dirichlet) 3.4.6. *The initial-boundary value problem for the scalar Eq. (3.4.12) with Dirichlet boundary conditions, is stated with initial condition*

$$u(0, \mathbf{x}) = \varphi(\mathbf{x}), \qquad \forall \, \mathbf{x} \in D, \tag{3.4.14}$$

and boundary conditions

$$\forall \, t \in [0, 1], \quad \forall \, \mathbf{x} \in \partial D : \quad u = \alpha^*(t; \mathbf{x} \in \partial D), \tag{3.4.15}$$

given as functions consistent, for $t = 0$, with the initial condition (3.4.14).

Problem (Neumann) 3.4.7. *The initial-boundary value problem for the scalar Eq. (3.4.12) with Dirichlet boundary conditions, is stated with initial condition (3.4.14) and Neumann boundary conditions*

$$\forall \, t \in [0, 1], \quad \forall \, \mathbf{x} \in \partial D : \quad \frac{\partial u}{\partial \mathbf{n}} = \gamma^*(t; \mathbf{x} \in \partial D), \tag{3.4.16}$$

given as functions of time and where $\mathbf{n}$ denotes the normal to ∂D directed inside D.

Remark 3.4.5. *If the model is defined by a system of equations, then initial and boundary conditions have to be assigned for each equation according to the rules stated above. For problems in unbounded domain the same reasoning developed for problems in one space dimension can be technically generalized to problems in more than one space domain.*

Example 3.4.2
Mathematical problems for the heat diffusion model

Consider the heat conduction problem

$$\frac{\partial u}{\partial t} = k \nabla^2 u + f(t, \mathbf{x}; u), \qquad \mathbf{x} \in \mathcal{D}, \tag{3.4.17}$$

which is well formulated if joined, for instance, to the initial condition

$$u(t = 0, \mathbf{x}) = u_{in}(\mathbf{x}), \qquad \mathbf{x} \in \mathcal{D}, \tag{3.4.18}$$

and to the boundary conditions

$$u(t, \mathbf{x}) = u_D(t, \mathbf{x}), \qquad \text{if } \mathbf{x} \in \partial \mathcal{D}_D,$$
$$\mathbf{n}(t, \mathbf{x}) \cdot \nabla u(t, \mathbf{x}) = u_N(t, \mathbf{x}), \qquad \text{if } \mathbf{x} \in \partial \mathcal{D}_N, \tag{3.4.19}$$

where $\partial\mathcal{D}_D$ and $\partial\mathcal{D}_N$ are a partition of the boundary $\partial\mathcal{D}$ and $\mathbf{n}$ is the normal to $\partial\mathcal{D}_N$.

$\square$

It is worth stressing again that the above statements of problems do not imply good position. This matter is dealt in the pertinent literature, e.g. Lions and Magenes (1968), and Dautray and Lions (1990), with reference to well defined mathematical problems. The above problems have been stated for bounded time intervals. If time is let to go to infinity, the statement is valid globally in time. In this case it is useful looking for the trend of the solutions asymptotically in time.

The statement of mathematical problems we have seen above has used different types of boundary conditions, always linear ones. However, in some cases of interest for the applications, non-linear boundary conditions are needed. This happens whenever the quantities that can be effectively measured at the boundaries are not the classical Dirichlet or Neumann conditions, or a linear combination of them.

It is not worth stressing that boundary conditions are not an abstract invention, but quantities, which have to be effectively measured on the real system. Only in such a way the prediction of the model will correspond to the real system under consideration. The example which follows refers to the vehicular traffic model presented in the Example 3.2.7 of Section 3.2. The measurements of the boundary conditions refer specifically to the flow. In fact, for simple technical reasons due to the available devices, the measurement of the flow is remarkably more precise than that of density. The following example illustrates the above reasonings in a practical case.

<hr>

Example 3.4.3
Traffic flow Model

Consider the macroscopic vehicular traffic model presented in Section 3.2, which is written as follows

$$\frac{\partial u}{\partial t} + c(u)\frac{\partial u}{\partial x} = \varepsilon\frac{\partial}{\partial x}\left[k(u)\frac{\partial u}{\partial x}\right], \tag{3.4.20}$$

corresponding to a model of the flow of the type

$$q = 1 - u\left[1 - \varepsilon(1-u)\frac{\partial u}{\partial x}\right], \tag{3.4.21}$$

where $u = u(t,x)$ and $q = q(t,x)$.

Suppose that the boundary conditions are given by the flow measurements as follows:

$$\begin{cases} q_\alpha(t) = 1 - \alpha(t)\left[1 - \varepsilon(1-\alpha(t))\gamma(t)\right], \\ q_\beta(t) = 1 - \alpha(t)\left[1 - \varepsilon(1-\beta(t))\delta(t)\right], \end{cases} \tag{3.4.22}$$

where $\alpha(t) = u(t,0), \quad \beta(t) = u(t,1), \quad \gamma(t) = \dfrac{\partial u(t,0)}{\partial x}, \quad \delta(t) = \dfrac{\partial u(t,1)}{\partial x}.$

It follows that if $q_\alpha(t)$ and $q_\beta(t)$ are given, then boundary conditions are identified as a non–linear combination of the Dirichlet and Neumann boundary conditions.

$\square$

The interested reader can find in Section 6.3 of Bellomo *et al.* (2007), how the above problem can be technically solved. It is plain that the above problem cannot be solved by solving system (3.4.22) with respect to α and β or γ and δ. On the other hand, the solution can be linked to the discretization schema.

Without entering into the details of technical calculations, we can show that it is necessary to derive the phenomenological relation (3.4.21) with respect to time and to link it to the equation of conservation of mass. The following model is obtained:

$$
\begin{cases}
\dfrac{\partial u}{\partial t} = -\dfrac{\partial q}{\partial x}\,, \\[2ex]
\dfrac{\partial q}{\partial t} = \left[(1 - 2u) + \varepsilon\,(2 - 3u)\,\dfrac{\partial q}{\partial x}\right]\dfrac{\partial q}{\partial x} - \varepsilon\,u(1 - u)\,\dfrac{\partial^2 q}{\partial x^2}\,.
\end{cases}
\tag{3.4.23}
$$

The boundary conditions for this problem are precisely $q_\alpha(t)$ and $q_\beta(t)$. Therefore, the problem can be solved with the appropriate Dirichlet type conditions on $x = 0$ and $x = 1$.

3.5 An Introduction to Analytic Methods for Linear Problems

The preceding sections have shown various examples of linear and nonlinear models. Similarly to the case of models stated in terms of ordinary differential equations, linearity has to be considered a very special case considering that all systems of real world are, at least in principle, nonlinear. In case, however special, of linear models and problems one can attempt to deal with analytic solutions. A brief account of mathematical methods to obtain analytic solutions is given in this section.

Consider first the relatively simple case of scalar linear models in one space dimension. Moreover, suppose that the solution $u = u(t, x)$ of some initial-boundary value problem is known, then the starting point of the search for analytic solutions is the representation of the solution in a Hilbert space. Specifically, consider a representation of a function $u = u(t, x)$ given by an expansion of the type

$$
u(t, x) = \sum_{i=0}^{\infty} c_i(t)\psi_i(x)\,,
\tag{3.5.1}
$$

where the functions ψ_i belong to a complete space of orthonormal functions defined in a suitable Hilbert space with weighted (the weight function is denoted by $w = w(x)$) inner product

$$
\langle f\,,\,g \rangle_w(t) = \int f(t, x)g(t, x)w(x)\,dx\,.
\tag{3.5.2}
$$

Consequently, the coefficients c_i are given by

$$c_i(t) = \langle u \,, \, \psi_i \rangle_w \,, \tag{3.5.3}$$

where the calculation of the integrals may need numerical computation. In this case, one may discretize the space variable and compute the integrals by weighted sums.

For practical applications u is **approximated** by u^n corresponding to the collocation I_x, then a truncated expansion is used

$$u(t,x) \cong u^n(t,x) = \sum_{i=0}^{n} c_i(t)\psi_i(x) \,, \tag{3.5.4}$$

where the coefficients c_i have to be computed as indicated above.

Various examples of orthonormal functions can be given in addition to the classical Fourier expansion by sinus and cosinus defined over the interval $[0, 2\pi]$ with weight $w = 1$. Some examples are given in what follows:

Example 3.5.1
Tchebyschev Polynomes

Tchebyschev polynomials are characterized by the following features:

- Range: $[-1, 1]$.

- Polynomials:

$$T_0 = 1 \,, \quad T_1 = x \,, \quad T_m = 2xT_{m-1} - T_{m-2} \,. \tag{3.5.5}$$

- Weight:

$$i = j \neq 0 : \frac{2/\pi}{1 - x^2} \,, \quad i = j = 0 : \frac{1/\pi}{1 - x^2} \,. \tag{3.5.6}$$

□

Example 3.5.2
Legendre Polynomials

Legendre polynomials are characterized by the following features:

- Range: $[-1, 1]$.

- Polynomials:

$$L_0 = 1 \,, \quad L_1 = x \,, \quad L_m = \frac{2m - 1}{m}xL_{m-1} - \frac{m - 1}{m}L_{m-2} \,. \tag{3.5.7}$$

- Weight:

$$i = j \neq 0 : \quad \frac{2}{2m+1} \,. \tag{3.5.8}$$

□

Example 3.5.3
Laguerre Polynomials

Laguerre polynomials are characterized by the following features:

- Range: $[0, \infty)$.

- Polynomials:

$$L_0^a = 1 \,, \quad L_1^a = a + 1 - x \,, \quad a > -1 \,, \tag{3.5.9}$$

and

$$L_m^a = \frac{1}{m}(2m - 1 + a - x)L_{m-1}^a - \frac{1}{m}(m - 1 + a)L_{m-2}^a \,. \tag{3.5.10}$$

- Weight:

$$i = j \neq 0 : \quad \frac{m!}{\Gamma(a + m + 1)} x^a e^{-x} \,. \tag{3.5.11}$$

□

Example 3.5.4
Hermite Polynomials

Hermite polynomials are characterized by the following features:

- Range: $(-\infty, \infty)$.

- Polynomials:

$$H_0 = 1 \,, \quad H_1 = x \,, \quad H_m = x H_{m-1} - (m - 1) H_{m-2} \,. \tag{3.5.12}$$

- Weight:

$$i = j \neq 0 : \quad \frac{m!}{\sqrt{2\pi}} e^{-x/2} \,. \tag{3.5.13}$$

□

The solution of mathematical problems consists in solving suitable evolution equations for the coefficients c_i which are obtained replacing the expression (3.5.4) into the partial differential equation and in implementing, still into the same expression, initial and boundary conditions. In the case of relatively simpler problems (e.g. linear differential equations with constant

coefficients) the solution can be recovered analytically, while in the general cases computational methods have to be used. Generally, the method leads to systems of ordinary differential equations of the type we have seen in Chapter 2.

Consider, in order to understand the application of the method, the following class of linear equations:

$$\frac{\partial}{\partial t}u = a(t)\frac{\partial}{\partial x}u + b(t)\frac{\partial^2}{\partial x^2}u\,, \tag{3.5.14}$$

and initial value problems without constraint at the boundaries.

Replacing the expression (3.5.4) in the evolution equation Eq. (3.5.14), yields a system of linear ordinary differential equations. In fact:

$$\frac{\partial}{\partial t}\sum_{j=0}^{n}c_j(t)\psi_j(x) = a(t)\frac{\partial}{\partial x}\sum_{j=0}^{n}c_j(t)\psi_j(x) + b(t)\frac{\partial^2}{\partial x^2}\sum_{j=0}^{n}c_j(t)\psi_j(x)\,. \tag{3.5.15}$$

By taking the inner product, an evolution equation for the coefficients can be obtained as follows:

$$\frac{dc_i}{dt} = a(t)\sum_{j=0}^{n}c_j(t)h_{ji}(t) + b(t)\sum_{j=0}^{n}c_j(t)k_{ji}(t)\,, \tag{3.5.16}$$

where

$$h_{ji} = \left\langle \frac{d\psi_j}{dx}\,,\ \psi_i \right\rangle\,, \tag{3.5.17}$$

and

$$k_{ji} = \left\langle \frac{d^2\psi_j}{dx^2}\,,\ \psi_i \right\rangle\,. \tag{3.5.18}$$

The above linear equation can be treated with methods of linear ordinary differential equations. Initial c_{i0} conditions have to be implemented for $t = 0$. Then using the same approximation, one has:

$$u(0,x) = u_0(x) \cong u_0^n(x) = \sum_{j=0}^{n}c_j(t)\psi_j(x)\,. \tag{3.5.19}$$

A similar reasoning can be applied to boundary conditions. Consider specifically the case of Dirichlet boundary conditions. Then one has:

$$u(t,0) = \alpha(t) \cong u^n(t,0) = \sum_{j=0}^{n}c_j(t)\psi_j(x=0)\,, \tag{3.5.20}$$

and

$$u(t,1) = \beta(t) \cong u^n(t,1) = \sum_{j=0}^{n}c_j(t)\psi_j(x=1)\,. \tag{3.5.21}$$

The solution of the above algebraic system allows computing the first and last coefficient in terms of the others, thus reducing the dimension of System (3.5.16). Convergence for $n \to \infty$ is

related to the application of classical convergence theorems for orthogonal functions in Hilbert spaces. Dealing with systems of equations simply means applying the above procedure to all equations.

In principle, the same method can be implemented for equations in several space dimension. Formally the procedure is the same, however the method generates technical computational complexity related to the large dimension of the system.

3.6 Discretization of Nonlinear Mathematical Models

Continuum models may be viewed as systems with infinite number of degrees of freedom. The analysis proposed in Section 3.5 has shown how one may look for analytic solutions in terms of an infinite expansion of functions in a suitable Hilbert space. This method can be unlikely applied to the solution of nonlinear problems and models, although, at least in principles, one may attempt to apply the same procedure. On the other hand, the technical application of the method immediately shows that the system of ordinary differential equations becomes nonlinear, and the computational complexity is to heavy to be technically tackled.

Then methods of computational mathematics need to be developed to approximate the continuous system, say:

$$\mathcal{L}\mathbf{u} = \mathcal{N}\mathbf{u}\,, \tag{3.6.1}$$

by a system with finite number of degrees of freedom:

$$\mathcal{L}\mathbf{u}^n = \mathcal{N}\mathbf{u}^n\,, \tag{3.6.2}$$

where n is such a number. In other words, the problem consists in approximating the continuous model (or problem) by a discrete model (or problem). Then the solution of the finite model can be obtained by methods reviewed in Chapter 2, while a technical analysis can possibly provide informations on the distance between the solution of the continuous model and the finite one.

Although these Lecture Notes deal with modelling rather than with computational methods, this section will however show how the above approximation can be developed for some simple cases. As we shall see, the analysis is rather simple in the case of problems in one space dimension only, while computational complexity problems arise when models, and related mathematical problems are in more than one space dimensions. So far this sections should be regarded as a brief introduction to the above problems to be properly dealt with referring to the specialized literature.

Discrete models can be obtained by continuous ones by decomposing the domain $\mathcal{D}$ of the space variable into a certain number of finite volumes $\mathcal{D}_i$:

$$\mathcal{D} = U_{i=1}^n \mathcal{D}_i\,, \qquad i = 1,\ldots,n\,, \tag{3.6.3}$$

and by taking averaged value of the state variable within each volume.

It follows that in each finite volume the dependent variable is $u_i = u_i(t)$, and that the mathematical model is a finite one consisting in a set of n equations providing the evolution of the u_i. The model is obtained by the same conservation and/or equilibrium equations of the continuous model. The variables u_i can be localized in the center of mass of each volume, while each finite element is assumed to be subject to the action of the continuous ones as well as from the boundaries for those elements which are localized on the boundary containing the system which is modelled.

The above procedure generates a finite model and mathematical problems stated in terms of a system of ordinary differential equations. The discretization method can be easily applied in the case of one space dimension. The examples which follow refer to the discretization of a model of an elastic string subject to Dirichlet boundary conditions, and to a model of diffusion phenomena with Neumann boundary conditions. Namely we refer to models already presented in Examples 3.2.1 and 3.2.2. Generalizations - and difficulties - to problems in more than one space dimension will be subsequently described.

Example 3.6.1
Discrete Models for a Vibrating String

Consider a discrete model corresponding to the vibrating string model described in Example 3.2.1 where, in this case, gravitation is not neglected and the vibration plane is supposed to be vertical.

Following the above listed modelling procedure, the space variable is discretized by the collocation

$$i = 0, \ldots, n+1 : \quad I_x = \{x_0 = 0, \ldots, x_i, \ldots, x_{n+1} = 1\}. \tag{3.6.4}$$

The **extrema** are fixed; hence two degrees of freedom, corresponding to the movement of the points on the boundary, are suppressed. A mass $m = M/(n+2)$ is placed in each collocation point. It is constrained to move along the vertical direction and is connected to the contiguous masses by linear springs with elastic constant k, as shown in Figure 3.6.1.
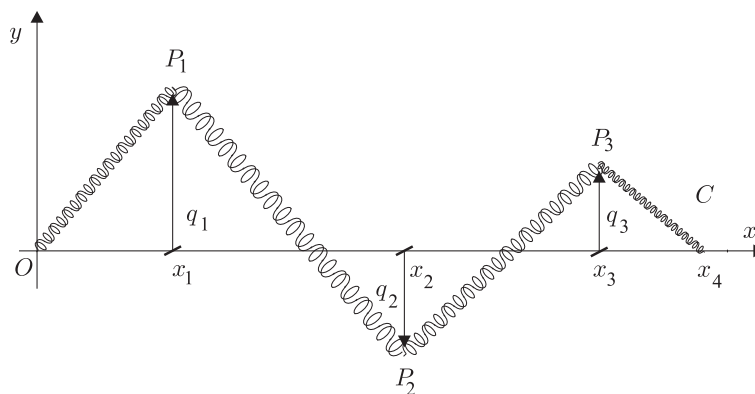

Figure 3.6.1 — Discrete model of a vibrating string.

The procedure provides a mechanical model with n degrees of freedom identified by the Lagrangian variable

$$\mathbf{q} = (q_1, \ldots, q_i, \ldots, q_n), \qquad q_i = q_i(t), \tag{3.6.5}$$

where q_i is the vertical displacement of the mass located in x_i. The mathematical model corresponding to the above mechanical model can be obtained by the following methods of classical mechanics. In detail, the kinetic energy is

$$E_c = \frac{1}{2} m \sum_{i=1}^{n} \left(\frac{dq_i}{dt} \right)^2, \tag{3.6.6}$$

while the potential is

$$U = \sum_{i=1}^{n} mg\, q_i - \frac{k}{2} \sum_{i=0}^{n} \left[(q_{i+1} - q_i)^2 + (x_{i+1} - x_i)^2 \right], \tag{3.6.7}$$

with $q_0 = q_{n+1} = 0$. The evolution model is as follows:

$$\frac{d^2 q_i}{dt^2} = g + \frac{k}{m} \left(q_{i+1} - 2q_i + q_{i-1} \right). \tag{3.6.8}$$

$\square$

It is worth remarking on a few connections between the above **finite** model and the original continuous model:

i) The derivation of the discrete model required the preliminary construction of a **mechanical model approximating** the continuous phenomenological model. Subsequently, modelling methods for models at the microscopic scale are applied to obtain the **finite mathematical model**.

ii) The system of ordinary differential equations is linear as it was the original continuous model. On the other hand, nonlinear models are needed for large deviations when the elastic term cannot be anymore assumed to be constant. The material behavior can be simulated assuming that c depends on the lengths of the stretched elements.

iii) Increasing the number of finite elements may increase accuracy. However, it also increases the dimension of the system of differential equations.

iv) The model with finite degrees of freedom satisfies the same linearity (or nonlinearity) properties of the continuous model.

v) The model has been derived assuming that each element moves in a vertical plane. On the other hand, the same procedure can be technically applied to the case of elements moving in the plane. This is a simple technical problem, while the continuous model implies severe technical difficulties.

The above model was derived following a finite element scheme. One can technically generalize them also to finite models derived in finite volume schemes as in the example which follow:

<div align="center">

Example 3.6.2

Discrete Models for Diffusion Phenomena

</div>

Consider the discrete model corresponding to the one-dimensional case of the heat diffusion model dealt with in Example 3.2.2. Obtained discretizing the space variable by the collocation (3.6.4).

A finite element corresponds to each point. Moreover, the heat flux at the ***extrema*** are prescribed, say $q_1 = q_1(t)$ and $q_n = q_n(t)$.

A mechanical model is obtained, which has n degrees of freedom and identified by the variable

$$\mathbf{u} = (u_1, \ldots, u_i, \ldots, u_n), \qquad u_i = u_i(t), \tag{3.6.9}$$

where u_i is the local temperature in the finite volume localized in x_i. The mathematical model is obtained applying to each finite volume the balance equation:

$$\frac{\partial u}{\partial t} = k_0 \frac{\partial^2 u}{\partial x^2}, \tag{3.6.10}$$

where the flux is modelled by applying Fourier's phenomenological model:

$$q = -h_0 \frac{\partial u}{\partial x} \tag{3.6.11}$$

The evolution model for an inner element is as follows:

$$\frac{du_i}{dt} = \frac{k_0}{H}[(u_{i+1} - 2u_i + u_{i-1})], \tag{3.6.12}$$

where space derivatives have been replaced by finite differences, and where H is the size of the volume. This crude approximation can be properly refined. The flux for the boundary elements is directly given by the boundary conditions.

In the nonlinear case the constant k_0 has to be replaced by a function of the local variable u.

<div align="right">

□

</div>

The above method is based on the idea of decomposing the continuous system into finite elements. Then the evolution equation for each element is derived using the same method used to derive the continuous model. A system of coupled equations is obtained where the coupling is related to the interactions between elements, in other words, $i - 1$ and $i + 1$-elements act on the i-element. Boundary conditions act on the first and last element.

The application of the method is quite immediate in one space dimension, on the other hand, various technical complexities occur in more than one space dimension, although the guiding

lines for the application of the method is precisely the same. The evolution in each sub-domain $\mathcal{D}_i$ is derived by local application of the above mentioned equilibrium and/or conservation equations, while the actions of the elements on the boundaries of $\mathcal{D}_i$ acts as boundary conditions.

An analogous result can be obtained by analytic interpolation methods of the variable $u = u(t, x)$ for $x \in [0, 1]$. In this case we shall talk about discretization methods by ***collocation-interpolation***. The description of the method refers both to interpolation of functions and to calculations of local derivatives. Moreover, let us define the collocation

$$i = 1, \ldots, n : \quad I_x = \{x_1 = 0, \ldots, x_i, \ldots, x_n = 1\}, \tag{3.6.13}$$

which may be equally spaced

$$x_i = (i-1)k, \qquad k = \frac{1}{n-1}. \tag{3.6.14}$$

or Tchebyschev type collocation with decreasing values of the measure $|x_i - x_j|$ towards the borders.

In general, $u = u(t, x)$ can be interpolated and approximated by means of by Lagrange polynomials as follows

$$u(t, x) \cong u^n(t, x) = \sum_{i=1}^{n} L_i(x) u_i(t), \tag{3.6.15}$$

where $u_i(t) = u(t, x_i)$ and where Lagrange polinomials are given by the following expressions

$$L_i(x) = \frac{(x - x_1) \ldots (x - x_{i-1})(x - x_{i+1}) \ldots (x - x_n)}{(x_i - x_1) \ldots (x_i - x_{i-1})(x_i - x_{i+1}) \ldots (x_i - x_n)}. \tag{3.6.16}$$

The above defined interpolations can be used to approximate the partial derivatives of the variable u in the nodal points of the discretization

$$\frac{\partial^r u}{\partial x^r}(t; x_i) \cong \sum_{h=1}^{n} a_{hi}^{(r)} u_h(t), \qquad a_{hi}^{(r)} = \frac{d^r L_h}{dx^r}(x_i), \tag{3.6.17}$$

for $r = 1, 2, \ldots$.

The value of the coefficients depends on the number of collocation points and on the type of collocation. Technical calculations provide, in the case of Lagrange polynomials, the following result

$$a_{hi}^{(1)} = \frac{\prod(x_i)}{(x_h - x_i)\prod(x_h)}, \qquad a_{ii}^{(1)} = \sum_{h \neq i} \frac{1}{x_i - x_h}, \tag{3.6.18}$$

where

$$\prod(x_i) = \prod_{p \neq i}(x_i - x_p), \qquad \prod(x_h) = \prod_{p \neq h}(x_h - x_p). \tag{3.6.19}$$

Higher order coefficients may be computed exploiting the following recurrence formula

$$a_{hi}^{(r+1)} = r\left(a_{hi}\,a_{hi}^{(r)} + \frac{a_{hi}^{(r-1)}}{x_h - x_i}\right)\,, \qquad a_{ii}^{(r+1)} = -\sum_{h \neq i} a_{hi}^{(r+1)}\,. \tag{3.6.20}$$

The same method can be used for time dependent functions in two space variables: $u = u(t,x,y) : \quad [0,1] \times [0,1] \times [0,\ell] \to [-1,1]$, such that $u(t;x,y)$ is a one to one map from $[0,1] \times [0,\ell]$ into $[-1,1]$, for every $t \in [0,1]$. Consider, in addition to the collocation I_x, the following

$$j = 1,\ldots,m : \quad I_y = \{y_1 = 0,\ldots,y_j,\ldots,y_m = 1\}\,. \tag{3.6.21}$$

It follows that

$$u = u(t,x,y) \cong u^{nm}(t,x,y) = \sum_{i=1}^{n}\sum_{j=1}^{m} L_i(x)L_j(y)u_{ij}(t)\,. \tag{3.6.22}$$

The approximation of the space derivatives in the collocation points is obtained by calculations analogous to the ones of the one-dimensional case:

$$\frac{\partial^r u}{\partial x^r}(t;x_i,y_j) \cong \sum_{h=1}^{n} a_{hi}^{(r)} u_{hj}(t)\,, \tag{3.6.23}$$

and

$$\frac{\partial^r u}{\partial y^r}(t;x_i,y_j) \cong \sum_{k=1}^{m} a_{kj}^{(r)} u_{ik}(t)\,, \tag{3.6.24}$$

while mixed type derivatives are given by

$$\frac{\partial^2 u}{\partial x \partial y}(t;x_i,y_j) \cong \sum_{h=1}^{n}\sum_{k=1}^{m} a_{hi}a_{kj}u_{hk}(t)\,, \tag{3.6.25}$$

where the coefficients a are given by the expressions reported above and depend, as we have seen, on the type of interpolation and number collocation points.

Both in one and two space dimension the interpolation is, by definition, exactly satisfied in the nodal points

$$u_i(t) = u^n(t,x_i)\,, \qquad u_{ij}(t) = u^{nm}(t,x_i,y_j)\,, \tag{3.6.26}$$

while partial derivatives are only approximated.

When problems in two space dimensions are not defined on non rectangular domains, then the interpolation method needs to be technically modified. When the domain is convex with respect to both axes and regular, then the following interpolation can be used

$$u = u(t,x,y) \cong u^{nm^*}(t,x,y) = \sum_{i=1}^{n}\sum_{j=1}^{m^*} L_i(x)L_j(y)u_{ij}(t)\,, \tag{3.6.27}$$

where the number of collocation points along the y-axis depends on the collocation on the x-axis.

The above collocation interpolation methods can be applied to obtain finite models approximating the continuous ones, and to solve the related initial-boundary value problems by approximating them by suitable initial value problems for ordinary differential equations. This method is explained, at a practical level, in the examples which follow:

Example 3.6.3
From Continuous to Finite Diffusion Models

Consider continuous model for diffusion phenomena corresponding to the following class of second order partial differential equations

$$\frac{\partial u}{\partial t} = \mu(x)\frac{\partial^2 u}{\partial x^2} + \varepsilon(x)\left(\frac{\partial u}{\partial x}\right)^2,\qquad(3.6.28)$$

where μ and ε are assumed to be given functions of the space variable.

The discretization of the model goes through the following steps:

1. The space variables are discretized into a suitable collocation I_x;

2. The dependent variable $u = u(t,x)$ is interpolated and approximated by the values $u_i(t) = u(t,x_i)$ as indicated in Eq. (3.6.15), and the space dependence is approximated using the same interpolation;

3. The finite model is obtained replacing the above interpolations into the continuous models and using the properties of the interpolating polynomials.

The result of above calculations yield a system of ordinary differential equations which defines the time evolution of the values of the variable u in the nodal points, that is the finite model. The above system can be written as follows:

$$\frac{du_i}{dt} = \mu(x_i)\sum_{j=1}^{n} a_{ji}^{(2)} u_j + \varepsilon(x_i)\left(\sum_{j=1}^{n} a_{ji}^{(1)} u_j\right)^2,\qquad(3.6.29)$$

for $i = 1,\dots,n$.

$\square$

Remark 3.6.1. *The above finite model can be used to solve the Dirichlet initial-boundary value problem simply by substituting the first and last equation by $u_1 = u(t,0)$ and $u_n = u(t,1)$. The differential system can then be solved by means of standard techniques for ordinary differential equations we have seen in Chapter 2.*

Remark 3.6.2. *The solution of Neumann problem can be developed analogously. The difference consists in dealing with the first and last equation. Imposing Neumann boundary*

conditions yields:

$$\begin{cases} \dfrac{\partial u}{\partial x}(t,0) = a_{11}^{(1)} u_1 + \displaystyle\sum_{j=2}^{n-1} a_{j1}^{(1)} u_j(t) + a_{n1}^{(1)} u_n \,, \\ \\ \dfrac{\partial u}{\partial x}(t,1) = a_{1n}^{(1)} u_1 + \displaystyle\sum_{j=2}^{n-1} a_{jn}^{(1)} u_j(t) + a_{nn}^{(1)} u_n \,. \end{cases} \qquad (3.6.30)$$

Then solving the above linear algebraic system with respect to u_1 and u_2 and substituting these terms into the first and last equation of the finite model yields the system of ordinary differential equations approximating the mathematical problem.

Remark 3.6.3. *Mixed type problems with Dirichlet boundary conditions on one side and Neumann boundary conditions on the other side can be dealt with following the same method we have seen above, using for the first or last equations one of the expression given by Eqs. (3.6.30) related to Neumann boundary conditions, while Dirichlet's condition is inserted by direct substitution.*

3.7 Critical Analysis

As we have seen, mathematical models derived at the macroscopic scale are generally stated in terms of partial differential equations. Moreover, models should be written in a suitable dimensionless form so that the independent variables are scaled in the interval $[0, 1]$, while the dependent variable is also scaled to be of the order of unity.

Discretization schemes toward computational solutions exploit directly the above formalization which refers both to the models and to the mathematical problems. Often, such a formalization is almost necessary to deal with the qualitative and quantitative analysis of models and problems. Therefore, the class of models, dealt with in this chapter, need a structure different from that one of discrete models which have been derived in terms of ordinary differential equations.

Looking at modelling aspects, one may observe that the various examples we have seen above have to be regarded as an approximation of physical reality. In fact, the reader can, for instance, recognize the following:

• All systems seen in this chapter are discrete: continuity assumptions are always an approximation of physical reality;

• Random features often occur either in the mathematical model or in the statement of the problem;

• Systems may be constituted by different interconnected systems. In this case one needs different models for each sub-system and the overall system should be viewed as a system of

systems. Therefore the mathematical statement of problems requires the statement of compatibility conditions between contiguous systems that may involve both initial and boundary conditions.

• Mathematical models are generally derived by equilibrium and/or conservation equations properly closed using phenomenological models describing the material behaviour of the system. Generally, these models are valid at equilibrium, while are used to describe dynamical behaviour far from equilibrium. Any attempt to improve modeling generates various types of nonlinearities.

Looking at computational aspects, the contents have been devoted simply to the approximation of continuous models by a suitable set of interconnected discrete models. The discretization has been obtained in two different ways:

i) Discretization of the volume occupied by the system into several contiguous volumes. Subsequently a finite model is derived in each volume supposing that the material is uniform in each volume. The model is obtained using the same equilibrium and/or conservation equations used for the derivation of the continuous model.

ii) Identification of a certain number of collocation points in the physical volume occupied by the system followed by a Lagrange type interpolation of the dependent variable corresponding to the collocation points. Subsequently partial derivatives, with respect to the space variable, are approximated by finite sums of the values of the dependent variables in the collocation points. Finally a system of ordinary differential equations, corresponding to a system of finite models, approximates the continuous model.

It may be argue that the first method discretizes the continuous model, with an infinite number of degrees of freedom, by a model with a finite number of degrees of freedom. On the other hand, the second method obtains an analogous result acting directly on the mathematical problem generated by the application of the model.

The above approach has been developed in the relatively simpler case of models and problems in one space dimension. Generalizations to more than one space dimension involve technical difficulties that are not dealt with in these Lecture Notes. A deeper insight into the application of collocation methods can be obtained by the book Bellomo *et al.* (2007), while finite elements methods for engineering applications are accurately dealt with in the book Kojić and Bathe (2005).

The reader is addressed to the pertinent literature Bellomo and Preziosi (1995) for alternative computational methods, for instance finite differences and spectral methods, and related convergence methods.

Finally, let us remark that models at the macroscopic scale can be suited to model systems of the inert matter, but not of the living systems. In fact, the averaging process ends up to kill the ability to express certain strategies. In some cases, the model includes random variables. For instance, in the vehicular traffic model of Section 3.2, the parameter ε, that attempts to model the ability of the driver to capture the local density conditions, can be modeled as a random

variable suitable to depict the stochastic distribution over the driver–vehicle microsystem.

In some cases, a stochastic process is added to model fluctuations. However, although the problem becomes very difficult, a deep insight into the ability of the model to capture the complexity of the interactions of living entities is not achieved. Therefore, a substantial improvement of the mathematical approach is necessary, as we shall see in the next chapter.

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Chapter 4

From Methods of Kinetic Theory to Modeling Living Systems

4.1 Introduction

Systems of real world are generally constituted by a large number of interacting elements. An example, which we have already examined in the preceding chapters, is a fluid of several interacting particles. In principle, one may model this system by microscopic type models related to the dynamics of each element in interaction with the others. However, Chapter 2 has shown that modeling systems with a large number of interacting elements generates complexity problems, due to an excessively large number of equations, which cannot be properly dealt with. This approach leads to a large number of equations with a computational time which exponentially increases with the number of equations, so that it may become too computationally complex or even impossible to deal with.

The macroscopic description, we have seen in Chapter 3, reduces the above complexity by dealing with quantities which are averaged, at each time, locally in space. The application of this modeling approach is possible when the number of elements is very large in a way that, given a small volume (in terms to be mathematically specified), it still contains a sufficiently large number of elements.

Intuitively one can realize that this approach cannot always be applied. For instance, this is the case of a diluted fluid, when the mean distance between particles is large with respect to their dimension and may even become of the same order of the container of the fluid. Therefore different methods need to be developed.

Methods of kinetic theory represent an alternative to the approach typical of continuum mechanics. Kinetic theory looks for evolution equations for the statistical distribution over the variable which describes the microscopic state of each element. Gross quantities (which are those delivered by macroscopic models) are obtained by suitable moments of the above statistical distribution.

This chapter gives a brief account to some classical models of the kinetic theory with special attention to the Boltzmann and Vlasov equations, which model the evolution of large systems

of **classical particles**. Subsequently, an introduction is proposed to models where the microscopic state of the interacting entities includes a variable related to a state different from those of classical mechanics. These entities are called, as we shall see, **active particles**. This mathematical approach can be used to model living, hence complex, systems.

After the above introduction a description of the contents of this chapter is given:

– Section 4.2 shows how the modeling of large systems of classical particles undergoing by short range interactions (collisions) can be described by the Boltzmann equation, the celebrated mathematical model of the (non-equilibrium) kinetic theory of diluted gases. Similarly, it is shown that the modeling long range interactions within a mean field description leads to Vlasov type models.

– Section 4.3 proposes some discretization schemes of the class of models reviewed in the preceding sections focusing on the Boltzmann equation. This approach leads to the so called Discrete Boltzmann equation.

– Section 4.4 presents the mathematical statement of problems related to the application of the above models to real flow description: typically the initial and the initial-boundary value problem.

– Section 4.5 initiates to tackle the difficult problem of modeling living systems focusing on the assessment of ten common characteristics of living systems. The contents identify the relevant characteristics that should be depicted models. Subsequently, the representation systems of active particles is presented. The derivation of a large class of evolution equations suitable to describe the evolution in time and space of the probability distribution over the microscopic state of the active particles is treated.

– Section 4.6 proposes some perspective ideas to develop the above mathematical approach, limited to the case of linearly additive interactions, to the more general, and realistic, case of nonlinear interactions. This section also reports about the modeling of hiding-learning phenomena.

– Section 4.7 also shows how the mathematical approach can be particularized to modeling a specific complex system. More precisely the contents focus on modeling vehicular traffic phenomena already treated in the preceding chapters, so that the interested reader can compare the approach of this present chapter to that of the previous ones.

– Section 4.8 proposes, in the same style of the preceding chapters, a critical analysis on the overall contents of these Lectures Notes.

Focusing on the models of the mathematical kinetic theory. The reader interested to additional information is addressed to the book by Cercignani *et al.* (1994) for an introduction to foundations of kinetic theory and applications, while analytic aspects, such as the well posedness of mathematical problems and asymptotic theory to obtain the macroscopic description from the microscopic one, are reported in the books Arlotti *et al.* (1995) and Glassey (1996).

As already mentioned, this chapter also presents some developments of the mathematical kinetic theory to model living, hence complex, systems. Some pioneers papers have been proposed

suitable generalizations and developments of the above mathematical approach to model large complex systems in different field of applied sciences. Among others, Prigogine and Hermann (1971) proposed a mathematical theory of traffic flow by Boltzmann type equations. The same approach has been applied to model the social behavior of colonies of insects by Jager and Segel (1992), cell populations with special attention to the immune competition Bellouquid and Delitala (2006), social systems Bertotti and Delitala (2004). A systematic presentation of the mathematical kinetic theory for active particles is proposed with various applications in the book Bellomo (2008). The class of models under consideration have been called, in the book Arlotti *et al.* (2003), ***generalized kinetic (Boltzmann) models***. Their common feature is that the model, similarly to the classical kinetic theory, is an evolution equation for the one particle distribution function over the microscopic state of the active particles interacting in a large system.

4.2 The Boltzmann Equation

A physical fluid is an assembly of disordered interacting particles free to move in all directions, inside a space domain $\Omega \subset \mathbb{R}^3$ possibly equal to the whole space $\mathbb{R}^3$. Assuming that the position of each particle is correctly identified by the coordinates of its center of mass:

$$\mathbf{x}_k, \qquad k = 1, \ldots, N, \tag{4.2.1}$$

the system may be reduced to a set of point masses in a fixed frame of reference. This is the case, for instance, if the shape of the particles is spherically symmetric, and hence rotational degrees of freedom can be ignored.

When the domain Ω is bounded, the particles interact with its walls Ω_w. If Ω contains obstacles, say sub-domains $\Omega^* \subset \Omega$ which restrict the free motion, then the particles interact also with the walls of Ω^*. In some instance, e.g. for flows around space ships, the obstacles are objects scattered throughout the surrounding space.

It is generally believed in physics, and in statistical mechanics in particular, that understanding the properties of a fluid follows from the detailed knowledge of the state of each of its atoms or molecules. In most fluids of practical interest, such states evolve according to the laws of classical mechanics which, for a system of N particles give the following set of ordinary differential equations:

$$\begin{cases} \dfrac{d\mathbf{x}_k}{dt} = \mathbf{v}_k, \\[2mm] m_k \dfrac{d\mathbf{v}_k}{dt} = \mathbf{F}_k = \mathbf{f}_k + \displaystyle\sum_{k'=1}^{N} \mathbf{f}_{k'k}, \end{cases} \tag{4.2.2}$$

with initial conditions:

$$\mathbf{x}_k(0) = \mathbf{x}_{k0}, \quad \mathbf{v}_k(0) = \mathbf{v}_{k0}, \quad k = 1, \ldots, N, \tag{4.2.3}$$

where $\mathbf{F}_k$ is the force referred to the mass m_k acting on each particle. $\mathbf{F}_k$ may be expressed as the superposition of an external field $\mathbf{f}_k$ and of the force $\mathbf{f}_{k'k}$ acting on the k-particle due to the action of all other particles. In general these forces are regular functions in the phase space, and $\mathbf{f}_{k'k}$ may be allowed to exhibit pole-discontinuities when the distance between particles is zero.

This approach prescribes that Eqs.(4.2.2) can be solved, and that the macroscopic properties of the fluid can be obtained as averages involving the microscopic information contained in such solution. However, it is very hard, if even possible, to implement such a program, unless suitable simplifications are introduced. Indeed, unavoidable inaccuracies in our knowledge of the initial conditions, the large value of N (about 10^{20} for a gas in normal conditions), and the mathematical complexity, result in the impossibility of retrieving and manipulating all the microscopic information provided by (4.2.2–4.2.3) and contained in $\{\mathbf{x}_k, \mathbf{v}_k\}$ for $k = 1, \ldots, N$. It is true that what is of interest is to extract from (4.2.2–4.2.3) the information sufficient to compute the time and space evolution of a restricted number of macroscopic observable such as the number density, mass velocity, temperature, and stress tensor. However, computing the macroscopic observable quantities using the solutions to Eq. (4.2.2) is an almost impossible task. This is not only because of the initial difficulty in dealing with a large system of ordinary differential equations, but also because afterwards one has to compute the averages which correctly define the macroscopic quantities. For instance, the mean mass density $E(\rho)$ should be obtained, for a system of identical particles, by examining the ratio:

$$E(\rho) = m\,\frac{\Delta n}{\Delta \mathbf{x}}\,, \qquad\qquad (4.2.4)$$

when the volume $\Delta \mathbf{x}$ tends to zero and the number of particles remains sufficiently large. Fluctuations cannot be avoided. Additional difficulties are related to the computation of the other macroscopic variables. Thus, constitutive relations are needed.

As we have seen, a different possible approach is that of fluid dynamics, see Truesdell and Rajagopal (2000). It consists in deriving the evolution equations, related to the above macroscopic observable quantities, under several strong assumptions, including the hypothesis of continuity of matter (continuum assumption). This constitutes a good approximation of a real system only if the mean distance between pairs of particles is small with respect to the characteristic lengths of the system, e.g. the typical length of Ω or of Ω^*. Conversely, if the intermolecular distances are of the same order of such lengths, the continuum assumption is no longer valid, and a discrepancy is expected between the description of continuum fluid dynamics and that furnished by Eqs. (4.2.2).

Therefore, considering that it is neither possible to deal with the equations of continuum fluid dynamics, nor with particle dynamics (4.2.3), a different model is needed. An alternative to the above descriptions is provided by the Boltzmann equation, the fundamental mathematical model of kinetic theory, which describes the evolution of a dilute monoatomic gas of a large number of identical particles undergoing elastic binary collisions.

Following Arlotti *et al.* (2003), we limit to recall the main features of the model, and we refer to the classical literature, among others Cercignani *et al.* (1994), for its derivation and its fundamental properties.

Let us consider a dilute monoatomic gas of particles modeled as mass points identified by unit mass, position $\mathbf{x}$ and velocity $\mathbf{v}$. The Boltzmann equation refers to the time evolution of the one-particle distribution function:

$$f = f(t, \mathbf{x}, \mathbf{v}), \quad f : \mathbb{R}_+ \times \Omega \times \mathbb{R}^3 \to \mathbb{R}_+ \,,$$

with the meaning that:

$$\int_B \int_A f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{x} \, d\mathbf{v} \tag{4.2.5}$$

gives the number of particles in a measurable set $A \times B \subset \Omega \times \mathbb{R}^3$, at time $t \geq 0$.

If f is known and integrable in the velocity space, the macroscopic observable quantities can be computed as expectation values of the corresponding microscopic functions. In particular,

$$\rho(t, \mathbf{x}) = \int_{\mathbb{R}^3} f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{v} \,, \tag{4.2.6}$$

and

$$\mathbf{u}(t, \mathbf{x}) = \frac{1}{\rho(t, \mathbf{x})} \int_{\mathbb{R}^3} \mathbf{v} \, f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{v} \,, \tag{4.2.7}$$

are, respectively, the mass density and the macroscopic velocity.

The internal energy is given by:

$$e(t, \mathbf{x}) = \frac{1}{2\rho(t, \mathbf{x})} \int_{\mathbb{R}^3} | \mathbf{v} - \mathbf{u}(t, \mathbf{x}) |^2 f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{v} \,. \tag{4.2.8}$$

In equilibrium conditions, the energy can be related (according to Boltzmann's principle) to the temperature by the relation:

$$e(t, \mathbf{x}) = \frac{3}{2} T(t, \mathbf{x}) \,,$$

where $T(t, \mathbf{x})$ is the temperature and, for simplicity of notation, we are assuming that the Boltzmann constant $k = 1$. This relation has to be handled carefully in nonequilibrium conditions, where the above principle cannot be straightforwardly applied.

The time dependence in the Boltzmann equation allows that, as time goes, the number of particles inside an infinitesimal volume $d\mathbf{x} \, d\mathbf{v}$ centered at the point $(\mathbf{x}, \mathbf{v})$ of the phase space may change if the system is away from equilibrium. Obviously, such a change is computed by balancing the incoming and outgoing particles in $d\mathbf{x} \, d\mathbf{v}$.

The idea behind this balance of losses and gains in $d\mathbf{x} \, d\mathbf{v}$ is that particles are lost or gained in $d\mathbf{x}$ by free streaming, while they leave or enter $d\mathbf{v}$ as the result of collisions with other particles.

This leads to the basic assumptions behind the phenomenological derivation of the Boltzmann equation, that in the case of absence of an external force field are:

- Gas particles move freely in the space. The collisions have instant in time and local in space character. During the collisions the conservation of momentum and energy holds according to the laws of classical mechanics.

- Collisions involving more than two particles are negligible.

- Collisions between pairs of particles are uncorrelated (molecular chaos hypothesis).

It should be remarked that, according to the first hypothesis, variations of the distribution function, inside $d\mathbf{x}$, are neglected. Therefore, the distribution function of the field particles which enter into the action domain of the test particles is actually approximated by the value of f in the position of the field particle.

Let us here recall that the momentum and energy conservation relations for a collision process $(\mathbf{v}, \mathbf{w}) \rightarrow (\mathbf{v}', \mathbf{w}')$ of two particles of simple gas are:

$$\begin{cases} \mathbf{v} + \mathbf{w} = \mathbf{v}' + \mathbf{w}' , \\ |\mathbf{v}|^2 + |\mathbf{w}|^2 = |\mathbf{v}'|^2 + |\mathbf{w}'|^2 . \end{cases} \tag{4.2.9}$$

The celebrated Boltzmann equation, which defines the evolution of the distribution function $f = f(t, \mathbf{x}, \mathbf{v})$ reads:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = J[f, f] , \tag{4.2.10}$$

where the collision operator J is given by:

$$J[f, f](t, \mathbf{x}, \mathbf{v}) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2_+} B(\mathbf{n}, \mathbf{w} - \mathbf{v})$$
$$\times \Big(f(t, \mathbf{x}, \mathbf{v}') f(t, \mathbf{x}, \mathbf{w}') - f(t, \mathbf{x}, \mathbf{v}) f(t, \mathbf{x}, \mathbf{w}) \Big) \, d\mathbf{n} \, d\mathbf{w} , \tag{4.2.11}$$

the post-collision velocities are given by:

$$\begin{cases} \mathbf{v}' = \mathbf{v} + ((\mathbf{w} - \mathbf{v}) \cdot \mathbf{n}) \, \mathbf{n} , \\ \mathbf{w}' = \mathbf{w} - ((\mathbf{w} - \mathbf{v}) \cdot \mathbf{n}) \, \mathbf{n} , \end{cases} \tag{4.2.12}$$

where we denote by a dot the scalar product, $\mathbf{n}$ is the unit vector in the direction of the apse-line bisecting the angle between $\mathbf{v} - \mathbf{w}$ and $\mathbf{w}' - \mathbf{v}'$, and

$$\mathbb{S}^2_+ = \{\mathbf{n} \in \mathbb{R}^3 : \quad |\mathbf{n}| = 1 , \quad (\mathbf{n} \cdot (\mathbf{w} - \mathbf{v})) \geq 0\} \tag{4.2.13}$$

is the domain of integration of the variable $\mathbf{n}$. Let us notice that Eq.(4.2.12) are reversible to respect pre and post collision velocities.

The form of the collision kernel B depends upon the particle interaction potential and we assume that B satisfies the following condition:

$$B \geq 0 , \quad B = B(\mathbf{n}, \mathbf{v}) \quad \text{is a function of} \quad \mathbf{n} \cdot \mathbf{v} \text{ and } |\mathbf{v}| \quad \text{only} . \tag{4.2.14}$$

Moreover, as usual in the subject, we will assume that B satisfies the Grad's angular cut-off potential condition, Grad (1963).

An important example of such a collision kernel B is the one corresponding to the hard sphere potential:

$$B(\mathbf{n}, \mathbf{v}) = \begin{cases} \mathbf{n} \cdot \mathbf{v} & \text{if } \mathbf{n} \cdot \mathbf{v} \geq 0 \,, \\ 0 & \text{otherwise.} \end{cases} \qquad (4.2.15)$$

The above picture on the variation of f, as a result of competition between free streaming and balance of losses and gains in $d\mathbf{x}\,d\mathbf{v}$, requires the size of the volume element $d\mathbf{x}\,d\mathbf{v}$ be large enough that the number of particles contained in it justifies the use of statistical methods. On the other hand, this number must be small enough that information contained in it should have local character. Clearly, these two features are not compatible in general, hence problems are expected in justifying the whole procedure. Hopefully, in the cases of practical interest, the molecule size does fall in a range of values which are small when compared to those of the volume elements $d\mathbf{x}$ which, in turn, can be considered as microscopic with respect to the observations scale.

With reference to the specialized literature, see for example by Cercignani *et al.* (1994) and Glassey (1996), we are now interested in reporting some fundamental properties of the Boltzmann model. In details:

$$\int_{\mathbb{R}^3} J[f, f]\, d\mathbf{v} = 0\,, \qquad (4.2.16)$$

$$\int_{\mathbb{R}^3} \mathbf{v} J[f, f]\, d\mathbf{v} = 0\,, \qquad (4.2.17)$$

and

$$\int_{\mathbb{R}^3} |\mathbf{v}|^2 J[f, f]\, d\mathbf{v} = 0\,, \qquad (4.2.18)$$

for each f such that the integrals make sense.

Moreover formal computations show that, if Ω is either $\mathbb{R}^3$ or the 3-dimensional torus T^3, any solution to the Boltzmann equation should satisfy the following conditions:

$$\int_{\mathbb{R}^3} \int_{\Omega} f(t, \mathbf{x}, \mathbf{v})\, d\mathbf{x}\, d\mathbf{v} = \int_{\mathbb{R}^3} \int_{\Omega} f(0, \mathbf{x}, \mathbf{v})\, d\mathbf{x}\, d\mathbf{v}\,, \qquad (4.2.19)$$

$$\int_{\mathbb{R}^3} \int_{\Omega} \mathbf{v}\, f(t, \mathbf{x}, \mathbf{v})\, d\mathbf{x}\, d\mathbf{v} = \int_{\mathbb{R}^3} \int_{\Omega} \mathbf{v}\, f(0, \mathbf{x}, \mathbf{v})\, d\mathbf{x}\, d\mathbf{v}\,, \qquad (4.2.20)$$

and

$$\int_{\mathbb{R}^3} \int_{\Omega} |\mathbf{v}|^2\, f(t, \mathbf{x}, \mathbf{v})\, d\mathbf{x}\, d\mathbf{v} = \int_{\mathbb{R}^3} \int_{\Omega} |\mathbf{v}|^2\, f(0, \mathbf{x}, \mathbf{v})\, d\mathbf{x}\, d\mathbf{v}\,. \qquad (4.2.21)$$

Let us now consider the equilibrium solutions of Eq. (4.2.10), i.e. the solutions of the equation:

$$J[f, f] = 0\,, \qquad (4.2.22)$$

we recall that the only solutions of Eq. (4.2.23) are the so-called local Maxwellian distributions given by:

$$M(t, \mathbf{x}, \mathbf{v}) = \frac{\rho(t, \mathbf{x})}{(2\pi\, T(t, \mathbf{x}))^{3/2}} \, \exp\left[-\frac{|\mathbf{v} - \mathbf{u}(t, \mathbf{x})|^2}{2\, T(t, \mathbf{x})} \right] , \qquad (4.2.23)$$

where ρ, T, and $\mathbf{u}$ are the macroscopic observable quantities.

An other interesting feature of the Boltzmann equation is described by the H functional:

$$H[f](t) = \int_{\mathbb{R}^3} \int_\Omega f(t, \mathbf{x}, \mathbf{v}) \log f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{x} \, d\mathbf{v} , \qquad (4.2.24)$$

if the term $f \log f$ is integrable for all $t > 0$. Indeed, the H-Theorem asserts that the H functional is formally decreasing along the solution:

$$\frac{d}{dt} H[f](t) = \int_{\mathbb{R}^3} \int_\Omega J[f,f](t, \mathbf{x}, \mathbf{v}) \log f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{x} \, d\mathbf{v} \leq 0 , \qquad (4.2.25)$$

where equality holds only at equilibrium, again for $\Omega = \mathbb{R}^3$ or $\Omega = T^3$.

If a positional macroscopic force $\mathbf{F}(\mathbf{x})$ is acting on the system, then the Boltzmann equation reads:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{F}(\mathbf{x}) \cdot \nabla_{\mathbf{v}} f = J[f, f] , \qquad (4.2.26)$$

The Boltzmann equation is such that the distribution function is modified only by external actions and short range interactions. On the other hand, various physical systems are such that also long range interactions may be significant.

To be more specific, consider the vector action $\mathcal{P} = \mathcal{P}(\mathbf{x}, \mathbf{v}, \mathbf{x}_*, \mathbf{v}_*)$ on the subject with microscopic state $\mathbf{x}, \mathbf{v}$ due to the subject with microscopic state $\mathbf{x}_*, \mathbf{v}_*$. The resultant action is:

$$\mathcal{F}[f](t, \mathbf{x}, \mathbf{v}) = \int_{\mathbb{R}^3 \times \mathcal{D}_\Omega} \mathcal{P}(\mathbf{x}, \mathbf{v}, \mathbf{x}_*, \mathbf{v}_*) \, f(t, \mathbf{x}_*, \mathbf{v}_*) \, d\mathbf{x}_* \, d\mathbf{v}_* , \qquad (4.2.26)$$

where $\mathcal{D}_\Omega$ is the domain around the test particle where the action of the field particle is effectively felt, in other words the action $\mathcal{P}$ decays with the distance between test and field particles and is equal to zero on the boundary of $\mathcal{D}_\Omega$. Based on the above assumptions, the mean field equation writes:

$$\frac{\partial f}{\partial t} + (\mathbf{v} \cdot \nabla_{\mathbf{x}}) f + \mathbf{F} \cdot \nabla_{\mathbf{v}} f + \nabla \cdot (\mathcal{F}[f] \, f) = 0 , \qquad (4.2.27)$$

where $\mathbf{F}$ is the positional macroscopic force is acting on the system delivered by Eq. (4.2.26).

4.3 Discrete Velocity Models

Classical models of the kinetic theory of gases have been presented in the preceding section. Following the line of Chapter 2 and 3, we shall now provide an outline of some methods to derive discrete velocity models also in view of the development of suitable computational schemes.

The discrete models of the Boltzmann equation can be obtained assuming that particles allowed to move with a finite number of velocities. The model is an evolution equation for the number densities N_i linked to the admissible velocities $\mathbf{v}_i$, for $i \in \mathbf{L} = \{1, \ldots, n\}$. The set $N = \{N_i\}_{i=1}^n$ corresponds, for certain aspects, to the one-particle distribution function of the continuous Boltzmann equation.

This model is called ***discrete Boltzmann equation***. The mathematical theory of the discrete kinetic theory was systematically developed in the Lecture Notes by Gatignol (1975), which provides a detailed analysis of the relevant aspects of the discrete kinetic theory: modeling, analysis of thermodynamic equilibrium and application to fluid-dynamic problems. The contents mainly refer to a simple monoatomic gas and to the related thermodynamic aspects. After such a fundamental contribution, several developments have been proposed in order to deal with more general physical systems: gas mixtures, chemically reacting gases, particles undergoing multiple collisions and so on. Analytic topics, such as the qualitative analysis of the initial value and of the initial-boundary value problem, have been object of continuous interest of applied mathematicians. The existing literature is reported in the review papers Platkowski and Illner (1988) and Bellomo and Gustafsson (1991).

The formal expression of the evolution equation is as follows:

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_i \cdot \nabla_{\mathbf{x}} \right) N_i = J_i[N] \,, \tag{4.3.1}$$

where

$$N_i = N_i(t, \mathbf{x}) : \quad (t, \mathbf{x}) \in [0, T] \times \mathbb{R}^\nu \to \mathbb{R}_+ \,, \quad \mathrm{i} = 1, \ldots, \mathrm{n} \,, \quad \nu = 1, 2, 3 \,, \tag{4.3.2}$$

and the binary collision terms is given by:

$$J_i[N] = \frac{1}{2} \sum_{j,h,k=1}^n A_{ij}^{hk} (N_h N_k - N_i N_j) \,. \tag{4.3.3}$$

The terms A_{ij}^{hk} are the so-called ***transition rates***:

$$(\mathbf{v}_i, \mathbf{v}_j) \longleftrightarrow (\mathbf{v}_h, \mathbf{v}_k) \,, \qquad i, j, h, k \in \mathbf{L} \,, \tag{4.3.4}$$

and where the collision scheme must be such that momentum and energy are preserved. These terms are positive constants which, according to the indistinguishability property of the gas particles and to the reversibility of the collisions, satisfy the following relations:

$$\mathbf{A} = A_{ji}^{hk} = A_{ij}^{kh} = A_{ji}^{kh} \,. \tag{4.3.5}$$

As for the Boltzmann equation, the qualitative analysis of discrete models needs the identification of the space of collision invariants and of the Maxwellian state. Specifically, the following definitions can be used:

> **Collision Invariant**
>
> A vector $\phi = \{\phi_i\}_{i \in \mathbf{L}} \in \mathbb{R}^m$ is defined **collision invariant** if:
>
> $$\langle \phi, J[N] \rangle = 0, \quad J[N] = \{J_{i \in \mathbf{L}} \in \mathbb{R}^m\}, \tag{4.3.6}$$
>
> where the inner product is defined in $\mathbb{R}^m$ and m is the cardinality of the set $\mathbf{L}$.

> **Space of the collision invariants**
>
> The set of the totality of collision invariants is called **space of the collision invariants** and is a linear subspace of $\mathbb{R}^m$. Such a space will be denoted, in what follows, by $\mathcal{M}$.

> **Maxwellian**
>
> Let $N_i > 0$ for any $i \in \mathbf{L}$, then the vector N is defined **Maxwellian** if $J[N] = 0$.

Moreover, the following propositions characterize the space of the collision invariants and the Maxwellian state:

Proposition 4.3.1. *Let $\phi \in \mathbb{R}^m$, then the following conditions are equivalent*
i) $\phi \in \mathcal{M}$, i.e. ϕ is a collision invariant;
ii) $\langle \phi, J[N] \rangle = 0$.

Proposition 4.3.2. *Let $N_i > 0$ for any $i \in \mathbf{L}$, then the following three conditions are equivalent*
i) N is a Maxwellian;
ii) $\{\log N_i\}_{i \in \mathbf{L}} \in \mathcal{M}$;
iii) $J[N] = 0$.

Consider now the classical H–Boltzmann function defined as:

$$H = \sum_{i \in \mathbf{L}} c_i N_i \log N_i. \tag{4.3.7}$$

Then, the evolution equation for the H–Boltzmann equation can be derived by multiplying the discrete Boltzmann equation by $1 + \log N_i$ and taking the sum over $i \in \mathbf{L}$. It can be technically verified that the time derivative of above functional is nonpositive and that the equality holds if and only if N is a Maxwellian.

Applied mathematicians have attempted in the last decade to design models with arbitrarily large number of velocities and hence to analyze convergence of discretized models toward the full Boltzmann equation. However, various technical difficulties have to be tackled as well documented in the paper Görsch (2002), such as:

i) The discretization schemes for each couples of incoming velocities do not assure a pair of outgoing velocities such that conservation of mass and momentum is preserved;

ii) Specific models may have a number of spurious collision invariants in addition to the classical ones corresponding to conservation of mass, linear momentum and energy;

iii) The convergence of the solutions of discretized equation to those of the full Boltzmann equation, when the number of discretization points tends to infinity, under suitable hypotheses which have to be properly defined.

A technical difficulty in dealing with the above convergence proof consists in obtaining an existence theorem for the Boltzmann equation in a function space which can be properly exploited for the development of the computational scheme.

An alternative consists in discretizing the velocity space by a suitable set of velocity modules, but letting the velocity free to assume all directions in the space. The formal expression of the evolution model is as follows:

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_i \cdot \nabla_{\mathbf{x}}\right) N_i(t, \mathbf{x}, \Omega) = J_i[f](t, \mathbf{x}, \Omega)\,, \tag{4.3.8}$$

where

$$N_i = N_i(t, \mathbf{x}, \Omega) : (t, \mathbf{x}) \in [0, T] \times \mathbb{R}^\nu \times \mathbb{R}^3 \to \mathbb{R}_+\,,\, \mathrm{i} = 1, \ldots, \mathrm{n}\,, \tag{4.3.9}$$

and where Ω is the unit vector which identifies the direction of the velocity, $\mathbf{v}_i = v_i\, \Omega$.

Example 4.3.1
Six Velocity Discrete Boltzmann Equation

Consider a one-component discrete velocity gas such that the particles can attain 6 velocities in the xy–plane. The velocity discretization is defined by:

$$\mathbf{v}_i = c\left[\cos(\frac{i-1}{3}\pi)\,\mathbf{i} + \sin(\frac{i-1}{3}\pi)\,\mathbf{j}\right] \qquad i = 1, \ldots, 6\,, \tag{4.3.10}$$

where $\mathbf{i}$ and $\mathbf{j}$ are the unit vectors of an orthogonal plane frame.

Such a velocity discretization generates head-on binary collisions with scattering in all directions:

$$(\mathbf{v}_i, \mathbf{v}_{i+3}) \longleftrightarrow (\mathbf{v}_h, \mathbf{v}_{h+3})\,, \quad h = 1, \ldots, 6\,,$$

that are the only nontrivial (generate a flux in the velocity space).

Detailed calculations provide the expression of the collisions operators. In particular the binary collision operator is simply obtained by joining the transition rates A_{ij}^{hk} to the corresponding transition probability densities a_{ij}^{hk} by $A_{ij}^{hk} = S|\mathbf{v}_i - \mathbf{v}_j|a_{ij}^{hk}$. The mathematical model follows from simple calculations.

□

4.4 Mathematical Problems

Mathematical problems related to the Boltzmann equation can be classified, as usual, into initial, initial-boundary and boundary value problems. However the statement of the problems is somewhat different from those models of continuous mechanics.

Consider first the initial value problem for the Boltzmann equation in absence of an external force field, in the whole space $\mathbb{R}^3$, and with given initial conditions:

$$f^0(\mathbf{x}, \mathbf{v}) = f(0, \mathbf{x}, \mathbf{v}) : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}_+ , \tag{4.4.1}$$

which are assumed to decay at infinity in space.

The integral form of the initial value problem for the Boltzmann equation, when $\mathbf{F} = \mathbf{0}$, reads:

$$f^{\#}(t, \mathbf{x}, \mathbf{v}) = f^0(\mathbf{x}, \mathbf{v}) + \int_0^t J^{\#}(s, \mathbf{x}, \mathbf{v}) \, ds , \tag{4.4.2}$$

where

$$f^{\#}(t, \mathbf{x}, \mathbf{v}) = f(t, \mathbf{x} + \mathbf{v} \, t, \mathbf{v}) , \tag{4.4.3}$$

and

$$J^{\#}(t, \mathbf{x}, \mathbf{v}) = J[f, f](t, \mathbf{x} + \mathbf{v} \, t, \mathbf{v}) . \tag{4.4.4}$$

The statement of the initial-boundary value problem requires the modeling of gas surface interaction phenomena. In particular, two specific problems, among several ones, can be stated:

- The **interior domain problem** which corresponds to a gas contained in a volume bounded by a solid surface;

- The **exterior domain problem**, which corresponds to a gas in the whole space $\mathbb{R}^3$ which contains an obstacle.

The surface of the solid wall is defined in both cases by Ω_w, the normal to the surface directed toward the gas is ν. Moreover, in order to define the boundary conditions on a solid wall, we need to define the partial incoming and outgoing traces f^+ and f^- on the boundary Ω_w, which, for continuous f, can be defined as follows:

$$\begin{cases} f^+(\mathbf{x}, \mathbf{v}) = f(\mathbf{x}, \mathbf{v}) , & \mathbf{x} \in \Omega_w , \quad \mathbf{v} \cdot \nu(\mathbf{x}) > 0 \\ f^+(\mathbf{x}, \mathbf{v}) = 0 , & \mathbf{x} \in \Omega_w , \quad \mathbf{v} \cdot \nu(\mathbf{x}) < 0 , \end{cases} \tag{4.4.5}$$

and

$$\begin{cases} f^-(\mathbf{x}, \mathbf{v}) = f(\mathbf{x}, \mathbf{v}) , & \mathbf{x} \in \Omega_w , \quad \mathbf{v} \cdot \nu(\mathbf{x}) < 0 \\ f^-(\mathbf{x}, \mathbf{v}) = 0 , & \mathbf{x} \in \Omega_w , \quad \mathbf{v} \cdot \nu(\mathbf{x}) > 0 . \end{cases} \tag{4.4.6}$$

Then the boundary condition may be formally defined as follows:

$$f^+(t, \mathbf{x}, \mathbf{v}) = \mathcal{R} \, f^-(t, \mathbf{x}, \mathbf{v}) , \tag{4.4.7}$$

where the operator $\mathcal{R}$, which maps the distribution function of the particles which collide with the surface into the one of particles leaving the surface is characterized, for a broad range of physical problems, by the following properties:

1. $\mathcal{R}$ *is linear, of local type with respect to* **x***, and is positive:*

$$f^- \geq 0 \Rightarrow \mathcal{R} f^- \geq 0 . \tag{4.4.8}$$

2. $\mathcal{R}$ *preserves mass, i.e. the flux of the incoming particles equals the one of the particles which leaves the surface.*

3. $\mathcal{R}$ *preserves local equilibrium at the boundary:* $\omega_w^+ = \mathcal{R} \omega_w^-$, *where* ω_w *is the Maxwellian distribution at the wall temperature.*

4. $\mathcal{R}$ *is dissipative, i.e. satisfies the inequality at the wall:*

$$\int_{\mathbb{R}^3} \langle \mathbf{v} \,, \mathbf{n} \rangle \left(f^- + \mathcal{R} f^- \right) \left(\log f + \frac{|\mathbf{v}|^2}{T} \right) d\mathbf{v} \leq 0 . \tag{4.4.9}$$

The formulation of the initial-boundary value problem, in the case of the **interior domain problem**, consists in linking the evolution equation (4.2.26) to the initial condition (4.4.1) and to the boundary condition (4.4.7) on the wall Ω_w. In the case of the **exterior domain problems**, in addition to the boundary conditions on the wall, suitable Maxwellian equilibrium conditions are assumed at infinity. If one deals with the boundary value problem, the statement of the boundary conditions must be linked to the **steady Boltzmann equation**, and the definitions of solutions are analogous to the ones we have seen for the initial value problem.

The mathematical statements we have just seen refer to the Boltzmann equation in absence of an external field, and hence the trajectories of the particles are straight lines. When an external field is acting on the particles, trajectories may be explicitly determined only by solving the equations of Newtonian dynamics.

Several books, for instance Glassey (1996), are available, for the interested reader, on the qualitative analysis of mathematical problems related to the application of the Boltzmann equation. The above cited book provides a detailed survey of existence theory for the Boltzmann and Vlasov equations.

4.5 Mathematical Methods to Model Living (Complex) Systems

This section presents, referring to the existing literature, a unified approach to model living systems by suitable development of the mathematical kinetic theory. The contents are presented starting from the identification of their main complexity features. Subsequently, a system approach is proposed by subdividing the overall system into functional subsystems and by

representing the state of them by a suitable probability distribution over the microscopic state of the entities composing each subsystem. Finally a mathematical framework is derived which may act as background paradigm for the derivation of specific models.

Therefore, this section offers the conceptual background for the derivation of models. The authors have attempted to unify various approaches that have been offered in the literature. Moreover, it will be discussed later how far this approach departs from the classical kinetic theory.

4.5.1 Ten Common Features of Complex Systems

As already mentioned, the mathematical approach to modeling living systems should attempt to capture, as far as it is possible, the complexity of all living systems. Of course, the authors do not naively claim that this is always possible. On the other hand it is an interesting and challenging field of applied mathematics, which can have a remarkable impact on life and applied sciences. The following sentences, extracted from Bellomo *et al.* (2010a) can possibly contribute to understand the aims of this section.

– The study of complex systems, namely systems of many individuals interacting in a nonlinear manner, has received in recent years a remarkable increase of interest among applied mathematicians, physicists as well as researchers in various other fields as economy or social sciences. ... Their collective overall behavior is determined by the dynamics of their interactions. On the other hand, a traditional modeling of individual dynamics does not lead in a straightforward way to a mathematical description of collective emerging behaviors. ... In particular it is very difficult to understand and model these systems based on the sole description of the dynamics and interactions of a few individual entities localized in space and time.

Starting from the above reasonings, let is attempt to identify ten, selected among several ones, common features and sources of complexity. The contents of Bellomo *et al.* (2009) is followed.

1. Ability to express a strategy: Living entities are capable to develop specific *strategies* and *organization abilities* that depend on the state of the surrounding environment. These can be expressed without the application of any external organizing principle. In general, they typically operate *out-of-equilibrium*. For example, a constant struggle with the environment is developed to remain in a particular out-of-equilibrium state, namely stay alive.

2. Heterogeneity: The ability to express a strategy is not the same for all entities: *Heterogeneity* characterizes a great part of living systems, namely, the characteristics of interacting entities can even differ from an entity to another belonging to the same structure. In biology, this is due to different phenotype expressions generated by the same genotype.

3. Interactions: Interactions are nonlinear (nonlinearly additive) and involve immediate neighbors, but in some cases also distant particles. Indeed, living systems have the ability to communicate and may possibly choose different observation paths.

4. Topology of interactions: In some cases, the topological distribution of a fixed number

of neighbors can play a prominent role in the development of the strategy and interactions. Namely, interactions do not involve all entities that are within an interaction domain.

5. Stochastic games: Interactions modify their state according to the strategy they develop. Living entities **play a game at each interaction** with an output that is technically related to their strategy often related to surviving and adaptation ability. This dynamics is also related to the fact that living systems receive a feedback from their environments, which enables them to learn from their experiences.

6. Large deviations: Interactions involving entities and those with the outer environment can lead to *large effects*, which in turn lead to even larger effects due to a natural trend far from equilibrium. Deviations can be also related to bifurcation phenomena.

7. Large number of components: *Complexity in living systems is induced by a large number of variables*, which are needed to describe their overall state. Therefore, the number of equations needed for the modeling approach may be too large to be practically treated. For instance, biological systems are different from the physical systems analyzed by statistical mechanics, which typically deals with systems containing many copies of a few interacting components, whereas cells contain from millions to a few copies of each of thousands of different components, each with specific interactions.

8. Learning ability: Living systems have the ability to learn from past experience. Therefore their strategic ability and the characteristics of interactions among living entities evolve in time. In some case some of the system attempts to escape from the other (hiding), while the other attempts to approach (learning).

9. Multiscale aspects: The study of complex living systems always needs a *multiscale approach*. For instance, the dynamics of a cell at the molecular (genetic) level determines the cellular behaviors. As a matter of fact, the structure of macroscopic tissues depends on such a dynamics.

10. Darwinian selection: All living systems are evolutionary. For instance birth processes can generate individuals more fitted to the environment, who in turn generate new individuals again more fitted to the outer environment. Neglecting this aspect means that the time scale of observation and modeling of the system itself is not long enough to observe evolutionary events. Such a time scale can be very short for cellular systems and very long for vertebrates. Therefore time is a key variable.

Of course, the interested reader can argue that some of the above features can be replaced by different ones. This is certainly true, however we leave this type of arguing to the personal initiative to go back to the intrinsic difficulty of the problem under consideration and, following Bellomo and Carbonaro (2011), we pose three **key questions** to applied mathematicians, that can possibly contribute to define methodological guidelines to modeling in view of a mathematical theory.

1. *Can mathematics contribute to reduce the complexity of the overall system by splitting it into suitable subsystems?*

2. *Can mathematics offer suitable tools to describe the five features proposed above as common to all complex biological systems?*

3. *How far is the state-of-the-art from the development of a biological-mathematical theory of living systems and how can an appropriate understanding of multiscale issues contribute to this ambitious objective?*

The modeling approach to complex systems should take into account the afore-said common complexity features and the three key questions. Then, it can be developed, according to the authors' bias, through four steps as follows:

Step 1: Derivation of a mathematical structure suitable to describe the evolution of a complex system in a way that the structure retains the common complexity features. It needs to be regarded as a potential ability to be characterized for each specific case study.

Step 2: The second step specifically refers to a well defined real system. It consists in selecting the specific complexity characteristics of the system under consideration and in adjusting the afore-said structure to the specific case.

Step 3: The third step consists in characterizing the variables and the parameters that characterize the model referring to the real system that is object of the modeling approach. This basically means modeling the interaction at the individual (microscopic scale).

Step 4: Validation of the model by comparison of the dynamics predicted by it with empirical data. More precisely, the model should show quantitative agreement with data that are quantitatively known and qualitative agreement with emerging behaviors that are observed in the real behavior.

Bearing in mind the problem of validation, some models (too many) artificially include empirical data. For instance trend to steady state conditions. This is not correct, prediction of the model should be a consequence of interactions at the microscopic scale. In general validation should be related to the ability of models to reproduce empirical data. However, quantitative empirical data are available only for steady state (may be equilibrium) conditions, while emerging behaviors are observed in dynamical conditions. These behaviors are observed and repeated only at a qualitative level as they are very sensitive to environmental conditions.

The validation of models of complex systems needs to be related to their ability to depict empirical data. In some cases, models may possibly describe emerging behaviors that have not yet been observed. In this case, specific experiments can be organized to verify these predictions.

4.5.2 Representation

Some preliminary reasonings on the modeling approach should be focused on the selection of the appropriate representation scale and on the related variable that are supposed to describe, in the mathematical model, the state of the system under consideration. This selection should however face the problem of reducing complexity. Some considerations, related to the key complexity features, are useful to the identify the strategy of the modeling approach.

1. The modeling of systems of the inert matter is developed within the framework of deterministic causality principles. Namely for a given cause, the effect is deterministically identified. This ***causality principle needs to be weakened, or even suppressed***, in the case of the living matter.

2. The description of the ***physical state of living systems*** needs the introduction of additional variables suitable to describe the strategy that each element of the system develops. Therefore, the use of models at the macroscopic scale ends up with killing the presence of such variable, which is, as previously mentioned, heterogeneously distributed.

3. If system is constituted by a large number of interacting living entities, one may call them ***active particles***, and their microscopic state should include, in addition to geometrical and mechanical variables, also an additional variable, called ***activity***. This variable should be appropriate to model the ability of each entity to express a specific strategy.

4. The ability to express a strategy is heterogeneously distributed over the active particles. Therefore, a modeling approach can be based on the description of the overall state of the system by a ***probability distribution function*** over such microscopic state.

5. ***Methods of the mathematical kinetic theory*** can be developed to model the evolution in time and space of the distribution function. For instance using a suitable balance in each elementary volume of the space of the microscopic states, where the inflow and outflow of particles in the said volume is determined by interactions among particles.

6. ***Living systems***, particularly in biology (e.g. multicellular systems), are constituted different types of active particles, so that several different functions are expressed. This is a relevant source of complexity. Therefore, it is useful reducing it ***by decomposing the system into suitable functional subsystems*** according to well defined rules that will be stated in the sequel.

7. A ***functional subsystem*** is a collection of active particles, which have the ability to express collectively the same ***activity*** regarded as a scalar variable. The whole system is constituted by several interacting functional subsystems. The link between a functional subsystem and its activity depends also on the specific phenomena under consideration.

8. The ***decomposition into functional subsystems*** is a flexible approach to be adapted at each particular investigation. Specifically, the identification of each functional sub-system is related to the activity they express as well as to the specificity of the investigation that is developed. Namely, given the same system, different decompositions can be developed corresponding to different specific investigation.

9. Active particles of the same functional subsystem may, however, differ for specific characteristics. For instance in a multicellular system, cells with a different genotype may however collectively express, with other cell, the same function. Therefore, ***different decomposition may correspond, according to the afore-said statements, to different composition of each functional subsystem***.

10. Considering that the subsystems composing a system may be ***linked by networks***, the modeling approach needs treating both interactions within the same functional subsystem in a node of the network and interactions involving functional subsystems of different nodes. In some cases nodes of the network may identify different sub systems. Dealing also with interactions among subsystems may need, in some cases, use of different scales.

Bearing all above in mind, let us consider a large system is constituted by interacting entities, called ***active particles*** organized into n interacting populations labeled by the indexes $i = 1, \ldots, n$. Each population corresponds to a ***functional subsystem***, namely active particles in each functional subsystem develop collectively a common strategy.

The variable charged to describe the state of each particles is called ***microscopic state***, which is denoted by the variable $\mathbf{w}$ that includes the geometrical and mechanical description as well as of the ***activity variable***. In the simplest case: $\mathbf{w} = \{\mathbf{x}, \mathbf{v}, u\}$, where $\mathbf{x} \in D_{\mathbf{x}}$ is ***position***, $\mathbf{v} \in D_{\mathbf{v}}$ is ***mechanical state***, e.g. linear velocity, and $u \in D_u$ is the ***activity***.

The description of the overall state of the system is defined by the ***generalized one-particle distribution function***:

$$f_i = f_i(t, \mathbf{x}, \mathbf{v}, u), \qquad i = 1, \ldots, n,$$

such that $f_i(t, \mathbf{x}, \mathbf{v}, u) \, d\mathbf{x} \, d\mathbf{v} \, du$ denotes the number of active particles whose state, at time t, is in the interval $[\mathbf{w}, \mathbf{w} + d\mathbf{w}]$. where $\mathbf{w} = \mathbf{x}, \mathbf{v}, u$ is an element of the ***space of the microscopic states***.

Remark 4.5.1. *If the number of active particles is constant in time, then the distribution function can be normalized with respect to such a number and consequently is a probability density.*

If f_i is known, moment calculations lead to the computing of macroscopic quantities. For instance, ***marginal densities*** are computed as follows:

$$f_i^m(t, \mathbf{x}, \mathbf{v}) = \int_{D_u} f_i(t, \mathbf{x}, \mathbf{v}, u) \, du, \tag{4.5.1}$$

$$f_i^a(t, \mathbf{x}, u) = \int_{D_{\mathbf{v}}} f_i(t, \mathbf{x}, \mathbf{v}, u) \, d\mathbf{v} \tag{4.5.2},$$

and

$$f_i^b(t, u) = \int_{D_{\mathbf{x}} \times D_{\mathbf{v}}} f_i(t, \mathbf{x}, \mathbf{v}, u) \, d\mathbf{x} \, d\mathbf{v}. \tag{4.5.3}$$

The ***local density*** of the ith functional subsystem is:

$$\nu[f_i](t, \mathbf{x}) = \int_{D_{\mathbf{v}} \times D_u} f_i(t, \mathbf{x}, \mathbf{v}, u) \, d\mathbf{v} \, du = \int_{D_{\mathbf{v}}} f_i^m(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{v}, \tag{4.5.4}$$

while integration over the volume $D_{\mathbf{x}}$ containing the particles gives the ***total size*** of the ith subsystem:

$$N_i[f_i](t) = \int_{D_{\mathbf{x}}} \nu[f_i](t, \mathbf{x}) \, d\mathbf{x}, \tag{4.5.5}$$

which can depend on time due to the role of proliferative or destructive interactions, as well as to the flux of particles through the boundaries of the volume.

First order moments provide either *linear mechanical macroscopic* quantities, or *linear activity macroscopic* quantities. More precisely, the *flux of particles*, at the time t in the position $\mathbf{x}$, is given by:

$$\mathbf{Q}[f_i](t, \mathbf{x}) = \int_{D_{\mathbf{v}} \times D_u} \mathbf{v} \, f_i(t, \mathbf{x}, \mathbf{v}, u) \, d\mathbf{v} \, du = \int_{D_{\mathbf{v}}} f_i^m(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{v} \,. \qquad (4.5.6)$$

The *mass velocity* of particles, at the time t in the position $\mathbf{x}$, is given by:

$$\mathbf{U}[f_i](t, \mathbf{x}) = \frac{1}{\nu_i[f_i](t, \mathbf{x})} \int_{D_{\mathbf{v}} \times D_u} \mathbf{v} \, f_i(t, \mathbf{x}, \mathbf{v}, u) \, d\mathbf{v} \, du \,. \qquad (4.5.7)$$

The **activity** terms are computed as follows:

$$a[f_i](t, \mathbf{x}) = \int_{D_{\mathbf{v}} \times D_u} u f_i(t, \mathbf{x}, \mathbf{v}, u) \, d\mathbf{v} \, du \,, \qquad (4.5.8)$$

while the *local activation density* is given by:

$$a^d[f_i](t, \mathbf{x}) = \frac{a_j[f_i](t, \mathbf{x})}{\nu_i[f_i](t, \mathbf{x})} = \frac{1}{\nu_i[f_i](t, \mathbf{x})} \int_{D_{\mathbf{v}} \times D_u} u f_i(t, \mathbf{x}, \mathbf{v}, u) \, d\mathbf{v} \, du \,. \qquad (4.5.9)$$

Integration over space provides global quantities:

$$A[f_i](t, \mathbf{x}) = \int_{\Omega} a[f_i](t, \mathbf{x}) \, d\mathbf{x} \,, \qquad A^d[f_i](t, \mathbf{x}) = \int_{\Omega} a^d[f_i](t, \mathbf{x}) \, d\mathbf{x} \,,$$

Second order moments yield quadratic quantities such as the *local quadratic activity*:

$$e[f_i](t, \mathbf{x}) = \int_{D_{\mathbf{v}} \times D_u} u^2 f_i(t, \mathbf{x}, \mathbf{v}, u) \, d\mathbf{v} \, du \,, \qquad (4.5.10)$$

while the *local quadratic density* is given by:

$$\varepsilon[f_i](t, \mathbf{x}) = \frac{e[f_i](t, \mathbf{x})}{\nu[f_i](t, \mathbf{x})} = \frac{1}{\nu[f_i](t, \mathbf{x})} \int_{D_{\mathbf{v}} \times D_u} u^2 f_i(t, \mathbf{x}, \mathbf{v}, u) \, d\mathbf{v} \, du \,, \qquad (4.5.11)$$

where the analogy between quadratic quantities and energy needs to be specified with reference the specific real system under consideration.

Remark 4.5.2. *Particular systems in life sciences are such that the **microscopic state is identified only by the activity variable**. Namely, space and velocity variables are not significant to describe the microscopic state of the active particles. In this case, the overall state of the system is described by the distribution function $f_i(t, u)$ over the activity variable only.*

Remark 4.5.3. *The **microscopic state may identified only by the space and activity variables**. Namely, the velocity variable is not significant to describe the microscopic state, while it is important to know the localization of the active particles. Therefore, the representation is given by $f_i(t, \mathbf{x}, u)$ and the definition of **vanishing variable** is used.*

Remark 4.5.4. *The space variable can be used, in some cases to identify the **regionalization** of active particles, where the activity variable is the same in each region, but the communication rules, namely the dynamics at the microscopic scale, differ from region to region. In this case the localization identifies different functional subsystems.*

It is useful in view of applications considering also the case of discrete variables such as **discrete velocities** defined by the set:

$$I_{\mathbf{v}} = \{\mathbf{v}_1, \ldots, \mathbf{v}_k, \ldots, \mathbf{v}_K\}, \quad k = 1, \ldots, K.$$

The representation is as follows:

$$f_i(t, \mathbf{x}, \mathbf{v}, u) = \sum_{k=1}^{K} f_i^k(t, \mathbf{x}) \, \delta(\mathbf{v} - \mathbf{v}_k), \qquad f_i^k(t, \mathbf{x}, u) = f_i(t, \mathbf{x}, u; \mathbf{v}_k). \tag{4.5.12}$$

Consider now the case of **discrete velocity, activity and space variable** where the discretization of the activity and space is delivered by the sets:

$$I_u = \{u_1, \ldots, \mathbf{x}_s, \ldots, u_S\}, \quad s = 1, \ldots, S,$$

and

$$I_{\mathbf{x}} = \{\mathbf{x}_1, \ldots, \mathbf{x}_r, \ldots, \mathbf{x}_R\}, \quad r = 1, \ldots, R.$$

In this general case, the representation is as follows:

$$f_i(t, \mathbf{x}, \mathbf{v}, u) = \sum_{s=1}^{S} \sum_{r=1}^{R} \sum_{k=1}^{K} f_i^{srk}(t) \, \delta(u - u_s) \, \delta(\mathbf{x} - \mathbf{x}_r) \, \delta(\mathbf{v} - \mathbf{v}_k), \tag{4.5.13}$$

where $f_i^{rk}(t) = f_i(t, \mathbf{x}_r, \mathbf{v}_k, u_s)$.

Calculation of macroscopic quantities is simply obtained by sums. For instance, the local density is given, respectively, by:

$$n_i(t, \mathbf{x}) = \sum_{k=1}^{K} \int_{D_u} f_i^k(t, \mathbf{x}, u) \, du, \quad \text{or} \quad n_i(t, \mathbf{x}) = \sum_{s=1}^{S} \sum_{k=1}^{K} f_i^{sk}(t, \mathbf{x}), \tag{4.5.14}$$

and so on.

Let us know apply the afore-said concepts, with tutorial aims, to the following examples:

------------------------------ *Example 4.5.1* ------------------------------
Vehicular Traffic

The representation, in view of the modeling approach, of vehicular traffic can be developed according to the following guidelines:

• **Micro-state:** The state of the micro-system is defined by position, velocity and activity;

• **Functional subsystems:** The simplest case consists in assuming one only functional subsystem. Otherwise, the decomposition can distinguish: Trucks, slow cars and fast cars. Multilane flows can be treated by inserting the lane in the micro-variable of as a functional subsystem.

Introducing various functional subsystems reduces the need of an heterogeneous activity variable to model the activity of each functional subsystem.

□

------------------------------ *Example 4.5.2* ------------------------------
Immune Competition

The representation of phenomena of the immune competition can take advantage of the following guidelines:

• **Micro-state:** The state of the micro-system is defined by the function (activity) expressed by cells of each functional subsystem;

• **Functional subsystems:** The simplest case consists in assuming two functional subsystems. One for cells with a pathologic state, one for the immune cells.

The modeling approach should include the onset of new functional subsystems related to Darwinian mutations.

□

------------------------------ *Example 4.5.3* ------------------------------
Social Dynamics

Social systems can be represented according to:

• **Micro-state:** The state of the micro-system is defined by the function (activity) expressed by individuals of each functional subsystem. It depends very much on the type of system under consideration.

• **Functional subsystems:** The simplest case consists in assuming one isolated functional subsystems. A general case consists in modeling several functional subsystems interacting in a network.

The localization can be used, for systems in a network, to identify different functional subsystems. The modeling approach should include the onset of new functional subsystems related to

aggregation and/or fragmentation events. New subsystems can also be generated by migration phenomena.

□

4.5.3 On the Kinetic Theory of Active Particles with Additive Interactions

Let us now deal with the derivation of mathematical structures suitable to derive the time and space evolution of the above distribution function. Preliminary to detailed calculations, a classification of models that are technically generated from the classical kinetic theory, is developed. In details:

• **Models of classical Kinetic Theory** are based on *classical interactions, localized or mean field, with conservation of mass momentum and energy.* The distribution function is as follows: $f = f(t, \mathbf{x}, \mathbf{v})$. If the dimension of the particles is finite, the microscopic state can include angular variables and velocities.

• The **Generalized Kinetic Theory** is based on *non-classical interactions, localized and mean field, without conservation of mass momentum and energy with the same rules for all particles (typically dissipative interactions).* The distribution function has the same structure as in the preceding case.

• The **Kinetic Theory for Active Particles** is based *interactions by stochastic games with randomly distributed rules.* The distribution function is as follows: $f = f(t, \mathbf{x}, \mathbf{v}, u)$.

A Particular case is when the rules are the same for all particles, namely homogeneous activity distribution. The distribution function is as follows:

$$f = f(t, \mathbf{x}, \mathbf{v}) \, \delta(u - u_0).$$

The strategy to derive equations follows the guidelines of the classical kinetic theory. Namely, by a balance equation for net flow of particles in the elementary volume of the space of the microscopic state by transport and interactions. The following active particles are involved in the interactions:

• **Test** particles with microscopic state, at the time t, defined by the variable $(\mathbf{x}, \mathbf{v}, u)$, whose distribution function is $f = f(t, \mathbf{x}, \mathbf{v}, u)$.

• **Field** particles with microscopic state, at the time t, defined by the variable $(\mathbf{x}^*, \mathbf{v}^*, u^*)$, whose distribution function is $f^* = f(t, \mathbf{x}^*, \mathbf{v}^*, u^*)$.

• **Candidate** particles with microscopic state, at the time t, defined by the variable $(\mathbf{x}_*, \mathbf{v}_*, u_*)$, whose distribution function is $f_* = f(t, \mathbf{x}_*, \mathbf{v}_*, u_*)$.

The **rules of interactions are as follows:** *The* **candidate** *particles with microscopic state defined, at the time t, by $(\mathbf{x}_*, \mathbf{v}_*, u_*)$, interacts with* **field** *particles with microscopic state, at the same time t, defined by $(\mathbf{x}^*, \mathbf{v}^*, u^*)$ and acquires, in probability the state of the*

test particles with microscopic state $(\mathbf{x}, \mathbf{v}, u)$. **Test** particles interacts with field particles and may lose their state.

The following interactions can be taken into account:

- **Conservative interactions** modify the microscopic state of particles;

- **Non conservative interactions** generate proliferation or destruction of particles in their microscopic state.

- **Onset of new functional subsystems**: both type of (above) interactions may generate a particle in a new functional subsystem.

The mathematical framework refers to the evolution in time and space of the test particle. The derivation related to the distribution functions f_i is based on the following balance of equations in the elementary volume of the phase space:

$$\frac{df_i}{dt}\,d\mathbf{x}\,d\mathbf{v} = \left(G_i[\mathbf{f}] - L_i[\mathbf{f}] + S_i[\mathbf{f}]\right) d\mathbf{x}\,d\mathbf{v}\,, \qquad (4.5.15)$$

where interactions of candidate and test particles refers to the field particles and $\mathbf{f} = \{f_i\}_{i=1}^n$. Moreover, for the ith functional subsystem:

$G_i[\mathbf{f}]$ denotes the **gain** of candidate particles into the state $\mathbf{x}\,\mathbf{v}, u$ of the test particle;

$L_i[\mathbf{f}]$ models the **loss** of test particles;

$S_i[\mathbf{f}]$ models **proliferation/destruction** of test particles in their microscopic state.

Let us consider the interactions between candidate or test particles of the hth functional subsystem and the field particles of the kth functional subsystem.

H.4.1. The candidate and test particles in $\mathbf{x}$, with state $\mathbf{v}_*, u_*$ and $\mathbf{v}, u$, respectively, interact with the field particles in $\mathbf{x}^*$, with state $\mathbf{v}^*, u^*$ located in its interaction domain Ω, $\mathbf{x}^* \in \Omega$.

H.4.2. Interactions are weighted by a suitable term $\eta_{hk}(\mathbf{v}_*, \mathbf{v}^*, u_*, u^*)$, that can be interpreted as an **interaction rate**, which depends on the local density in the position of the field particles.

H.4.3. The distance and topological distribution of the intensity of the interactions is weighted by a function $p_{hk}(\mathbf{x}, \mathbf{x}^*)$ such that:

$$\int_\Omega p_{hk}(\mathbf{x}, \mathbf{x}^*)\,d\mathbf{x}^* = 1\,.$$

H.4.4. The candidate particle modifies its state according to the probability density $\mathcal{A}$ defined as follows:

$$\mathcal{A}_{hk}(\mathbf{v}_* \to \mathbf{v},\, u_* \to u|\mathbf{v}_*, \mathbf{v}^*, u_*, u^*)$$

where $\mathcal{A}_{hk}$ denotes the probability density that a candidate particles of the h-subsystems with state $\mathbf{v}_*, u_*$ reaches the state $\mathbf{v}, u$ after an interaction with the field particles k-subsystems with state $\mathbf{v}^*, u^*$, while the test particle looses its state $\mathbf{v}$ and u after interactions with field particles with velocity $\mathbf{v}^*$ and activity u^*.

H.4.5. The test particle, in $\mathbf{x}$, can proliferate, due to encounters with field particles in $\mathbf{x}^*$, with rate $\mu^i_{hk}(\mathbf{x}, \mathbf{x}^*)$, which denotes the proliferation rate into the functional subsystem i, due the encounter of particles belonging the functional subsystems h and k. Destructive events can occur only within the same functional subsystem with rate $\mu^i_{ik}(\mathbf{x}, \mathbf{x}^*)$.

Conjecture 4.1. *Interactions modify the activity variable according to topological stochastic games, however independently on the distribution of the velocity variable, while modification of the velocity of the interacting particles depends also on the activity variable.*

$$\mathcal{A}_{hk}(\cdot) = \mathcal{B}_{hk}(u_* \to u, \,|u_*, u^*) \times \mathcal{C}_{hk}(\mathbf{v}_* \to \mathbf{v}\,|\mathbf{v}_*, \mathbf{v}^*, u_*, u^*)\,,$$

where $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ are, for positive defined f, probability densities:

$$\int_{D_{\mathbf{v}} \times D_u} \mathcal{A}_{hk}(\mathbf{v}_* \to \mathbf{v}, \, u_* \to u\,|\mathbf{v}_*, \mathbf{v}^*, u_*, u^*)\, d\mathbf{v}\, du = 1\,, \quad \forall\ \mathbf{v}_*, \mathbf{v}^*\, u_*, u^*\,,$$

and

$$\int_{D_u} \mathcal{B}_{hk}(u_* \to u, \,|u_*, u^*)\, du = 1\,, \quad \forall\ u_*, u^*\,,$$

$$\int_{D_{\mathbf{v}}} \mathcal{C}_{hk}(\mathbf{v}_* \to \mathbf{v}\,|\mathbf{v}_*, \mathbf{v}^*, u_*, u^*)\, d\mathbf{v} = 1\,, \quad \forall\ \mathbf{v}_*, \mathbf{v}^*\, u_*, u^*\,.$$

Conjecture 4.2. *The encounter rate, namely, the frequency of interactions depends on velocity and activity of the interacting pairs:* $\eta_{ij}(\mathbf{v}_*, \mathbf{v}^*, u_*, u^*)$, $\quad \eta_{hk}(\mathbf{v}, \mathbf{v}^*, u, u^*)$.

Conjecture 4.3. *The weight function, which models the intensity of interactions depends on the localization of the interacting pairs:* $p_{ij}(\mathbf{x}, \mathbf{x}^*)$, $\quad p_{hk}(\mathbf{x}, \mathbf{x}^*)$.

Using the afore-said conjectures yields:

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_i \cdot \nabla_{\mathbf{x}}\right) f_i(t, \mathbf{x}, \mathbf{v}, u) = \left[\sum_{j=1}^{n}\left(G_{ij}[\mathbf{f}] - L_{ij}[\mathbf{f}]\right) + \sum_{h=1}^{n}\sum_{k=1}^{n} S^i_{hk}[\mathbf{f}]\right](t, \mathbf{x}, \mathbf{v}, u)\,, \quad (4.5.16)$$

where

$$G_{ij} = \int_{\Omega \times D^2_{\mathbf{v}} \times D^2_u} \eta_{ij}(\mathbf{v}_*, \mathbf{v}^*, u_*, u^*) p_{ij}(\mathbf{x}, \mathbf{x}^*)\, \mathcal{B}_{ij}(u_* \to u|u_*, u^*)\, \mathcal{C}_{ij}(\mathbf{v}_* \to \mathbf{v}\,|\mathbf{v}_*, \mathbf{v}^*, u_*, u^*)$$
$$\times\, f_i(t, \mathbf{x}, \mathbf{v}_*, u_*) f_j(t, \mathbf{x}^*, \mathbf{v}^*, u^*)\, d\mathbf{x}^*\, d\mathbf{v}_*\, d\mathbf{v}^*\, du_*\, du^*\,, \qquad (4.5.17)$$

$$L_{ij} = f_i(t, \mathbf{x}, \mathbf{v}) \int_{\Omega \times D_{\mathbf{v}} \times D_u} \eta_{ij}(\mathbf{v}, \mathbf{v}^*, u, u^*) p_{ij}(\mathbf{x}, \mathbf{x}^*)\, f_j(t, \mathbf{x}^*, \mathbf{v}^*, u^*)\, d\mathbf{v}^*\, du^*\, d\mathbf{x}^*\,, \qquad (4.5.18)$$

and

$$S^i_{hk} = \int_{\Omega \times D_{\mathbf{v}} \times D^2_u} \eta_{hk}(\mathbf{v}, \mathbf{v}^*, u, u^*) p_{hk}(\mathbf{x}, \mathbf{x}^*)\, \mu^i_{hk}(u, u^*)$$
$$\times\, f_h(t, \mathbf{x}, \mathbf{v}, u_*) f_k(t, \mathbf{x}^*, \mathbf{v}^*, u^*)\, d\mathbf{x}^*\, d\mathbf{v}^*\, du_*\, du^*\,. \qquad (4.5.19)$$

Let us now consider the case of open systems. Modeling **external actions at the microscopic scale** means modeling the action of functional subsystems generated by the outer system delivered by the distribution functions:

$$g_r(t, \mathbf{x}, w), \quad r = 1, \ldots, m, \quad w \in D_w = D_u, \tag{4.5.20}$$

which depends on time, space and on a variable w modeling the activity of the outer functional subsystem.

Reasonings analogous to those we have seen above lead to the derivation of the mathematical structures. The relatively simpler spatially homogeneous case correspond to the following system:

$$\frac{\partial f_i}{\partial t}(t, u) + \mathcal{F}_i(t) \frac{\partial f_i}{\partial u}(t, u) = J_i[\mathbf{f}](t, u) + Q_i[\mathbf{f}](t, u)$$

$$= \sum_{j=1}^{n} \int_{D_u \times D_u} \eta_{ij}(u_*, u^*) \mathcal{B}_{ij}(u_* \to u | u_*, u^*) f_i(t, u_*) f_j(t, u^*) \, du_* du^*$$

$$- f_i(t, u) \sum_{j=1}^{n} \int_{D_u} \eta_{ij}(u, u^*) f_j(t, u^*) \, du^*$$

$$+ \sum_{h=1}^{n} \sum_{k=1}^{n} \int_{D_u \times D_u} \eta_{hk}(u_*, u^*) \mu_{hk}^i(u, u^*) f_h(t, u_*) f_k(t, u^*) \, du_* du^*$$

$$+ \sum_{j=1}^{m} \int_{D_u \times D_v} \eta_{ij}^e(u_*, w^*) \mathcal{B}_{ij}^e(u_* \to u | u_*, v^*) f_i(t, u_*) g_j(t, w^*) du_* dw^*$$

$$- f_i(t, u) \sum_{j=1}^{m} \int_{D_v} \eta_{ij}^e(u, w^*) g_j(t, w^*) \, dv^*$$

$$+ \sum_{h=1}^{r} \sum_{k=1}^{m} \int_{D_u} \int_{D_u} \eta_{hk}^e(u_*, w^*) \mu_{hk}^e(i)(u_*, w^*; u) f_h(t, u_*) g_k(t, w^*) du_* dw^* . \tag{4.5.21}$$

where:

η_{hk}^e models the encounter rates between the kth external action with state v^* and the hth **candidate particle** with state u_*, and similarly for η_{ij}^e.

$\mathcal{B}_{ij}^e(u_* \to u | u_*, v^*)$ denotes the probability density that the candidate particle of the ith functional subsystem with state u_*, falls into the state u of the same functional subsystem due to interactions with the jth action with state v^*.

$\mu_{hk}^e(i)(u_*, v^*; u)$ models the net proliferation into the ith population, due to interactions, which occur with rate η_{hk}, of the **candidate** particle of the population h^{th} with state u_* with the kth action with state v^*.

More complex, but technically analogous calculations can be developed when the space variable is included in the microscopic state.

4.6 Some Preliminary Ideas on the Modeling of Nonlinear Interactions

It is well understood that interactions involving living entities may be nonlinearly additive. A brief introduction is given in this subsection. Some sources of nonlinearity are the following:

• Encounter rate depending on the distribution function due to the ***hiding and learning dynamics***;

• Table of games conditioned by the distribution function;

• Nonlinearity induced by topological distribution of the interacting entities.

The modeling of the ***learning dynamics*** refers to the seminal paper by Cucker and Smale (2002). This paper presents a deep and exhaustive understanding of the approximation of sparse data, viewed as learning, i.e. the information to be learned.

Here some preliminary ideas are proposed, referring to Bellomo (2010), on the modeling approach to ***hiding and learning*** dynamics of two interacting functional subsystems, where the first one escapes, while the second one hunts. The mathematical structure, which is a particular case of (4.5.21), can be used:

$$\frac{\partial f_i}{\partial t}(t, u) = \sum_{j=1}^{2} \int_{D_u \times D_u} \eta_{ij}(u_*, u^*)\, \mathcal{B}_{ij}(u_* \to u | u_*, u^*)\, f_i(t, u_*)\, f_j(t, u^*)\, du_*\, du^*$$

$$- f_i(t, u) \sum_{j=1}^{2} \int_{D_u} \eta_{ij}(u, u^*)\, [1 - \mu_{ij}(u, u^*)]\, f_j(t, u^*)\, du^*. \qquad (4.6.1)$$

where: η_{ij} and $\mu_{ij}(u, u^*)$ the encounter rate and the proliferation rate related to the candidate active particle, with state u_*, of the hth functional subsystem and the field active particle, with state u^*, of the jth functional subsystem. Moreover, $\mathcal{B}_{ij}$ is the probability density that a candidate particle, with state u_*, of the ith functional subsystem ends up into the state u of the test particle of the same functional subsystem after the interaction with the field particle, with state u^*, of the jth functional subsystem.

The mathematical structure can be specialized into a mathematical model when the interaction terms η_{ij} and $\mathcal{B}_{ij}$ are properly modeled according to a dynamics of hiding and learning actions. Specifically, let us consider the encounter rate in the following general form

$$\eta_{ij} = \eta_{ij}^0\ e^{-c\,\beta_{ij}^2(t|\mathbf{f}, u_*, u^*)}, \qquad (4.6.2)$$

where c is a positive constant and $\beta_{ij}^2(t|\mathbf{f})$ models the distance between the two interacting particles. In details, the following cases can be considered:

I $-$ β_{ij} ***is equal to zero:*** This assumption corresponds to simplest approach that consists in assuming that the encounter rate is identified only by the interacting pairs, so that it is a constant η_{ij}^0 for each pair of interacting functional subsystems.

II $- \beta_{ij}$ **is the distance between the microscopic states of the two interacting pairs:** This amounts to suppose that β_{ij} is given by the difference between the microscopic state of the interacting particles, and it can be related to the interaction rate as follows:

$$\beta_{ij}(u_*, u^*) = \sqrt{(u_* - u^*)^2}, \qquad \eta_{ij} = \eta_{ij}^0 \ e^{-c\,(u_* - u^*)^2}. \tag{4.6.3}$$

III $- \beta_{ij}$ **is given by the distance between the shapes of the distribution of the two interacting subsystems:** This corresponds to suppose that it is given by the difference between the shapes of the interacting particles. More precisely distance β_{ij} between the ith and the jth functional subsystem can be defined as follows:

$$\beta_{ij}^2(t|\mathbf{f}) = \int_{D_u} (f_i - f_j)^2(t, u) \, du, \tag{4.6.4}$$

hence

$$\eta_{ij} = \eta_{ij}^0 \ e^{-c\beta_{ij}^2(t|\mathbf{f})} = \eta_{ij}^0 \ e^{-c \int_{D_u} (f_i - f_j)^2(t, u) \, du}. \tag{4.6.5}$$

More in general, the distance β_{ij} can be given by the norm of the difference between f_i and f_j in the appropriate metric space.

The dynamics is given by the following equation:

$$\frac{\partial f_i}{\partial t}(t, u) = \sum_{j=1}^{2} \int_{D_u \times D_u} \eta_{ij}^0 \, e^{-c\,\beta_{ij}^2(t|\mathbf{f})} \, \mathcal{B}_{ij}(u_* \to u|u_*, u^*) \, f_i(t, u_*) \, f_j(t, u^*) \, du_* \, du^*$$

$$- f_i(t, u) \sum_{j=1}^{2} \int_{D_u} \eta_{ij}^0 \, e^{-c\,\beta_{ij}^2(t|\mathbf{f})} \left[1 - \mu_{ij}(u, u^*)\right] f_j(t, u^*) \, du^*. \tag{4.6.6}$$

This structure can be generalized to include the **generation of new functional subsystems** as follows:

$$\frac{\partial f_i}{\partial t}(t, u) = \sum_{h=1}^{p} \sum_{k=1}^{p} \int_{D_u \times D_u} \eta_{hk}^0 \, e^{-c\,\beta_{hk}^2(t|\mathbf{f})} \, \mathcal{B}_{hk}^i(u_* \to u|u_*, u^*) \, f_h(t, u_*) \, f_k(t, u^*) \, du_* \, du^*$$

$$- f_i(t, u) \sum_{k=1}^{p} \int_{D_u} \eta_{ik}^0 \, e^{-c\,\beta_{ik}^2(t|\mathbf{f})} \, f_k(t, u^*) \, du_*$$

$$+ \sum_{h=1}^{p} \sum_{k=1}^{p} \int_{D_u \times D_u} \eta_{hk}^0 \, e^{-c\,\beta_{hk}^2(t|\mathbf{f})} \mu_{hk}^i(u_*, u^*) f_h(t, u_*) \, f_k(t, u^*) \, du_* \, du^*, \tag{4.6.7}$$

where $\mathcal{B}_{hk}^i$ is the probability density that a candidate particle of the hth functional subsystem, with state u_* ends up into the state u of the ith functional subsystem after the interaction with the field particle of the kth functional subsystem, with state u^*. Moreover, μ_{hk}^i is the proliferative/destructive rate in the ith f.s. of the test particle, due to the encounter between the hth candidate particle, with state u_*, of the kth particle (field), with state u^*.

Example 4.6.1
Modeling Hiding Learning Dynamics

A simple approach of modeling the terms $\mathcal{B}_{ij}$, for two functional subsystems, can be obtained by supposing that the output of the interaction is defined by the most probable value m_{ij} and the variance σ_{ij}. In general it can be assumed that encounters within the same functional subsystem do not modify the state of the interacting pair:

• The candidate particle with activity u_* does not shows any modification of its state related when it encounters a field particle of the same subsystem: $m_{11} = m_{22} = u_*$.

• The candidate particle of the first subsystem, with activity u_*, shows a trend to increase the distance when it encounters the candidate particle of the second subsystem:

$$\begin{cases} m_{12} = u_* - \varepsilon_1 \left(u^* - u_* \right), & \text{if} \quad u_* > u^* \\ m_{12} = u_* + \varepsilon_1 \left(u^* - u_* \right), & \text{if} \quad u_* \leq u^* \end{cases}$$

• The candidate particle, with activity u_*, of the second subsystem shows a trend to reduce the distance with respect to the state of the candidate particle of the first subsystem:

$$\begin{cases} m_{21} = u_* - \varepsilon_2 \left(u^* - u_* \right), & \text{if} \quad u_* < u^* \\ m_{21} = u_* + \varepsilon_2 \left(u^* - u_* \right), & \text{if} \quad u_* \geq u^* \end{cases}$$

$\square$

Let us now consider the case of nonlinear interactions where the term $\mathcal{B}_{ij}$, depend on the distribution function of the interaction particles, for instance by the moments of such distribution. The evolution equation for functional subsystems undergoing conservative interactions is as follows:

$$\frac{\partial f_i}{\partial t}(t, u) = J_i[\mathbf{f}](t, u) = \sum_{j=1}^{n} J_{ij}[f_i, f_j](t, u)$$

$$= \sum_{j=1}^{n} \int_{D_u \times D_u} \eta_{ij}(t|f_i, f_j) \, \mathcal{B}_{ij}(u_* \to u|u_*, u^*, \mathcal{E}^p[f_i], \mathcal{E}^p[f_j]) \, f_i(t, u_*) \, f_j(t, u^*) \, du_* \, du^*$$

$$- f_i(t, u) \sum_{j=1}^{n} \int_{D_u} \eta_{ij}(t|f_i, f_j) \, f_j(t, u^*) \, du^*, \tag{4.6.8}$$

More precisely, the idea is that the candidate particle interacts with the field particles within its space interaction domain and feels an action identified by the low order moments of the field active particles. The action can be also related, whether consistent with the specific system under consideration, to their most probable value, see Bellomo *et al.* (2010b). This paper also shows that the interaction domain of the candidate particle with state u_* may not be the whole

domain D_u but a subset $\Omega_{u_*} \subseteq D_u$, which contains the field particles $u^* \in \Omega_{u_*}$ that are able to interact with candidate particle. Thus interactions only occur if the distance, in the space of microscopic states of the interacting particles, are sufficiently small. Therefore a positive function $\omega(u_*, u^*)$, normalized with respect to integration over u^*, is introduced to take into account such dynamics. This function, which weight the interactions among the active particles, is assumed to have a compact support in the domain of influence $\Omega_{u_*} \subseteq D_u$ of the interactions. Moreover:

$$\int_{D_u} \omega(u_*, u^*) \, du^* = \int_{\Omega_{u_*}} \omega(u_*, u^*) \, du^* = 1. \tag{4.6.9}$$

Accordingly we define the pth order weighted moment as follows:

$$\mathcal{E}_w^p[f_i](t, u_*) = \int_{D_u} (u^*)^p \, \omega(u_*, u^*) \, f_i(t, u^*) \, du^* = \int_{\Omega_{u_*}} (u^*)^p \, \omega(u_*, u^*) \, f_i(t, u^*) \, du^*. \tag{4.6.10}$$

The mathematical structure is as follow:

$$\frac{\partial f_i}{\partial t}(t, u) = Q_i[\mathbf{f}](t, u) = \sum_{h,k=1}^{n} Q_{hk}[f_h, f_k](t, u)$$

$$= \sum_{h=1}^{n} \sum_{k=1}^{n} \int_{D_u \times D_u} \eta_{hk}^0 e^{-c\beta_{hk}^2(t|f_h, f_k)} \mathcal{B}_{hk}^i(u_* \to u | u_*, u^*, \mathcal{E}_w^p[f_h], \mathcal{E}_w^p[f_k]) f_h(t, u_*) f_k(t, u^*) du_* du^*$$

$$- f_i(t, u) \sum_{k=1}^{n} \int_{D_u} \eta_{ik}^0 e^{-c\beta_{ik}^2(t|f_i, f_k)} f_k(t, u^*) \, du_*$$

$$- \sum_{h=1}^{n} \sum_{k=1}^{n} \int_{D_u \times D_u} \eta_{hk}^0 e^{-c\beta_{hk}^2(t|f_h, f_k)} \mu_{hk}^i(u_*, u^*) f_h(t, u_*) f_k(t, u^*) \, du_* \, du^*. \tag{4.6.11}$$

where the number of particles is not any more constant in time due to the term that models proliferative and/or destructive events. In details:

• μ_{hk}^i models the proliferative/destructive rate of particles of the hth functional subsystem, with state u_*, into the state u of the ith functional subsystem due to the encounter with the particle (field) of the kth functional subsystem, with state u^*. In particular, destructive events occur only within the functional subsystem of the field particles.

• $\mathcal{B}_{hk}^i$ models the probability density that a candidate particle of the hth functional subsystem, and with state u_*, ends up into the state u of the ith functional subsystem after the interaction with the field particle, with state u^*, of the kth functional subsystem.

The application of the mathematical approach we have seen in the preceding and in this sections can be practically applied to model ***vehicular traffic dynamics***, namely a class of complex systems already treated various times in these Lectures Notes. Three aspects will be considered, and treated in the forthcoming examples; namely, the derivation of the mathematical structure suitable to capture the complexity of the system under consideration, the

derivation of the table of games modeling interactions at the microscopic scale and the validation by using empirical data. The book by Kerner (2004) offers a valuable collection of experimental results followed by a sharp interpretation based on the physics of traffic, while the review papers by Helbing (2001) and Bellomo and Dogbè (2011) provide the mathematical background for the kinetic theory approach to modeling vehicular traffic phenomena.

Let us recall, repeating some concepts of the preceding chapters, that the modeling should be developed by using dimensionless quantities. Referring specifically to the maximum density n_M of vehicles corresponding to bumper-to-bumper traffic jam, and to the maximum admissible mean velocity V_M which can be reached, in average, by vehicles running in free flow conditions, while a fast isolated vehicle can reach velocities larger that V_M. More precisely, a limit velocity can be defined as follows: $V_\ell = (1+\mu)V_M$, with $\mu > 0$, such that no vehicle can reach, simply by mechanical reasons, a velocity larger than V_ℓ. Moreover, it is convenient, to identify the critical time T_c as the ratio between ℓ and V_M. Moreover, t is the dimensionless time variable obtained referring the real time t_r to a suitable critical time $T_c = \ell/V_M$, while x is the dimensionless space variable obtained dividing the real space x_r by the length ℓ of the road.

The modeling approach can be based on a strategy defined by the following reasonings:

• *Increasing the complexity of the model increases the number of parameters to be identified.*

• *The system is with finite degrees of freedom. However, microscopic models induce considerable errors in the computation of macroscopic quantities.*

• *The flow is not continuous, hence hydrodynamic models should not be used. Moreover, it is difficult to evaluate the entity of the approximation induced by macro-models.*

• *The number of individual entities is not large enough to allow the use of continuous distribution functions within the framework of the mathematical kinetic theory. Moreover, interactions are not localized, considering that drivers adapt the dynamics of the vehicle to the flow conditions in the visibility zone.*

• *Individual entities cannot be regarded as classical particles, but as active particles due to their ability to modify their dynamics according to specific strategies.*

The examples proposed in the following tackle the afore-said specific modeling issues and refer to the recent paper Bianca and Coscia (2011).

Example 4.6.2
Representation and Mathematical Structure of Vehicular Traffic

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Let us consider **discrete velocity models**, where the velocity variable belongs to the following set: $I_v = \{v_1 = 0, \ldots, v_i, \ldots, v_n = 1\}$. The corresponding discrete representation is obtained by linking the discrete distribution functions to each v_i: $f_i = f_i(t,x) : \mathbb{R}_+ \times [0,1] \to \mathbb{R}_+$, for $i = 1, \ldots, n$.

Macroscopic quantities are obtained by weighted sums. For instance, dimensionless number

density and flow are given by:

$$\rho(t, x) = \sum_{i=1}^{n} f_i(t, x),$$

and

$$q(t, x) = \sum_{i=1}^{n} v_i f_i(t, x), \qquad q(t, x) = \xi(t, x)\rho(t, x).$$

The mathematical structure to be used for the derivation of models can be based on the following assumptions:

• Interactions are distributed over a (dimensionless) characteristic length $\xi > 0$, which can be interpreted as the ***visibility length*** of the drivers: a vehicle located at a point $x \in D_x$ is supposed to be affected in average by all vehicles comprised within a certain ***visibility zone***.

• ***Interactions are weighted*** by means of a proper function $w(x, y)$, and occur with intensity according to the free space locally available in the visibility zone. Considering that a vehicle is essentially an anisotropic particle, in the sense that it reacts mainly to frontal stimuli than to rear ones, it is assumed that the visibility zone does not include any stretch behind the vehicles.

Accordingly, the mathematical structure to generate specific models is as follows:

$$\frac{\partial f_i}{\partial t} + v_i \frac{\partial f_i}{\partial x} = \sum_{h=1}^{n} \sum_{k=1}^{n} \int_{x}^{x+\xi} \eta[\rho](t, y) A_{hk}^{i}[\rho; \alpha] f_h(t, x) f_k(t, y) w(x, y)\, dy$$

$$- f_i(t, x) \sum_{h=1}^{n} \int_{x}^{x+\xi} \eta[\rho](t, y) f_h(t, y) w(x, y)\, dy, \qquad (4.6.12)$$

where

$$w(x, y) \geq 0, \quad \int_{x}^{x+\xi} w(x, y)\, dy = 1,$$

while

$$A_{hk}^{i}[\rho; \alpha] \geq 0, \quad \sum_{i=1}^{n} A_{hk}^{i}[\rho; \alpha] = 1, \quad \forall h, k = 1, \ldots, n, \quad \rho(t, x) \in [0, 1).$$

denotes the probability density that a candidate particle with velocity v_h falls into the state v_i after an encounter with a field particle with velocity v_k and α is a parametr to be properly characterized.

$\square$

Example 4.6.3
Modeling Interactions of Vehicles

The modeling of interactions, according to Bianca and Coscia (2011) uses a parameter $\alpha \in [0,1]$ is related to the quality of the road:

$$\alpha = \frac{\rho_c}{\rho_{cM}}, \quad \alpha \in [0,1],$$

where ρ_{cM} is the maximal admissible value corresponding to the best highway in optimal environmental conditions.

The velocity is discretized by coupling of a steady grid when the density ρ is less than the critical one ρ_c and with an adaptive grid when ρ is greater than ρ_c:

$$\begin{cases} v_i = 2\,\dfrac{i-1}{n-1} & \text{if} \quad 0 \le \rho \le \rho_c, \\[2mm] v_i = (1+\alpha)\,(1-\rho^3)^2\,\dfrac{i-1}{n-1} & \text{if} \quad \rho_c < \rho \le 1, \end{cases}$$

for $i \in \{1, \ldots, n\}$

The encounter rate n_{hk}, for $h, k \in \{1, \ldots, n\}$, is assumed as follows: $\eta_{hk} = |v_h - v_k|$. The Table of the Games A_{hk}^i can be derived according to the following assumptions:

i) The trend of the candidate particle to change its velocity decreases in probability when the "distance" $|v_h - v_k|$ between the velocity of the candidate and field vehicle decreases.

ii) The candidate vehicle h can attain only a velocity $v_i \in \{v_h, v_{h-1}, \ldots, v_k\}$ if it interacts with a field vehicle with velocity v_k such that $v_h > v_k$ while if the candidate vehicle interacts with a field vehicle such that $v_h < v_k$ it can only attain a velocity $v_i \in \{v_h, v_{h+1}, \ldots, v_k\}$.

iii) If the candidate and field vehicles have the same velocity, the interaction does not imply a change in velocity.

iv) When a candidate vehicle, with velocity v_h, encounters a field vehicle, with velocity $v_k > v_h$ (***faster vehicle***), the candidate vehicle has a trend to increase its velocity from v_h to v_k.

v) When a candidate vehicle, with velocity v_h, encounters a field vehicle, with velocity $v_k < v_h$ (***slower vehicle***), the candidate vehicle has a trend to decrease its velocity from v_h to v_k.

Detailed calculations reported in the afore stated paper provide the following results:

$$\begin{cases} k < h, \quad i = h: \quad A_{hk}^i = 1 - \varepsilon_{hk}, \\[2mm] k < h, \quad k \le i < h: \quad A_{hk}^i = \dfrac{\varepsilon_{hk}}{|h-k|}, \\[2mm] k > h, \quad h < i \le h: \quad A_{hk}^i = \dfrac{\varepsilon_{hk}}{|h-k|}, \\[2mm] k > h, \quad i = h: \quad A_{hk}^i = 1 - \varepsilon_{hk}, \end{cases}$$

where

$$\varepsilon_{hk} = \alpha \, \frac{1 - \rho}{|h - k|^2} \, .$$

$\square$

Let us finally consider the problem of the validation of models. Three types of empirical data can be classified:

Quantitative data, which provide accurate data of macroscopic quantities such as number density, mean velocity, and/or flow. Models are required to have the ability to reproduce them quantitatively.

Qualitative data on emerging behaviors, which corresponds to specific conditions, for instance in vehicular traffic interactions of clusters of fast and slow vehicles, bottlenecks. Model are required to reproduce qualitatively emerging behaviors.

Data on individual behaviors, which should be used to design models for the table of games.

A remarkable difficulty is that quantitative and qualitative empirical data *provide macroscopic quantities, while the dynamics is ruled at the microscopic scale*. Moreover:

• The averaging process which leads to macroscopic quantities introduces unavoidable fluctuations due not only to measurement errors, but also to the stochastic and granular essence of the flow, where deceleration and acceleration of vehicles are observed even in almost steady flow *stop and go dynamics*;

• Generally, experimental results refer to *steady state conditions, while rarely traffic reach a steady state*;

• Empirical data show *results very sensitive to the quality of environmental conditions*. Therefore, it is impossible to identify a unique deterministic representation.

• Kerner (2004) remarks that additional transitions can be observed when the flow is congested, for instance related to a considerable dispersion of data. Moreover, transitions have to be interpreted carefully due to *their variability with environmental conditions*.

• *The use of quantitative data as a direct input* to derive models is an abuse as, at least in principles, a careful modeling of microscopic interactions should provide the above result.

The interested reader can obtain a deeper understanding of the topic treated in this section by Bianca and Coscia (2010), where it is shown that their model remarkably reproduce all quantitative features of the velocity diagram studied by Kerner (2004). This diagram reports the mean velocity versus density and shows that there exists a critical density ρ_c such that for $\rho < \rho_c$ the mean velocity maintains its maximum value, while for $\rho > \rho_c$ a sharp decay indicates the transition from free to congested flow. This characteristic, and specifically ρ_c, depends on the quality of the outer environment. Additional information is obtained by Delitala and Tosin (2007), where it is shown that various emerging behaviors are reproduced by their model.

4.7 Critical Analysis

A concise introduction to some models of the kinetic theory for classical and active particles has been given in this chapter, while suitable bibliographical indications have been provided toward a deeper knowledge on the topics treated in this chapter have been given.

The substantial difference between models for classical and active particles refers to microscopic interactions. Classical particles follow deterministic laws of Newtonian mechanics, namely if both the input velocities and the impact parameter are assigned, then the output velocities can be computed. On the other hand, interactions for active particles are stochastic. Moreover the activity variable can modify the mechanical variables due to the strategy of the particles to modify their dynamics.

Although this chapter does not report specific applications, some bibliographical indications can be given. Specifically, the Boltzmann equation has been applied to study a variety of fluid dynamic problems at large Knudsen number. Various applications are documented in the books by Kogan (1969). The Vlasov equation has been applied to study various problems in plasma physics, see for example Schram (1991).

The Kinetic Theory of Active Particles has been used to model some interesting complex systems in applied sciences which are constituted by a large number of interacting entities such that their microscopic state includes, in addition to geometrical and mechanical variable, an additional microscopic state related to their behavior, which will be called ***characteristic microscopic variable***, or simply: ***activity***. Microscopic interactions do not follow rules of mechanics (classical or quantum), but are governed by a somehow organized behavior which is able to modify laws of mechanics.

As already mentioned in Chapter 1, mathematical models of the kinetic theory are used to overcame complexity problems induced by the need of modeling large systems of interacting individuals, where the number of equations needed to describe the system is not computationally tractable. The representation offered by methods of the mathematical kinetic theory is elegant and efficient. On the other hand the derivation of equations is based on heuristic assumptions (for instance the factorization of the joint probability density), that cannot be rigorously justified. Therefore, models of the kinetic theory have to be regarded as an approximation of the physical reality considering that even the structures, that the models refer to, are based on mathematical approximations. Of course, various approaches to improve the above mentioned approximations have been developed. However, we do not discuss this difficult topic in these Lecture Notes.

Technically, different are the complexity problems related to models of active particles. In fact, velocities of elements of living systems are always bounded, as documented in all applications dealt with in the book Bellomo (2008). Therefore, complexity problems are related to modeling microscopic interactions rather than to the development of computational algorithms. Discretization can be viewed as an approach to capture the main feature of the activity variable in view of modeling microscopic interactions.

Finally, let us stress again that the various reasonings proposed in this chapter have to be regarded simply as a brief introduction to modeling systems in applied and life sciences by the approach of the classical and generalized kinetic theory. This brief introduction has the objective to motivate the reader to a deeper insight, that may possibly start from the bibliography cited in this chapter.

Chapter 5

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