

# Introduction

All truly wise thoughts have been thought already thousands of times; but to make them truly ours, we must think them over again honestly, till they take root in our personal experience.

*Johann Wolfgang von Goethe (1749–1832)*

## Historical note

The first attempt to describe the physical reality in a quantitative way, presumably, dates back to the Pythagoreans, with their effort to explain the tangible world by means of integer numbers. The establishment of mathematics as the proper language to decipher natural phenomena lagged behind until the 17th century, when Galileo inaugurated modern physics with his major work (1638): *Discorsi e dimostrazioni matematiche intorno a due nuove scienze* (Discourses and mathematical demonstrations concerning two new sciences). Half a century later, in 1687, Newton published the *Philosophiae Naturalis Principia Mathematica* (The Mathematical Principles of Natural Philosophy) which laid the foundations of classical mechanics. The publication of the *Principia* represents the *summa* of the scientific revolution, in which Science, as we know it today, was born.

From a conceptual point of view, the main legacy of Galileo and Newton is the idea that Nature obeys unchanging laws which can be formulated in mathematical language, therefrom physical events can be predicted with certainty. These ideas were later translated in the philosophical proposition of *determinism*, as expressed in a rather vivid way by Laplace (1814) in his book *Essai philosophique sur les probabilités* (Philosophical Essay on Probability):

*We must consider the present state of Universe as the effect of its past state and the cause of its future state. An intelligence that would know all forces of nature and the respective situation of all its elements, if furthermore it was large enough to be able to analyze all these data,*

*would embrace in the same expression the motions of the largest bodies of Universe as well as those of the slightest atom: nothing would be uncertain for this intelligence, all future and all past would be as known as present.*

The above statement was widely recognized as the landmark of scientific thinking: a good scientific theory must describe a natural phenomenon by using mathematical methods; once the temporal evolution equations of the phenomenon are known and the initial conditions are determined, the state of the system can be known at each future time by solving such equations. Nowadays, the quoted text is often cited and criticized in some popular science books as too naive. In contrast with how often asserted, it should be emphasized that Laplace was not as naive about the true relevance of the determinism. Actually, he was aware of the practical difficulties of a strictly deterministic approach to many everyday life phenomena which exhibit unpredictable behaviors as, for instance, the weather. How do we reconcile Laplace's deterministic assumption with the "irregularity" and "unpredictability" of many observed phenomena? Laplace himself gave an answer to this question, in the same book, identifying the origin of the irregularity in our imperfect knowledge of the system:

*The curve described by a simple molecule of air or vapor is regulated in a manner just as certain as the planetary orbits; the only difference between them is that which comes from our ignorance. Probability is relative, in part to this ignorance, in part to our knowledge.*

A fairer interpretation of Laplace's image of "mathematical intelligence" probably lies in his desire to underline the importance of prediction in science, as it transparently appears from a famous anecdote quoted by Cohen and Stewart (1994). When Napoleon received Laplace's masterpiece *Mécanique Céleste* told him *M. Laplace, they tell me you have written this large book on the system of the universe, and have never even mentioned its Creator.* And Laplace answered *I did not need to make such assumption.* So that Napoleon replied: *Ah! That is a beautiful assumption, it explains many things,* and Laplace: *This hypothesis, Sire, does explain everything, but does not permit to predict anything. As a scholar, I must provide you with works permitting predictions.*

The main reason for the almost unanimous consensus of 19th century scientists about determinism has to be, perhaps, searched in the great successes of Celestial Mechanics in making accurate predictions of planetary motions. In particular, we should mention the spectacular discovery of Neptune after its existence was predicted — theoretically deduced — by Le Verrier and Adams using Newtonian mechanics. Nevertheless, still within the 19th century, other phenomena not as regular as planet motions were active subject of research, from which statistical physics originated. For example, in 1873, Maxwell gave a conference with the significant title: *Does the progress of Physical Science tend to give any advantage to*

*the opinion of Necessity (or Determinism) over that of the Contingency of Events and the Freedom of the Will?*

The great Scottish scientist realized that, in some cases, system details are so fine that lie beyond any possibility of control. Since *the same antecedents never again concur, and nothing ever happens twice*, he criticized as empirically empty the well recognized law *from the same antecedents the same consequences follow*. Actually, he went even further by recognizing the possible failure of the weaker version *from like antecedents like consequences follow*, as instability mechanisms can be present.

Ironically, the first<sup>1</sup> clear example of what we know today as Chaos — a paradigm for deterministic irregular and unpredictable phenomena — was found in Celestial Mechanics, the science of regular and predictable phenomena *par excellence*. This is the case of the longstanding *three-body problem* — i.e. the motion of three gravitationally interacting bodies such as, e.g. Moon-Earth-Sun [Gutzwiller (1998)] — which was already in the nightmares of Newton, Euler, Lagrange and many others. Given the law of gravity, the initial positions and velocities of the three bodies, the subsequent positions and velocities are determined by the equations of mechanics. In spite of the deterministic nature of the system, Poincaré (1892, 1893, 1899) found that the evolution can be chaotic, meaning that small perturbations in the initial state, such as a slight change in one body's initial position, might lead to dramatic differences in the later states of the system.

The deep implication of these results is that determinism and predictability are distinct problems. However, Poincaré's discoveries did not receive the due attention for a quite long time. Probably, there are two main reasons for such a delay. First, in the early 20th century, scientists and philosophers lost interest in classical mechanics<sup>2</sup> because they were primarily attracted by two new revolutionary theories: relativity and quantum mechanics. Second, an important role in the recognition of the importance and ubiquity of Chaos has been played by the development of the computer, which came much after Poincaré's contribution. In fact, only thanks to the advent of computer and scientific visualization was possible to (numerically) compute and see the staggering complexity of chaotic behaviors emerging from non-linear deterministic systems.

A widespread view claims that the line of scientific research opened by Poincaré remained neglected until 1963, when meteorologist Lorenz rediscovered deterministic chaos while studying the evolution of a simple model of the atmosphere. Consequently, often, it is claimed that the new paradigm of deterministic chaos began in

---

<sup>1</sup>In 1898 chaos was noticed also by Hadamard who found that a negative curvature system displaying sensitive dependence on the initial conditions.

<sup>2</sup>It is interesting to mention the case of the young Fermi who, in 1923, obtained interesting results in classical mechanics from which he argued (erroneously) that Hamiltonian systems, in general, are ergodic. This conclusion has been generally accepted (at least by the physics community) Following Fermi's 1923 work, even in the absence of a rigorous demonstration, the ergodicity problem seemed, at least to physicists, essentially solved. It seems that Fermi was not very worried of the lacking of rigor of his "proof", likely the main reason was his (and more generally of the large part of the physics community) interest in the development of quantum physics.

the sixties. This is not true, as mathematicians never forgot the legacy of Poincaré, although it was not so well known by physicists. Although this is not the proper place for precise historical<sup>3</sup> considerations, it is important to give, at least, an idea of the variegated history of dynamical systems and its interconnections with other fields before the (re)discovery of chaos, and its modern developments. The schematic list below, containing the most relevant contributions, serves to this aim:

- [early 20th century] Stability theory and qualitative analysis of differential equations, which started with Poincaré and Lyapunov and continues with Birkhoff and the soviet school.
- [starting from the '20s] Control theory with the work of Andronov, van der Pol and Wiener.
- [mid '20s and '40s-'50s] Investigation of nonlinear models for population dynamics and ecological systems by Volterra and Lotka and, later, the study of the logistic map by von Neumann and Ulam.
- [ '30s] Birkhoff and von Neumann studies of ergodic theory. The seminal work of Krylov on mixing and the foundations of statistical mechanics.<sup>4</sup>
- [1948–1960] Information theory born already mature with Shannon's work and was introduced in dynamical systems theory, during the fifties, by Kolmogorov and Sinai.
- [1955] Fermi-Pasta-Ulam (FPU) numerical experiment on nonlinear Hamiltonian systems showed that ergodicity is a non-generic property.
- [1954–1963] The KAM theorem for the regular behavior of almost integrable Hamiltonian systems, which was proposed by Kolmogorov and subsequently completed by Arnold and Moser.

This, non exhaustive, list demonstrates how claiming chaos as a new paradigmatic theory born in the sixties is not supported by facts.<sup>5</sup>

It is worth concluding this brief historical introduction by mentioning some of the most important steps which lead to “modern” (say after 1960) development of dynamical systems in physics.

The pioneering contributions of Lorenz, Hénon and Heiles, and Chirikov, showing that even simple low dimensional deterministic systems can exhibit irregular and unpredictable behaviors, brought chaos to the attention of the physics community. The first clear evidence of the physical relevance of chaos to important phenomena, such as turbulence, came with the works of Ruelle, Takens and Newhouse on the onset of chaos. Afterwards, brilliant experiments on the onset of chaos in Rayleigh-Bénard convection (Libchaber, Swinney, Gollub and Giglio) confirmed

---

<sup>3</sup>For throughout introduction to dynamical systems history see the nice work of Aubin and Dalmedico (2002).

<sup>4</sup>His thesis *Mixing processes in phase space* appeared posthumously in 1950, when it was translated in English [Krylov (1979)] the book came as a big surprise in the West.

<sup>5</sup>For a detailed discussion about the use and abuse of chaos see *Science of Chaos or Chaos in Science?* by Bricmont (1995).

the theoretical predictions, boosting the interest of physicists in nonlinear dynamical systems. Another crucial moment for the development of dynamical systems theory was the disclosure of the connections among chaos, critical phenomena and scaling subsequent to the works of Feigenbaum<sup>6</sup> on the universality of the period doubling mechanism for the transition to chaos. The thermodynamic formalism, originally proposed by Ruelle and then “translated” in more physical terms with the introduction of multifractals and periodic orbits expansion, disclosed the deep connection between chaos and statistical mechanics. Fundamental in providing the suitable (practical) tools for the investigation of chaotic dynamical systems were: the introduction of efficient numerical methods for the computation of Lyapunov exponents (Benettin, Galgani, Giorgilli and Strelcyn), the fractal dimension (Grassberger and Procaccia), and the embedding technique, pioneered by Takens, which constitutes a bridge between theory and experiments.

The physics of chaotic dynamical systems benefited of many contributions from mathematicians which were very active after 1960 among whom we should remember Bowen, Ruelle, Sinai and Smale.

## Overview of the book

The book is divided into two parts.

**Part I: Introduction to Dynamical Systems and Chaos** (Chapters 1–7) aims to provide basic results, concepts and tools on dynamical systems, encompassing stability theory, classical examples of chaos, ergodic theory, fractals and multifractals, characteristic Lyapunov exponents and the transition to chaos.

**Part II: Advanced Topics and Applications: From Information Theory to Turbulence** (Chapters 8–14) introduces the reader to the applications of dynamical systems in celestial and fluid mechanics, population biology and chemistry. It also introduces more sophisticated tools of analysis in terms of information theory concepts and their generalization, together with a review of high dimensional systems from chaotic extended systems to turbulence.

Chapters are organized in main text and call-out *boxes*, which serve as appendices with various scopes. Some boxes are meant to make the book self-consistent by recalling some basic notions, e.g. Box B.1 and B.6 are devoted to Hamiltonian dynamics and Markov Chains, respectively. Some others present examples of technical or pedagogical interest, e.g. Box B.14 deals with the resonance overlap criterion while Box B.23 shows an example of use of discrete mapping to describe Halley comet dynamics. Most of boxes focuses on technical aspects or deepening of some aspects which are only briefly considered in the main text. Furthermore, Chapters from 2 to 9 end with a few exercises and suggestions for numerical experiences meant helping to master the presented concepts and tools.

---

<sup>6</sup>Actually also other authors obtained independently the same results, see Derrida *et al.* (1979).

Chapters are organized as follows.

The first three Chapters are meant to be a gentle introduction to chaos, and set the language and notation used in the rest of the book. In particular, Chapter 1 aims to introduce newcomers to the main aspects of chaotic dynamics with the aid of a specific example, namely the nonlinear pendulum, in terms of which the distinction between determinism and predictability is clarified. The definition of dissipative and conservative (Hamiltonian) dynamical systems, the basic language and notation, together with a brief account of linear and nonlinear stability analysis are presented in Chapter 2. Three classical examples of chaotic behavior — the logistic map, the Lorenz system and the Hénon-Heiles model — are reviewed in Chapter 3

With Chapter 4 it starts the formal treatment of chaotic dynamical systems. In particular, the basic notions of ergodic theory and mixing are introduced, and concepts such as invariant and natural measure discussed. Moreover, the analogies between chaotic systems and Markov Chains are emphasized. Chapter 5 defines and explains how to compute the basic tools and indicators for the characterization of chaotic systems such the multifractal description of strange attractors, the stretching and folding mechanism, the characteristic Lyapunov exponents and the finite time Lyapunov exponents.

The first part of the book ends with Chapter 6 and 7 which discuss, emphasizing the universal aspects, the problem of the transition from order to chaos in dissipative and Hamiltonian systems, respectively.

The second part of the book starts with Chapter 8 which introduces the Kolmogorov-Sinai entropy and deals with information theory and, in particular, its connection with algorithmic complexity, the problem of compression and the characterization of "randomness" in chaotic systems. Chapter 9 extends the information theory approach introducing the  $\varepsilon$ -entropy which generalizes Shannon and Kolmogorov-Sinai entropies to a coarse-grained description level. With similar purposes, it is also discussed the Finite Size Lyapunov Exponents, an extension to the usual Lyapunov exponents accounting for finite perturbations.

Chapter 10 reviews the practical and theoretical issues inherent to computer simulations and experimental data analysis of chaotic systems. In particular, it accounts for the effects of round-off errors and the problem of discretization in digital computations. As for the data analysis, the main methods and their limitations are discussed. Further, it is discussed the longstanding issue of distinguishing chaos from noise and model building from time series.

Chapter 11 is devoted to some important applications of low dimensional Hamiltonian and dissipative chaotic systems encompassing celestial mechanics, transport in fluids, population dynamics, chemistry and the problem of synchronization.

High dimensional systems with their complex spatiotemporal behaviors and connection to statistical mechanics are discussed in Chapters 12 and 13. In the former, after briefly reviewing the systems of interest, we focus on three main aspects: the

generalizations of the Lyapunov exponents needed to account for the spatiotemporal evolution of perturbations; the description of some phenomena in terms of non-equilibrium statistical mechanics; the description of high dimensional systems at a coarse-grained level and its connection to the problem of model building. The latter Chapter focuses on fluid mechanics with emphasis on turbulence. In particular, we discuss the statistical mechanics description of perfect fluids, the phenomenology of two- and three-dimensional turbulence, the general problem of the reduction of partial differential equations to systems with a finite number of degrees of freedom and various aspects of the predictability problem in turbulent flows.

At last, in Chapter 14 starting from the seminal paper by Fermi, Pasta and Ulam (FPU) we discuss a specific research issue, namely the relationship between statistical mechanics and the chaotic properties of the underlying dynamics. This Chapter will give us the opportunity to reconsider some subtle issues which stand at the foundation of statistical mechanics. Especially, the discussion on FPU numerical experiments has a great pedagogical value in showing how, in a typical research program, only with a clever combination of theory, computer simulations, probabilistic arguments and conjectures is possible a real progress.

The book ends with an epilogue containing some general considerations on the role of models, computer simulations and the impact of chaos in the scientific research activity in the last decades.

## Hints on how to use/read this book

Some possible paths to the use of this book are:

- A) For a basic course aiming to introduce chaos and dynamical system: the first five Chapters and parts of Chapter 6 and 7, depending if the emphasis of the course is on dissipative or Hamiltonian systems, part of Chapter 8 for the Kolmogorov-Sinai entropy;
- B) For an advanced general course: the first part, Chapters 8 and 10.
- C) For advanced topical courses: the first part and a selection of the second part, for instance
  - C.1) Chapters 8 and 9 for an information theory, or computer science, oriented course;
  - C.2) Chapters 8-10 for researchers and/or graduate students, interested in the treatment of experimental data and modeling;
  - C.3) Section 11.3 for a tour on chaos in chemistry and biology;
  - C.4) Chapters 12, 13 and 14 if the main interest is in high dimensional systems;
  - C.5) Section 11.2 and Chapter 13 for a tour on chaos and fluid mechanics;
  - C.6) Sections 12.4 and 13.2 plus Chapter 14 for a tour on chaos and statistical mechanics.

We encourage all who wish to comment on the book to contact us through the book homepage URL: <http://denali.phys.uniroma1.it/~chaosbookCCV09/> where errata and solutions to the exercises will be maintained.