Thermal Convection: Patterns, Evolution and Stability

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Thermal Convection
To a red rose

... to my sons
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Preface

Most of the fluid motion we are accustomed to on Earth is driven by gravity. The presence of Earth creates a gravitational field that acts to attract objects with a force that is inversely proportional to the square of the distance between the mass centre of the object and the centre of Earth. A very common example of gravity’s impact on fluids is the creation of flows around our bodies, around the flame of a candle, in a container of water heated from below or from the side and in atmospheric and oceanic circulation at every scale.

The presence of flows of gravitational origin is not limited to fluids that affect our lives every day. They are also found inside planetary bodies. This is the reason why, for instance, continents ‘move’ (the ‘solid’ Earth itself undergoes a fluid-like internal circulation on time-scales of millions of years, the surface expression of which is continental drift) and a magnetic field is present around our planet (as a consequence of liquid metal motion in the Earth ‘core’).

Gravitational attraction is a fundamental property of matter that exists throughout the known universe; hence fluid motion of a gravitational origin also occurs in and around other celestial bodies and is presumed to play an important role in the dynamics of stars like the Sun.

Instability of such flows and their transition to turbulence are widespread phenomena in the natural environment at several scales and are at the root of typical problems in meteorology, oceanography, geophysics and astrophysics.

The possible origin of natural flows, however, is not limited to the action of the gravitational force. Other volume or ‘surface’ forces may be involved in the process related to the generation of fluid motion and ensuing evolutionary progress.

In particular, in the presence of a free interface (e.g. a surface separating two immiscible liquids or a liquid and a gas), surface tension-driven convection (also referred to as ‘Marangoni’ flow) may arise as a consequence of temperature or concentration gradients.

In such a context, it should be stressed that the universal nature of all these fluid phenomena makes their study fundamental not only to science, but also to engineering and industrial practical applications (e.g. the processing of metal alloys and inorganic or organic emulsions, cooling systems, the production of semiconductor crystals and various biological and biotechnological processes). The study of these topics has extensive background application in many fields.

As a relevant and important example, most widely used technologies for single-crystalline materials (e.g. horizontal and vertical Bridgman growth, Czochralski method, floating-zone technique) are affected by the presence of fluid convection. All conventional melt growth configurations require, in fact, the application of thermal gradients across the phase boundary: the axial and/or radial components of these gradients are destabilizing and provide driving forces for free convection in all fluid phases involved. Melt growth processes are, therefore, subject to varying heat- and mass-transfer conditions, which in recent years have been found to be directly or indirectly responsible for most bulk deficiencies in many materials. In particular, instabilities of the melt flow usually lead to three-dimensional oscillatory effects which strongly affect the quality of the growing crystals at microscopic scale length and therefore are very undesirable.
Some of these effects are known to be independent of gravity, that is, they are related to the other types of forces mentioned before.

Along these lines, it is worth mentioning that (because in many circumstances the influence of gravity on fluids is strong and masks or overshadows these important factors), a number of experiments have been carried out in recent years on orbiting platforms (the so-called ‘microgravity’ conditions). The peculiar behaviour of physical systems in space, and ultimately the interest in this ‘new’ environment, have come from the virtual disappearance of the gravity forces and related effects mentioned above and the appearance of phenomena unobservable on Earth, especially those driven by surface forces (that become largely predominant when terrestrial gravity is removed). The use of such an environment has also led, however, to the identification of a new type of fluid motion induced by the presence of ‘vibrations’ of the considered orbiting platform (usually referred to as g-jitters). This kind of convection, initially studied due to its perturbing and undesired influence on microgravity experiments, has recently witnessed renewed interest due to its possible application in terrestrial conditions as a means to ‘control’ flow intensity and patterning in other types of convection (as a possible variant to the use of magnetic fields traditionally employed for such a purpose).

**Aims and Scope**

As a natural consequence of all the arguments illustrated above, the present book is devoted to a critical, focused and ‘comparative’ study of all these different types of thermal convection.

Gravitational (also referred to in the literature as ‘natural’ or buoyancy), surface tension-driven, vibrational and magnetic flows are considered in various geometric models (infinite horizontal and vertical layers, open and closed geometries, shallow and tall cavities, cubic and parallelepipeds, slots, annular and spherical configurations, cylindrical enclosures, floating zones, liquid bridges, etc., many of which have enjoyed widespread use over recent years as ‘paradigm’ models for the study of these topics), under various heating conditions (from below, from above or from the side), for different fluids (liquid metals, molten salts and semiconductors, gases, water, oils, many organic and inorganic transparent liquids, etc.) and possible combinations of all these variants.

A significant effort is provided to illustrate the genesis of these kinds of flows, the governing nondimensional parameters, the scaling properties, their structure and, in particular, the stability behaviour and the possible bifurcations to different patterns of symmetry and/or spatiotemporal regimes. The book presents, in fact, a discussion of the main modes of two- and three-dimensional flows, pattern defects and the scenarios of convection-regime changes (together with the related transitional stages of evolution). To name some examples: striped patterns, various types of planforms (related to Rayleigh–Bénard or Marangoni–Bénard convection), textures (hexagons, squares, triangles, diamonds, spirals, panam structures, targets, spoke pattern), rhombic, square and star-like ‘lattices’ or ‘super-lattices’ (in vibrational convection), multiplume and multicellular configurations, cats-eye structures, patterns exhibiting the shape of a ‘flower’, a variety of symmetry-breaking effects, and so on.

A categorization and description of many kinds (both canonical and ‘exotic’) of instability are provided; to name just a few: Eckhaus, oscillatory skewed varicose, cross-roll, bimodal, the Busse oscillatory instability, zig-zag, knot, oscillatory blob, spiral-defect chaos, transverse hydrodynamic modes, oscillatory longitudinal rolls, transverse, longitudinal and oblique hydrothermal waves, steady and oscillatory multicellular flows, pulsating and rotating regimes, and so on, with the related discussion not limited to the first bifurcation of the flow, but also considering secondary, tertiary and high-order states.

Some emphasis is also given to the transition to chaos, related theories and possible means of flow control.
The analysis, moreover, does not cover only the cases in which all these types of convection (thermogravitational, thermocapillary, thermovibrational) act separately. Significant space is also devoted to elucidate the possible ‘interplay’ of several effects in situations where driving forces of different nature are simultaneously responsible for the generation of fluid motion. This subject (hybrid or mixed convection) is of particular importance as the identification of the most dominant mechanism and/or the mutual interference of different mechanisms involved with a comparable intensity may help researchers in elaborating rational guidelines relating to physical factors that can increase the probability of success in practical technological processes.

A number of existing analyses are reviewed and discussed through a focused and critical comparison of experimental and numerical results and theoretical arguments introduced over the years by investigators to explain the observed phenomena. The text has elicited information from about 100 of the author’s relevant and recent papers and about 1000 analyses available in the literature to illustrate possible approaches to the considered problems, practical applications and the ensuing insights into the physics.

A deductive approach is followed with systems of growing complexity being treated as the discussion progresses.

The book, however, is not limited to a systematic survey of landmark and recent results in the literature. Specific experimental and numerical examples are conceived and presented to provide inputs for an increased understanding of the underlying fluid flow mechanisms. Of course, an important part of these examples is based on numerical simulations (CFD). This branch of fluid dynamics complements experimental and theoretical fluid dynamics by providing an alternative cost-effective means of simulating real processes. It offers the means of testing theoretical advances for conditions often unavailable experimentally or having a prohibitive cost.

To summarize, the book progresses with the aid and support of both experimental results and numerical simulations for a better representation of the structure of convection and moves through very focused examples and situations, many of which are of a prototypical nature (some unpublished and heretofore unseen material is used to support the discussions).

The declared objectives are:

(a) to provide the reader with an ensemble picture of the subject (illustrating the state-of-the-art and providing researchers from universities and industry with a basis on which they are able to estimate the possible impact of a variety of parameters);

(b) to clarify some still unresolved controversies pertaining to the physical nature of the dominant driving force responsible for asymmetric/oscillatory convection in various natural phenomena and/or technologically important processes;

(c) to elucidate some unexpected theoretical kinships existing among fluid-mechanical behaviours arising in different contexts (such a philosophy, in particular, being used in the attempt to build a common theoretical source for the community of fluid physicists under the optimistic idea that an ongoing, mutually beneficial dialogue is established among different branches of research in these fields).

Each chapter of the book deals with a different aspect of the aforementioned topics, providing the necessary background information (i.e. literature, fundamental concepts, equations and mathematical models, information on the experimental and numerical techniques, etc.), focusing on the latest advances, describing in detail the insights into the physics provided by the experiments and/or numerical simulations and introducing (where necessary) theoretical and critical links with the other book chapters and related topics.

As anticipated, the final goal of such a treatise is to help the scientific community significantly in elaborating and validating new, more complex models, in accelerating the current trend towards predictable and reproducible natural phenomena and finally in establishing an adequate scientific foundation to industrial processes which are still conducted on a largely empirical basis.
In practice, the text is conceived in order to be a useful reference guide for other specialists in these disciplines (including professionals in the metallurgy and foundry field; researchers and scientists who are now coordinating their efforts to improve the quality of semiconductor or macromolecular crystals; organic chemists and materials scientists; and atmosphere and planetary physicists) and also an advanced-level text for students taking part in courses on the physics of fluids, fluid mechanics, the behaviour and evolution of nonlinear systems, environmental phenomena and materials engineering. It is directed at readers already engaged or starting to be engaged in these topics. Physicists, engineers, designers and students will find the necessary information and revealing insights into the behaviour of many phenomena (including, as outlined before, both historical developments and very recent contributions).

Finally, it is also worth pointing out that the study of pattern formation (convective flows can form more or less ordered spatial structures) also falls under the broader heading of nonequilibrium phenomena. Beyond practical applications, it is therefore clear that these problems also exert an appeal to researchers and scientists as a consequence of the complexity of the possible stages of evolution, of the nonlinear behaviour and because these organized structures are aesthetically and philosophically pleasing as well as irresistible to theoretical physicists.

This complexity is shared with other systems in Nature and constitutes a remarkable challenge for any theoretical model. Indeed, convection problems are a rich source of material propaedeutical to the development of new ideas concerning the relationship between order and chaos in fluid dynamics and, in general, between simplicity and complexity in the structure and behaviour of systems governed by nonlinear equations.

In view of the foregoing discussion, there is no doubt that elucidating the mechanisms for the formation and evolution of hydrodynamic structures can be regarded as a subject of paramount importance not only for the aforementioned meteorology, oceanography, astrophysics, geophysics and (on a smaller scale) crystal growth, the processing of metal alloys and a variety of other technological processes, but also from an ‘ideological’ synergetic point of view for further progress in the understanding of pattern-forming systems of different nature.

Unlike earlier books on the subject, here, even if partial differential equations and related methods of solution are widely used in the text and CFD is actually at the root of many of the proposed examples, the heavy mathematical background underlying and governing the behaviours illustrated is kept to the minimum. Much of the available space is devoted to the description (both qualitative and quantitative) of the spatial and temporal convection structures, related thresholds in terms of characteristic numbers and to the ‘physics’. This is done under the optimistic hope that such a philosophy may significantly increase the readability of the book and, in particular, make it understandable also to those individuals who are not ‘pure’ fluid physicists or mathematicians.

In the same spirit, the use of jargon is limited as much as possible and most of the mathematical arguments are concentrated in the first chapter (this chapter is devoted to the description of the numerical algorithms used to perform the time integration, to compute directly the steady or oscillatory states and to investigate their stability), allowing readers who are not interested in these aspects to skip them and jump directly into the results.

Marcello Lappa
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This book is a composite of many ideas. It was authored between 2006 and 2009 in the pleasant atmosphere provided by my writing desk and warm lamp at home, especially in the evening and at night.

It was originally conceived (in 2005) as an enriched version of Chapter 2 of my earlier monograph *Fluids, Materials and Microgravity*, published in 2004 by Elsevier Science, for which I was preparing a second edition. After writing about 100 pages, I realized, however, that the subject of thermal convection would deserve its own separate and exhaustive treatment.

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article authors, reviewers, experts in various fields and other Editorial Board members, to whom collectively I also express my appreciation.

As a concluding remark, let me also point out that the overt intention of including so many references (there are more than 1000) is to encourage readers and students to follow up on various details and, most importantly, not to limit their readings to the relatively synthetic and didactic account I have provided here. It is obvious that if one tries to survey the developments of the last 200 years, one cannot follow carefully all the twigs of the tree. It is also evident that one will possibly emphasize some results due to personal taste, interests and experiences. Let me apologize for this right at the beginning.

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1

Equations, General Concepts and Methods of Analysis

1.1 Pattern Formation and Nonlinear Dynamics

Regular structures arise everywhere in Nature and virtually every technological process involves their formation at some stage. By injecting energy into a dynamic system, typically an initial equilibrium state becomes unstable above a certain threshold and, as a result of this instability, well-defined space–time structures emerge.

Beyond the specific situation or system considered, these structures are characterized by a recognizable level of self-organization (i.e. a precise morphology and/or topology in space and/or lines of evolution in time) and under certain idealizations it is natural to consider the process leading to their formation as the life of the considered dynamic system. The features of this life as \( t \to \infty \) then determine the characteristic aspects of these structures, be they perfect or irregular.

In general, there exist, between the limiting purely regular and irregular field distributions in space (and/or time), numerous intermediate situations. One of the most remarkable achievements obtained in recent years is the discovery that these dynamics and the related transitional stages are largely determined by a sort of obscure dialectics between the tendency that every natural system exhibits towards order or disorder, self-organization or chaos. This seems to be an intrinsic feature of the way in which our Universe (and all the dynamic systems which are contained within it) works. Among other things, it also constitutes one of the most fascinating philosophical questions to which humankind is trying to find a decisive answer.

The fact that strikingly well-ordered and similar phenomena are found across disciplines is indeed an important impetus for research in this theoretical field. It stands at the intersection of many scientific branches, which make it a multi-domain field of investigations and a truly interdisciplinary science.

The problem has always been widely open and has been approached from different directions and by different research groups with various backgrounds and perspectives. In particular, the similarity in fundamental mechanisms and the accompanying mathematics has brought together scientists from many fields, such as fundamental fluid dynamics (e.g. Cross and Hohenberg,
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1993), meteorology, oceanography, astrophysics, geophysics, material science (e.g. Langer, 1980), chemistry (e.g. Weaire and Rivier, 1984; Henisch, 1991), surface science (e.g. Zander et al., 1990), biology (e.g. Gierer and Meinhardt, 1972), medicine and so on (the reader is also referred to the discussions in the preface of this book).

This synergy has led over the years to the establishment of a common, elegant theoretical framework that is now generally referred to as the field of pattern formation or, in other acceptations, the study of the related stability and possible evolution.

The above-mentioned commonality, whose most evident articulation has been over recent years the definition of general objectives and a general modus operandi (as discussed below), can be regarded as the spark at the root of the present work.

The principal objectives of such research are (i) the analysis of the hierarchy of instabilities and the birth of various structures in the course of evolution from an initial state, (ii) the investigation of the mutual transformation of these structures as some control conditions are varied and (iii) understanding the cause-and-effect relationships at the root of the observed behaviours.

The common modus operandi consists of a general way of thinking, which, from a more precise mathematical point of view, means the adoption of specific tools of analysis and techniques to be used when the dynamics of interest do not follow linear laws (i.e. are not characterized by a direct proportionality between cause and effect).

Although the above arguments are often used narrowly to describe this field, in general they may be applied to describe more or less everything that happens in the Universe. Hence these statements can hardly be used as rigorous definitions.

In practice, this topic must be placed in a more precise theoretical context by introducing some necessary concepts and notions. Such a theoretical melange is propaedeutical to a better recognition, definition and characterization of the aforementioned phenomena. Also, these general considerations facilitate the subsequent introduction of more complex notions and will significantly help the reader in the understanding of the theoretical explanations and arguments given throughout this chapter. Some of them, such as stability, instability and evolution, have been already used above without providing, however, an adequate basis (we shall come back to these later in this chapter). Other fundamental and propaedeutical ingredients are illustrated and elaborated in Section 1.1.1. Many of them are not independent of one another and the related relationships are difficult to discern, which requires careful treatment.

1.1.1 Some Fundamental Concepts: Pattern, Interrelation and Scale

Given the complexity of the considered topic, following the elegant approach of Bar-Yam (2001), it is convenient to start the discussion from the introduction of three simple (but illuminating) ideas only. The first is the concept of pattern per se. The other ones are the definitions of interrelation and scale.

To some extent, these concepts simplify the problem by abstracting from specific cases the features which are essential in the description of pattern formation. In the process of abstraction we get a more general problem in which thermal convection (the subject of this book) is just one effective realization.

A pattern is

- a set of relationships that can be identified by observations of a system, or an ensemble of sub-systems
- a simple type of emergent property of a system, where a pattern is a feature of the system as a whole but does not apply to constituent sub-parts of the system.
- a property of a system by which the description of the system becomes relatively simple and short with respect to detailing the characteristics of its components.
A simple type of pattern is a repetitive structure in space. Shifting the view by one repeat length leads to seeing the same thing (this may occur along a single direction or along more than one direction). Similarly to repeating patterns in space, we can also have a repeating pattern in time (this may occur in the form of a simple harmonic process or as the superposition of many of these behaviours with different amplitude and frequency). Generally, a pattern can have both features.

We also think of patterns as prototypes or exemplars. This is the sense in which we use it to describe a given structure (in space or in time) with well-defined features. In this case the pattern is not about the relationships within the structure, but about the possibility of repeating such a scenario many times in certain (well-defined and reproducible) circumstances.

The connection between the pattern as repetition and the pattern as prototype is just like the relationship between two types of properties: properties that appear as a consequence of the mutual interference among components of a system and properties that arise from interaction of a system with its environment (the larger system of which it is a part).

**Interrelation** is

- what parts of a system do as a consequence of mutual interplay that they would not do by themselves: collective behaviour
- what a system does by virtue of interaction with its environment that it would not do by itself, for example its function.

According to the first statement, interrelation refers to understanding how ensemble properties arise from the cooperative behaviour of parts. More generally, it refers to how behaviour at a larger scale of the system arises from detailed structures and interdependencies on a finer scale. In practice, it is about how a macroscopic scenario arises from microscopic behaviours (for interesting effective examples in various fields not covered by the present book, the reader is referred to, for example, Piccolo et al., 2002; Carotenuto et al., 2002; Lappa et al., 2002, 2003b, Lappa, 2002b, 2003c,d, 2005c; Lappa and Castagnolo, 2003; and references cited therein).

According to the second statement, interrelation refers to all the properties that we assign to a system due to interaction between it and its environment.

In practice, the second aspect of interrelation may be linked theoretically to the first aspect because the system can be viewed along with parts of its environment as together forming a larger system. The collective behaviours due to the relationships of the larger system’s parts reflect the relationships of the original system and its environment. In general, however, there is a tendency to separate expressly the interdependence between the components of a system that creates its recognizable identification (i.e. the pattern) from its environment: The point of transition from the system to its environment is generally referred to as the ‘boundary’ of the system; such a boundary, together with its functions, that is, the related protocols of interaction with the external environment, are typically regarded as an additional property of the considered system.

**Scale** is

- the size of a system or an appropriate reference quantity for a property that one is describing
- the required precision of observation or description.

A somewhat related concept is that of *scaling* or *scalings* that refer to some general analytical relationships which can be established between certain properties of the considered system and fundamental reference quantities (e.g. a length scale).

Additional useful and important ideas such as dissipative structures, stability, bifurcation, uniqueness, multiplicity of solutions and attractor will be introduced in the following sections as required and with an increasing degree of complexity as the discussion progresses. It will be illustrated how these interwoven definitions can be applied to systems that are vastly different in their meaning, shape, scales and physics.
In particular, starting from the derivation of the governing (balance) equations of a dynamic system from the microscopic collective behaviour of its molecules, it will be shown how all these concepts have extensive background application at large scales (when discussing the properties of the natural patterns provided by laboratory or numerical experiments) and again at relatively small scales (both in space and time) when the considered system approaches a special condition known as ‘spatiotemporal chaos’ in which it exhibits an increasing degree of complexity and finer (sub-)structures.

1.1.2 PDEs, Symmetry and Nonequilibrium Phenomena

From a purely mathematical point of view, in typical pattern-formation phenomena organized structures are formed due to intrinsic nonlinearities of the considered system.

It is a well-known and universally recognized concept that Nature does not follow a linear pattern, and linearity, if it exists in Nature, is a special case of nonlinearity.

Trying to provide a definition for nonlinearity (or of nonlinear science) makes almost no sense given the excessive level of abstraction that would be required by such an attempt.

From an intuitive standpoint, however, nonlinearity can be regarded as ‘a feedback loop’ acting as an intrinsic property of the system that feeds information back into the system where it is iterated or used multiplicatively.

This feedback loop is created when, as explained before, the system parts are connected in a network of specialized functions. This leads to collective behaviours more complex than those of the individual constituent components; the related feedback loop and iterative process make the system extremely sensitive to its (even though very small) internal variations. It is by virtue of these mechanisms that these systems contain their own capacity for transformation (requiring only the right conditions for activation) and that we speak about nonlinear behaviour.

In general, studies of pattern formation use a common set of fundamental concepts to describe how non-equilibrium processes cause structures to appear. The theoretical starting point is usually a set of deterministic equations governing the possible evolutionary progress of the considered system. Obviously, these equations, typically in the form of partial differential equations (PDEs), are nonlinear.

As explained above, nonlinearity of these equations reflects how the system parts interfere with one another exchanging some kind of information. This, however, is not the only factor playing a significant role. In canonical studies on these subjects the nonlinear model equations are often considered on finite spatial domains and (according to the earlier discussion on the concept of interrelation, Section 1.1.1) need a specification for the system interaction with its environment. These interactions are generally modelled as additional mathematical constraints known as ‘boundary conditions’. Obviously, these conditions are also vital in determining the pattern-selection processes and underlying mechanisms.

It is also worth noting that, beyond the mathematical form (i.e. the functional dependences relating the system properties to those of the environment) of the these protocols of interaction, the spatial shape of the system boundary per se can significantly enter the dynamics (e.g. Lappa et al., 2002; Lappa, 2005a,b, 2006a).

Along these lines, over the years simplified (easy to handle) configurations (where well-established parameters can be fixed and the behaviour of the system in response to changes of these parameters can be investigated) have been conceived by researchers. In general, well-defined geometric shapes make mathematical analysis and computations simpler and some boundary conditions are more attractive than others. For these reasons they have enjoyed widespread use in the definition and ensuing analysis of this subject.
These simple geometric domains and mathematically friendly boundary conditions usually imply symmetry. Such symmetries may be present because of the domain geometry or as a result of some modelling assumptions (large systems are often discussed using periodic boundary conditions).

Symmetry is a very important ingredient (together with nonlinearity) in pattern formation phenomena.

The aforementioned partial differential equations are often invariant under some groups ($G$) of Euclidean transformations (translations, rotations and reflections of the physical space). Any PDE that is posed on a domain and is invariant under a group $G$ will inherit those symmetries in $G$ that preserve the domain and the boundary conditions (symmetries enter into problems of this type from the invariance properties of the governing equations and the shape of the boundary of the considered system, the container in the case of a fluid).

Remarkably, the existence of these symmetries implies the possibility of symmetry breaking, which is one of the fundamental concepts at the root of pattern formation phenomena (it is strictly associated, in particular, with some fundamental companion notions such as stability and bifurcation that will be treated later in this chapter together with related tools of analysis).

Although much progress towards possible techniques for the integration of the governing equations and the study of stability and bifurcation of related solutions has been achieved in recent years, fundamental challenges remain, many of which are of a ‘philosophical’ or ‘archetypical’ nature.

Systems that are driven out of equilibrium often show similar patterns, although the underlying processes can be quite different. One challenge is to find measures that can quantitatively assess the similarity of different patterns.

The deep question of whether universality classes exist for patterning behaviour, however, is still unanswered. The characterization of dynamics that are complex in both space and time (the aforementioned spatiotemporal chaos, Section 1.1.1) is far from complete. It is known that sudden changes from ‘normal’ to alternate realities are common. A minute change in one variable can yield a vastly disproportionate change in the system at a later time (Section 1.8.3).

In some situations, these systems are deterministic (i.e. there is a unique, well-defined consequent to every state), but in other circumstances they exhibit a stochastic or random behaviour (there is more than one consequent chosen from some probability distribution, for example the ‘perfect’ coin toss has two consequents with equal probability for each initial state).

Some researchers have modelled some of these behaviours as the patterns formed by nonlinear systems were controlled by one or more ‘attractors’ (and it is known that more complex patterns, such as fractals, are formed by strange attractors), but the underlying mechanisms are still obscure.

In such a context, fluid convection induced by body and/or surface forces can certainly be regarded as one of the most distinguished physical phenomena to test existing theories and concepts and probe new ideas about dynamic systems.

First studies of these subjects can be tracked back to almost 2000 years ago. Indeed, the origin of the word convection should be ascribed to the Latin word convectiones which means ‘transport’, and the word thermal has its root in the Greek prefix thermo- ($\theta\epsilon\rho\mu\delta\varsigma$, meaning heat, hot, warm) and/or in the derived Latin word thermanticus, (meaning ‘which transports heat’).

Over the last century, fluid dynamics has motivated much of the basic research on pattern formation and books are still being published on this subject. As an example, every year the international journal The Physics of Fluids devotes one issue to illustrate the variety and beauty of natural fluid flows (under the heading ‘a gallery of fluid motion’); the formation of patterns in fluids is also the primary focus of journals focused expressly on technological and industrial applications (the international journal Fluid Dynamics and Materials Processing, above all).
Indeed, convection problems of the type considered in the present book (thermogravitational, thermal Marangoni and thermovibrational flows) can provide fundamental information on the relationship between determinism and chaos in fluid dynamics and, in general, between simplicity and complexity in the structure and behaviour of systems governed by nonlinear equations.

In the case of fluids, the governing equations correspond to the Navier–Stokes equations, one of the most intensively studied set of PDEs.

1.2 The Navier–Stokes Equations

1.2.1 A Satisfying Microscopic Derivation of the Balance Equations

The Navier–Stokes equations, named after Claude-Louis Navier and George Gabriel Stokes, describe the motion of fluid substances such as gases, liquids and even solids of geological sizes and time-scales. These equations establish that changes in momentum in infinitesimal volumes of fluid are simply the sum of dissipative viscous forces, changes in pressure, gravity, surface tension (in the presence of a free surface) and other forces acting on the fluid: an application of Newton’s second law (Navier, 1822; Stokes, 1845).

They are one of the most useful sets of equations because they describe the physics of a large number of phenomena of academic and practical interest. They may be used to model weather, ocean currents, flow around an airfoil (wing), fluid motion inside a crucible used for crystal growth or for the treatment of metal alloys, blood flow in an artery and even motion of stars inside a galaxy.

Although fluid dynamics is a well-established discipline, its focus has shifted over the years and the range of applications has diversified. As such, these equations, in both full and simplified forms, are used in the design of aircraft and cars, the study of natural convection, the design of power stations, the analysis of the effects of pollution, the study of biokinetics of protein crystals (e.g. Lappa, 2003b, 2004d, 2005c) and the biomechanics of biological tissues (e.g. Lappa, 2003e, 2004e, 2006b) and so on. Coupled with Maxwell’s equations, they can be used to model and study magnetohydrodynamics in typical problems of crystal growth or Earth-core dynamics.

There are many ways to derive these equations. They can be introduced starting directly from the conservation of mass and momentum being written for an arbitrary macroscopic control volume (this is the usual ‘point of view’ taken by engineers), as an application of Newton’s second law to a continuum (this is the usual ‘point of view’ taken by physicists). In these treatments, the (geometric) continuum hypothesis is invoked from the start (the underlying idea is that ‘matter’ occupies all points of the space of interest and that properties of the fluid can be represented by piecewise continuous functions of space and time, as long as length and time scales are not too small).

The Navier–Stokes equations can be also derived from microscopic models, i.e. by obtaining these classical partial differential equations as the scaling limits of large microscopic systems (the mathematician’s point of view). The latter strategy provides a wealth of additional aspects that are overlooked or somehow ‘hidden’ when using other approaches (e.g. the meaning of the ‘mass velocity’, the relationship between the stress tensor and the exchange of momentum at a molecular level) and which otherwise have to be introduced on empirical bases.

Here the goal is to stake out some common ground by providing a synergetic synthesis of the distinct approaches/points of view.

Towards this end, it is worth noting that the microscopic approach for deriving the Navier–Stokes equations can be elaborated in its simplest form by reinterpreting (at a different length scale) the descriptive models originally introduced for Maxwell’s equations, that is, explaining the macrophysical properties of fluids based on microscopic models of their constituent particles (i.e. deriving thermodynamic and hydrodynamic limits for stochastic particle systems, i.e. ‘building’ a macroscopic state from microscopic statistics).
Lorentz (1902) was the first to give a derivation of Maxwell’s equations in material bodies from the fundamental equations of his electron theory by averaging the microscopic field quantities over physically infinitesimal space and time regions (a century ago, Lorentz deduced the macroscopic Maxwell equations by spatially averaging a set of postulated equations for the microscopic electromagnetic field). This procedure has with only slight modifications been taken over by various authors. A straightforward derivation of Maxwell’s equations from electron theory was given by Mazur and Nijboer (1953) on the basis of ensemble averaging. The formalism used was analogous to that applied by Kirkwood (1946) and Irving and Kirkwood (1950).

This philosophy gives justice to the fundamental discontinuous nature of matter. Moreover, it allows the establishment of a fruitful theoretical link to the concepts elaborated in Section 1.1.

At first glance, recalling the ideas illustrated in Section 1.1.1, the infinite variety of flow patterns and convective spatiotemporal structures displayed by fluids could be simply regarded as the ensemble behaviour created by the collective motion of the molecules of which the considered fluid consists.

It will be shown in the following sections how, at a deeper level of analysis, an intimate correspondence can be established between the theoretical concept of the set of system parts mentioned in Section 1.1.1 (connected in a network of specialized functions responsible for nonlinear dynamics) and a set of elementary volumes (or parcels) of fluid exchanging at any instant mass, momentum and energy such as the biological cells of a living organism (e.g. Lappa, 2008).

Remarkably, such exchange is basically responsible for the nonlinear nature of the Navier–Stokes equations. The macroscopic protocols of interaction among the various subparts (the so-called convective fluxes introduced in Section 1.2.3), in fact, admit mathematical representation in which some of the system variables are involved multiplicatively.

Not to be too cryptic and to prevent the flavour being too philosophical, hereafter the discussion progresses with the support of precise mathematical arguments.

1.2.2 A Statistical Mechanical Theory of Transport Processes

As outlined before, in their final form the Navier–Stokes equations assume a fluid to be a continuum, whereas in reality a fluid is a collection of discrete molecules. To model the underlying microscopic physics, statistical mechanics begins considering the characterization of a generic ensemble of \( N \) particles as defined in classical mechanics, that is, in terms of the complete specification (at a given instant) of the individual particle position \( \mathbf{r}_i \), particle mass \( m_i \) and velocity \( \mathbf{c}_i \); moreover, the following obvious relationships are used (a microscopic application of Newton’s laws):

\[
\sum_{i=1}^{N} m_i = \text{constant} \quad (1.1a)
\]

\[
f = m_i \frac{d\mathbf{c}_i}{dt} \quad (1.1b)
\]

The considered system consisting of \( N \) particles is assumed to be hosted in a generic volume \( D_{\text{REV}} \) (further necessary information on the nature of this volume will be provided later in this section).

In the following, the generic quantity associated with a single particle is denoted by \( \Pi_i \), and its time derivative by \( \dot{\Pi}_i \). Moreover, given a generic function \( a \), the symbol \( < a > \) is used to indicate its ‘average’ value from a stochastic standpoint.

In such a context, the density of the generic quantity \( \Pi_i \) is introduced as a function \( P_{\Pi_i}(\mathbf{r}, t) \) defined in such a way that its integral computed over the domain \( D_{\text{REV}} \) gives the stochastic average value of the sum of all the quantities \( \Pi_i \) related to the particles hosted in \( D_{\text{REV}} \).

From a mathematical point of view, the definition of the density function \( P_{\Pi_i}(\mathbf{r}, t) \) can be based on the well-known Dirac function \( \delta(r) \) [whose properties are: \( \delta(s) = 0 \) for \( s \neq 0 \), \( \delta = \infty \) for \( s = 0 \)].
and $\int_D \delta dD = 1$ if the generic domain $D$ contains the origin $s = 0$. It reads

$$P_{\Pi}(\mathbf{r}, t) = \left\langle \sum_{i=1}^{N} \Pi_i \delta(\mathbf{r} - \mathbf{r}_i) \right\rangle$$

(1.2)

In fact, taking into account the properties of the Dirac function:

$$\int_{D_{REV}} P_{\Pi}(\mathbf{r}, t) dD = \left\langle \sum_{i=1}^{N} \Pi_i \int_{D_{REV}} \delta(\mathbf{r} - \mathbf{r}_i) dD \right\rangle = \left\langle \sum_{i=1}^{N} \Pi_i \right\rangle$$

(1.3)

which satisfies the definition given above for $P_{\Pi}(\mathbf{r}, t)$.

By taking the derivative with respect to time of Eq. (1.2):

$$\frac{\partial}{\partial t} P_{\Pi}(\mathbf{r}, t) = \left\langle \sum_{i=1}^{N} \left[ \Pi_i \delta(\mathbf{r} - \mathbf{r}_i) + \Pi_i \frac{\partial}{\partial t} \delta(\mathbf{r} - \mathbf{r}_i) \right] \right\rangle$$

(1.4)

and since from a mathematical point of view

$$\frac{\partial}{\partial t} \delta[\mathbf{r} - \mathbf{r}_i(t)] = \frac{\partial}{\partial \mathbf{r}} \delta[\mathbf{r} - \mathbf{r}_i(t)] \frac{\partial}{\partial t} [\mathbf{r} - \mathbf{r}_i(t)] = -\mathbf{c}_i \cdot \nabla \delta(\mathbf{r} - \mathbf{r}_i)$$

(1.5)

Eq. (1.4) becomes

$$\frac{\partial}{\partial t} P_{\Pi}(\mathbf{r}, t) = \left\langle \sum_{i=1}^{N} \left[ \Pi_i \delta(\mathbf{r} - \mathbf{r}_i) - \Pi_i \nabla \cdot [\mathbf{c}_i \delta(\mathbf{r} - \mathbf{r}_i)] \right] \right\rangle$$

(1.6)

Introducing

$$\Phi_P = \left\langle \sum_{i=1}^{N} \left[ \Pi_i \mathbf{c}_i \delta(\mathbf{r} - \mathbf{r}_i) \right] \right\rangle$$

(1.7a)

$$P^* = \left\langle \sum_{i=1}^{N} \left[ \Pi_i \delta(\mathbf{r} - \mathbf{r}_i) \right] \right\rangle$$

(1.7b)

Eq. (1.4) can be rewritten as

$$\frac{\partial}{\partial t} P_{\Pi}(\mathbf{r}, t) + \nabla \cdot \Phi_P = P^*$$

(1.8)

which is known as the general balance equation, where $\Phi_P$ and $P^*$ are known as flux density and production density, respectively. In such an equation $P_{\Pi}(\mathbf{r}, t)$ and $P^*$ have the same tensorial order (e.g. both are scalars or vectors), whereas $\Phi_P$ has a larger order [e.g. it is a vector if $P_{\Pi}(\mathbf{r}, t)$ is a scalar and becomes a tensor with order two when $P_{\Pi}(\mathbf{r}, t)$ has order one].

At this stage, some additional insights can be provided about the 'nature' of the volume $D_{REV}$ used for determining Eq. (1.8). In classical thermodynamics, the problem of deriving governing laws is typically investigated in the limit as $N \to \infty$ and $D \to \infty$, while the density $n = N/D$ remains constant (this is called the thermodynamic limit).

The various properties of the system are separated into extensive and intensive quantities. Extensive quantities are proportional to the effective size of the system, whereas intensive quantities are independent of the size of the system (this reflects the intuition that local properties of a macroscopic object do not depend on the size of the system). As a relevant example, all the quantities appearing in Eq. (1.8) are intensive macroscopic quantities.