Understanding Complex Systems

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Santo Banerjee
Lamberto Rondoni *Editors*

Applications of Chaos and Nonlinear Dynamics in Science and Engineering - Vol. 4

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Understanding Complex Systems

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Applications of Chaos and Nonlinear Dynamics in Science and Engineering - Vol. 4

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Preface

This is the fourth volume of the collection of essays entitled *Applications of Chaos and Nonlinear Dynamics in Science and Engineering*, which has been addressed to Master and Ph.D. Students, as well as to specialists of disciplines other than the hard sciences, in order to help them familiarize with the theory and the applications of nonlinearity, and its use in describing complex phenomena.

As illustrated in the previous volumes, terms such as nonlinear dynamics, chaos and complexity have pervaded the vocabulary of almost all fields of science and technology. As a matter of fact, current mathematical descriptions of evolving phenomena consist of nonlinear ordinary or partial differential equations, of various kinds of stochastic processes and of nonlinear space and time discrete iterative schemes. In the deterministic cases, a typical situation is that in which the propagation of uncertainties is exponential in time, a phenomenon known as sensitive dependence on initial conditions, and concisely and suggestively called deterministic chaos.

To understand the reasons why certain terms have become common in many different fields, it suffices to observe that nonlinearities appear in feedback phenomena, which are ubiquitous in nature, and generically in the evolution equations of systems consisting of interacting parts or interacting with an external environment. Furthermore, any measurement one may perform, like any estimate of the initial state of any material object, is bound to be affected by uncertainties, which propagate in time leading to the conclusion that a degree of unpredictability is intrinsic, in practice as well as in principle, to all time dependent phenomena. For this reason, the study of nonlinear evolutions is commonly associated with statistical concepts, and relies on measures such as the Lyapunov exponents and various kinds of dynamical entropies.

In the previous volumes, we have presented a vast collection of examples, treated explicitly and in moderately technical terms. Indeed, these concepts have in the past decades turned useful in countless practical applications—beyond the mathematical and physical literature in which they have been mostly developed—ranging from engineering to biology, medicine, computer and telecommunication sciences, etc. We have thus followed an approach which we deem suitable to a vast

readership, proposing essays written in the form of tutorials. In this last volume, we complete our survey and introduction to nonlinear, chaotic and complex phenomena, considering some issues of higher theoretical content than in the previous volumes, but preserving the mildly technical style of the previous volumes.

Part I concerns nonlinearities in transport of energy and matter, with one contribution by L. Stricker and L. Rondoni on models of heat transport and their mechanical properties, one contribution on the general theory of diffusion, by G. Boffetta, G. Lacorata and A. Vulpiani, and one contribution by M. Colangeli on the relation between the Boltzmann equation and hydrodynamics.

In Part II, we have three contributions on chaos and synchronization in complex networks: one by J. Stroud, M. Barahona and T. Pereira on modular networks, one by P. Carl on the evolution of climate, and one by A. Tai and S. Jalan on the use of random matrices. The chapters are well illustrated with recent developments on the subject area and possible practical applications.

Part III has two contributions on phase space reconstruction and on biological patterns, respectively, by S. K. Palit, S. Mukherjee, S. Banerjee, M.R.K. Ariffin and D. K. Bhattacharya, and by M. Banerjee. The theories are well illustrated and supported with analytical and numerical results.

Part IV concerns the use of chaos in field programmable gate arrays. This chapter is very useful as an introduction to the subject area.

We hope that this collection of examples, combined with those reported in the previous three volumes have covered a sufficiently wide spectrum of subjects, in terms suitable to a wide audience, interested in importing dynamical concepts in their disciplines, without recourse to sophisticated mathematical tools. The concepts of nonlinear dynamics are indeed proving more and more useful in all fields of research.

Serdang, Malaysia S. Banerjee
Torino, Italy L. Rondoni
26 January 2015

Contents

Part I Nonlinearity in Transport, Mechanical Models and Hydrodynamics

1 Microscopic Models for Vibrations in Mechanical Systems Under Equilibrium and Non-equilibrium Conditions 3
Laura Stricker and Lamberto Rondoni

2 Chaos, Transport and Diffusion 31
Guido Boffetta, Guglielmo Lacorata, and Angelo Vulpiani

3 Small Scale Hydrodynamics 65
Matteo Colangeli

Part II Chaos, Synchronization and Complex Networks

4 Dynamics of Cluster Synchronisation in Modular Networks: Implications for Structural and Functional Networks 107
Jake Stroud, Mauricio Barahona, and Tiago Pereira

5 Synchronous Motions Across the Instrumental Climate Record 131
Peter Carl

6 Application of Random Matrix Theory to Complex Networks 195
Aparna Rai and Sarika Jalan

Part III Attractor Reconstructions and Ecology/Biological Patterns

7 Some Time-Delay Finding Measures and Attractor Reconstruction ... 215
Sanjay Kumar Palit, Sayan Mukherjee, Santo Banerjee, M.R.K. Ariffin, and D.K. Bhattacharya

8 Turing and Non-Turing Patterns in Two-Dimensional Prey-Predator Models 257
Malay Banerjee

Part IV Chaos and Field Programmable Gate Array

9 Realizing Chaotic Systems on Field Programmable Gate Arrays: An Introduction 283
Bharathwaj Muthuswamy and Santo Banerjee

Part I
Nonlinearity in Transport, Mechanical Models and Hydrodynamics

Chapter 1
Microscopic Models for Vibrations in Mechanical Systems Under Equilibrium and Non-equilibrium Conditions

Laura Stricker and Lamberto Rondoni

Abstract Equilibrium Thermodynamics studies states of macroscopic objects that do not change in time when isolated from their environment. This requires chemical, mechanical and thermal equilibrium which together amount to thermodynamic equilibrium. A non-equilibrium state can be established putting the system in contact with more than one reservoir of heat, mass, or other physical quantities. The dynamical evolution of a system of particles representing a macroscopic bar in both equilibrium and non-equilibrium conditions is illustrated by means of a simple one-dimensional molecular dynamics model, illustrating how macroscopic phenomena may be qualitatively understood with microscopic toy models. In particular, a system of hard point-particles undergoing only binary collisions is considered. A conservative force is applied on one of the end particles to reproduce the cohesion of the bar. Non-equilibrium conditions are obtained by adding two deterministic thermostats acting on the first and on the last particle of the bar. In the equilibrium case, we determine the values of macroscopic and microscopic proprieties of the system, such as length, linear density, specific kinetic energy, average energy per particle, and position of the centre of mass of control groups located in different parts of the bar. In the non-equilibrium case, we focus on length oscillations, and we demonstrate their dependence on the characteristic parameters of the thermostats. Although highly idealized, this model reproduces an important qualitative aspect of metal bars: hardening.

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1.1 Introduction: Thermal Baths

Chains of oscillators constitute a very popular kind of models, used to understand the behaviour of macroscopic objects from the point of view of their microscopic constituents. The first of these models is the Fermi–Pasta–Ulam model [9], which consists of a linear chain of interacting particles providing a minimal framework for studies of ergodicity, dynamical relaxation and diffusion laws, with given interparticle interaction potentials, initial and boundary conditions [3, 10, 13]. In this tutorial, we demonstrate that the conceptually simple framework of one-dimensional N-particle systems can be consistently used to model the qualitative thermo-mechanical behaviour of solids. In particular, we consider a chain of particles, with one fixed and one free end, to study the variations of length, in response to external forces or to temperature changes. We provide both theoretical considerations and numerical results from molecular dynamics simulations, which allow direct access to any quantity of interest. These kinds of chains have been considered mostly to study heat conduction, cf. [3, 10, 13] for recent reviews on the subject, and [4–6] for some of the few works on thermo-mechanical properties.

In the theoretical study of statistical mechanics, a proper modelling of the interaction with thermal reservoirs has a crucial role. At equilibrium, this is usually done by means of well-established methods, such as the micro-canonical molecular dynamics and Monte Carlo simulations. Out of equilibrium, the lack of a general theoretical framework enforces the definition of the interaction with thermal baths. From a conceptual point of view, the procedure requires considering non-equilibrium states in the infinite system limit. For example, one could imagine to have an infinite chain of particles, with initial conditions such that all the atoms on the right and those on the left of a certain finite subset are in equilibrium at different temperatures. The subset defines the system that we want to study. However, the only case in which the above mentioned approach can be fully worked out is the case of harmonic chains [14–17]. In such a system, it is possible to derive the degrees of freedom corresponding to the reservoirs' dynamics. Therefore the existence of stationary non-equilibrium states of the system can be proved at the cost of dealing, however, with arbitrarily large energy fluctuations. In general, when non-linear effects appear, the evolution of the heat baths cannot be described anymore by means of standard techniques. However, non-linear chains can still be studied, by assuming that the non-linearity is restrained to the system of interest, while the semi-infinite particle chains (i.e. the two reservoirs) can undergo only linear interactions [1].

Following this approach, the existence of an invariant measure (not explicitly know) has been proved for non-equilibrium systems, in chains of highly non linear coupled oscillators undergoing large temperature gradients [8]. This is analogous to energy conservation in equilibrium systems.

1.1.1 Stochastic Baths

A traditional way to implement the interaction with reservoirs is the introduction of simultaneous random forces and dissipation, in agreement with the fluctuation-dissipation theorem. Hence, the reservoirs are not influenced by the dynamics of the system. For instance, in the case of a chain of particles with equal mass m, the following system of Langevin equations is derived:

$$m\ddot{q}_i = F\left(q_i - q_{i-q}\right) - F(q_{i+1} - q_i) + (\xi_+ - \lambda_+\dot{q}_i)\,\delta_{i1} + (\xi_- - \lambda_-\dot{q}_i)\,\delta_{iN} \tag{1.1}$$

where $(\xi_+ - \lambda_+\dot{q}_i)\,\delta_{i1}$, $(\xi_- - \lambda_-\dot{q}_i)\,\delta_{iN}$ are the forces acting respectively on the first and the Nth particle.

λ_- and λ_+ are the dissipation coefficients producing the slowing down forces $-\lambda_+\dot{q}_i\delta_{i1}$, $-\lambda_-\dot{q}_i\delta_{iN}$. ξ_- and ξ_+ are the independent Wiener processes (stochastic forces) with vanishing average, and variance $2\lambda_\pm k_B T_\pm$, with T the absolute temperature and k_B the Boltzmann constant. For non-linear forces, this model can be treated only numerically.

Once the non-equilibrium steady state condition is reached, the average heat flux can be derived from the temperature profile. The average energy exchanged between the first particle and the adjacent reservoir is the *heat flux j*

$$j\,(\lambda, N) = \frac{\lambda_+}{m_1}\,(T_+ - T_1)$$

Similarly at the other extreme of the system of interest. Then, at the microscopic level one commonly considers each reservoir as an ideal one-dimensional gas of particles with mass $M_\pm$, interacting with the chain through elastic collisions [18]. A simple strategy consists in selecting a random sequence of instants t_i, in which every thermostated atom collides with a particle of the corresponding reservoir. A natural choice for the distribution $W(\tau)$ of the intervals τ among consecutive collisions is the Poissonian distribution

$$W\,(\tau) = \frac{1}{\tau}e^{-\frac{\tau}{\overline{\tau}}}$$

with $\overline{\tau}$ the average collision time. If we consider the reservoir positioned on the left of the system of interest, the velocity of the first particle changes due to collisions from $\dot{q}_{1B}$ (before collision) to $\dot{q}_{1A}$ (after collision)

$$\dot{q}_{1A} = \dot{q}_{1B} + \frac{2M_+}{m + M_+}\,(v - \dot{q}_{1B})$$

where the gas particles velocity v is a random variable with a Maxwellian probability distribution $P(v)$

$$P_+(v) = \sqrt{\frac{M_+}{2\pi k_B T_+}} \cdot e^{-\frac{M_+ v^2}{2k_B T_+}}$$

When $M_\pm = m$, the procedure simplifies and it amounts to equating the particle velocity after collision to the random variable v, so that the colliding particles merely exchange their velocities. In the limit case $M_\pm << m$, the interaction with the heat baths become of Langevin kind, as in (1.1), with $\lambda_\pm = 2M_\pm/\overline{\tau}$. This method is computationally easier, because it does not imply dealing with stochastic differential equations and integration can be performed with conventional algorithms. Moreover, it is physically consistent, because damping is not imposed a priori in the model, but is intrinsically generated by the dynamics. A similar approach, consists in determining the collision times for the interaction with "thermal walls" located at the two extremes of the particle chain. This method has the advantage of allowing the inclusion of pressure effects. In this case, the velocity of the thermostated particles is randomized at every collision with the wall. The sign of the component of the velocity normal to the wall has be inverted, while its absolute value must be distributed following a Maxwellian distribution centered on the wall temperature [19].

1.1.2 Deterministic Baths

Different kinds of deterministic heat baths are commonly used [7, 11] in order to give a self-consistent description of non-equilibrium processes and to overcome the difficulties related to stochastic processes. Two possible modelling strategies are the application of the thermostating forces only to the extremes of the particles chain or to the whole chain.

1.1.2.1 Application of Forces to the Extremes of the Particle Chain

Non-equilibrium conditions are reached by applying two forces at the extremes of the particles chain. The most popular scheme in the molecular dynamics community is the *Nosè–Hoover thermostat* [7]. With this thermostat, the evolution of the particles in contact with the thermal bath α is governed by the equation:

$$m\ddot{q}_i = F(q_i - q_{i-1}) - F(q_{i+1} - q_i) - \begin{cases} \zeta_+ \dot{q}_i & if \quad i \in S_+ \\ \zeta_- \dot{q}_i & if \quad i \in S_- \end{cases} \tag{1.2}$$