FOCUS ISSUE: Chaos and Irreversibility

Chaos and irreversibility: Introductory Comments

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In the last few years, novel approaches from the theory of dynamical systems and chaos have been successfully applied to nonequilibrium statistical mechanics and thermodynamics. On the other hand, the advent of fast computers has greatly broadened the possibilities of simulating nonequilibrium molecular systems and hence of establishing connections between microscopic level dynamical properties and macroscopic behavior. The convergence of these results is shedding new light on the long-standing problem of irreversibility and its relationship to the microscopic chaos in the motion of atoms and molecules in matter. This field of research is today undergoing a rapid development at the frontier of mathematics, physics and chemistry.

An International Graduate School and Workshop was organized at the Bolyai College of the Eötvös University, Budapest on the subject of CHAOS AND IRREVERSIBILITY (Classical Aspects) in August 31–September 6, 1997 under the auspices of the Eötvös University, the International Erwin Schrödinger Institute (Vienna), and the European Commission's Training and Mobility of Researchers Program. The aim of the school was to give an introduction to this new field, whereas in the workshop the most recent results were presented.

One of the most gratifying outcomes of this event was to achieve a balance among the three above-mentioned subject areas. Excellent opportunities were provided for better understanding and comparing the different approaches, and for assessing the limits of their validity. Moreover, consensus was achieved for the first time on key questions such as:

- Microscopic chaos plays an important role in the onset of transport processes and hence in the origin of irreversible behavior.
- Equilibrium states and nonequilibrium steady states are associated with completely different structures (smooth and fractal, respectively).
- Low-dimensional model dynamical systems can be extended to emulate spatially extended dynamics modeling transport processes. This also provides interesting insights on how entropy and entropy production-like quantities can emerge from the dynamics.

In a subject experiencing such rapid development, it was also natural to encounter different views, sometimes opposing but more often complementing each other. This was the case, for instance, when modeling nonequilibrium steady states, either through time-reversible but dissipative dynamics or via a purely conservative dynamics in which nonequilibrium is introduced by deterministic boundary conditions. Coarse graining was a second such issue. Some authors hold the view that mapping the deterministic dynamics into a probabilistic process by projecting onto a partition or by accounting for noise and/or fluctuations allows one to incorporate several key concepts. Others objected to this view on the grounds that it coarsens the fine, multifractal structure of the invariant manifolds. Related to this is, finally, the ''minus sign'' question: how to cope with the fact that the Gibbs entropy's time derivative is negative in a dissipative system—just the type of systems for which one would expect to find a positive entropy production.

The present focus issue contains papers written by invited speakers to the Budapest School and Workshop including two colleagues who were unable to attend. We regret that limitations of space did not allow us to incorporate all the workshop contributions and to open the issue to other potential contributors.

The contributions are about equally divided between reviews on the subject, usually ending with recent unpublished results, and research articles. The first article, by G. Nicolis and D. Daems, starts with a general survey of the probabilistic aspects of dynamical systems. It concludes with some new results on the connection between entropy production and phase space dynamics using the probabilistic approach.

The remaining articles can be grouped according to four broad categories:

- Thermostatted systems (G. Morriss and C. Dettmann; D. Searles, D. Evans, and D. Isbister; Ph. Choquard; E. G. D. Cohen and L. Rondoni; W. G. Hoover and H. Posch).
- General properties of nonequilibrium systems from a dynamical system point of view (L. Rondoni and S. Stöcker; G. Gallavotti; S. Goldstein, J. L. Lebowitz, and Ya. Sinai).
- Simple map models for transport, reactive and other irre-

versible processes (W. Breymann, T. Tél, and J. Vollmer; P. Gaspard and R. Klages; S. Tasaki, T. Gilbert, and J. R. Dorfman).

- Methods for computing the various indicators of microscopic chaos in many-particle systems (J. R. Dorfman, A. Latz, and H. van Beijeren; Lj. Milanovic, H. Posch, and W. G. Hoover).

We hope that the present focus issue of *Chaos* will serve as a jumping off point for new ideas and new developments in this field.