

NONLINEARITY, FLUCTUATIONS, AND COMPLEXITY

Université Libre de Bruxelles, Bruxelles, Belgique

March 16-19, 2005

Summary

The conference “Nonlinearity, Fluctuations, and Complexity” was held at the Université Libre de Bruxelles from March 16 till March 19, 2005. It gathered 93 participants among which 35 speakers for an overview of the state of the art in our understanding of nonlinear phenomena and complex systems on the basis of the physico-chemical laws of thermodynamics, statistical mechanics, and the theory of stochastic processes.

During the conference, experts on both theoretical and experimental aspects of reaction-diffusion systems, complex systems, nonlinear dynamics, stochastic processes, mesoscopic systems, as well as classical and quantum statistical mechanics have presented their most recent results and discussed of their implications and applications. The interdisciplinary character of the conference was the occasion for the cross-fertilization of the different disciplines. Moreover, the conference has also contributed to formulate strategies for developing the modeling of nonlinear phenomena, complex systems, and mesoscopic dynamical behaviors.

One of the key issues discussed at the conference was to obtain an understanding of nonlinear phenomena and complex systems in a unified multiscale approach relating the microscopic, stochastic and macroscopic levels of description, which is a goal stated in the STOCHDYN programme: *questions of fundamental importance include the transition from a dynamical to a stochastic description and from a Hamiltonian to a thermodynamic formalism. New connections, such as the relation between microscopic chaos and dissipative processes have to be further explored.*

The conference included a celebration of the 65th birthday of Professor Grégoire Nicolis who has made many prominent contributions to the field and has formed many scientists.

The conference has been financially support by the STOCHDYN programme of ESF, the International Solvay Institutes of Physics and Chemistry, the Fonds National de la Recherche Scientifique (FNRS Belgium), the Communauté française de Belgique, and the Université Libre de Bruxelles.

Description of the scientific content

One of the important scientific problems of our time is to understand the complexification of matter and the emergence of natural complex systems on the basis of the physico-chemical laws of thermodynamics, statistical mechanics, and the theory of stochastic processes. It is now well established that the stochastic modeling allows to tackle the complexity of nonlinear systems. The dominant role of fluctuations at the mesoscopic scale can be amplified to the macroscopic scale by the effect of nonequilibrium instabilities, leading to the emergence of new phenomena unexpected at the lower level of organization. The synergy between noise and nonlinearity can induce order-disorder competitions which play a key role in understanding the complex structures arising in spatially extended systems.

In order to discuss the different aspects of the field, the conference was organized in 7 sessions:

COMPLEXITY
REACTION-DIFFUSION SYSTEMS I & II
STATISTICAL MECHANICS
NONLINEAR DYNAMICS
QUANTUM SYSTEMS
MESOSCOPIC SYSTEMS

Session on COMPLEXITY:

Complexity has many different facets discussed in mathematics, physics, chemistry, and biology. In mathematics, algorithmic and computational complexities have been defined which give tools to understand, in particular, how randomness and probabilities can be logically introduced in the description of a system (G. Chaitin). Besides, natural sciences provide several examples of complex systems which are systems composed on interacting entities having some collective behavior which is neither purely regular nor completely random. Famous and evident examples of complex systems are found in biology such as the process of biological evolution (P. Schuster) and the brain of upper vertebrates (T. Arecchi), both of which were discussed at the conference on the basis of nonlinear dynamics in such

high-dimensional phase spaces that statistical aspects become important. Two further examples were discussed, namely, the synchronization of interacting nephrons in kidneys (E. Mosekilde) and the collective behavior of populations of social insects (J.L. Deneubourg). The modeling of such complex systems involves both stochastic and nonlinear aspects.

Sessions I and II on REACTION-DIFFUSION SYSTEMS:

Interestingly, complexity is also the feature of physico-chemical systems, in particular, under nonequilibrium constraints which drive their self-organization into spatio-temporal patterns of various kinds. This structuration of matter is the result of nonequilibrium instabilities due to different possible mechanisms. The most well-known mechanism involves the coupling between diffusion and reaction as it is the case in the so-called reaction-diffusion systems which have been much studied during the last decade. The most recent advances on reaction-diffusion systems have led to the engineering of devices in which the reaction-diffusion process is under external control by either optical (K. Showalter) or electrochemical (J.L. Hudson) means. Such controls allow the monitoring of the collective dynamics of the reaction-diffusion system. Experimental work on reaction-diffusion processes have also been reported in micro emulsions (I. Epstein). The most recent theoretical studies concern spiral waves in chaotic systems (R. Kapral), fractional reaction-diffusion in complex media (K. Seki), and the mathematical derivation of limit-cycle solutions of the nonlinear ODE's (J.W. Turner). Besides reaction-diffusion, there exist other mechanisms which have been reported at the conference: instabilities due to the coupling of reaction with mechanics in special gels leading to oscillations (J. Boissonade), to the coupling between diffusion and electrochemical processes at interfaces leading to corrosion (A. Mikhailov), and to the coupling of reaction with hydrodynamic advection as it is the case for plankton at the surface of oceans (T. Tél). Finally, it has been theoretically demonstrated by P. Coulet that information can be stored in a spatially periodic pattern under appropriate conditions.

Session on STATISTICAL MECHANICS:

Statistical mechanics is the basic theory allowing us to connect the microscopic dynamics of interacting particles to the macroscopic properties of a system. Molecular fluctuations described by stochastic processes arise on mesoscopic scales. We are here at the core of the problem of providing a unified multiscale approach relating the microscopic, stochastic and macroscopic levels of description. Recent advances show that structures and dynamics are already important on quite small scales and that the macroscopic description can be deduced from this observation in many circumstances. The diffusion of colloidal particles can be studied in great detail in quasi one- and two-dimensional confined geometries, showing anomalous behavior which can be explained in terms of pair distribution functions (S. A. Rice). Unusual aspects of diffusion also arise in the presence of a magnetic field (J. Piasecki) or in lattices where special types of biased random walks can be described in terms of a diffusion equation with position and time exchanged (J.P. Boon). Open questions were discussed about the applications of kinetic theory to self-gravitating systems, shock waves at very large Mach number, and Bose-Einstein condensates (Y. Pomeau). Moreover, a derivation of Fourier's law was reported for a chain of coupled anharmonic oscillators (J. Bricmont).

Session on NONLINEAR DYNAMICS:

Many natural systems present collective behavior which can be described in terms of nonlinear dynamics. The variety of such systems is very large from macroscopic media sustaining combustion processes and plasmas, to systems of particles moving in some substrate. Nonlinear behavior is often studied in models capturing the essence of the phenomenon. This is the case for combustion in solids where nonlinear flame waves can be modeled in terms of propagation on coupled one-dimensional rods (B. Matkowsky). The coupling between the motion of electrons and ions can lead to solitary waves and special conduction properties (M. Velarde) as well as to ratchet effects in parametrically driven Frenkel-Kontorova chains (C. Baesens). In plasmas, kinetic master equations can be derived from the nonlinear dynamics in the presence of strong chaotic behavior (Y. Elskens). Such connections between dynamics and kinetics is also possible for active Brownian particles (R. Klages). Finally, a report was given on nonlinear dynamics in systems with delays which have many applications in nonlinear optics, chemistry, biology, and engineering (T. Erneux).

Session on QUANTUM SYSTEMS:

Several talks were devoted to quantum systems, especially, about the derivation of transport and irreversible properties in nonequilibrium quantum systems. A systematic derivation of nonequilibrium steady states in open quantum systems was presented showing, in particular, how nonequilibrium constraints such as electric currents can affect the Peierls transition (S. Tasaki). A derivation of entropy production was proposed for a quantum version of the Kac

ring model (C. Maes). A new method for the numerical simulation of the relaxation of a two-level quantum subsystem coupled to a classical heat was also presented (D. MacKernan). Besides, it was shown that topological quantum effects can arise by a kind of Aharonov-Bohm effect in models of intertwined conducting molecules (H. L. Frisch).

Session on MESOSCOPIC SYSTEMS:

The theory of stochastic processes plays its fundamental role in the description of mesoscopic systems. In these systems, the stochasticity arises not only because of the molecular fluctuations but also because the systems may present some micro heterogeneities and undergo some instabilities. This is the case for the combustion of small conglomerated solid particles where a stochastic multiscale modeling can be set up for the propagation of combustion waves (F. Baras). The stochastic description is also required to understand processes of heterogeneous catalysis such as the oxidation of CO on Pt in the presence of a surface reconstruction (A. Provata). Furthermore, mathematical studies of reaction and diffusion in restricted geometries such as fractals have been reported (J. Bentz and J. Kozak).

Assessment of the results and perspectives

The conference was a real success. First of all, a broad range of new results on nonlinear phenomena and complex systems were reported establishing the state of the art of the field. The conference has shown the unity of the field by the existence of appropriate concepts and methods to connect the different levels of descriptions from the microscopic to the macroscopic scales. The theory of stochastic processes and statistical mechanics are instrumental in connecting the microscopic and macroscopic levels of description while demonstrating the existence of specific properties associated with the mesoscopic fluctuations. Nonlinear effects appear by the collective behavior between the individual entities interacting within the system. These nonlinear properties may still be affected by the fluctuations on the mesoscopic scales. The combination between the nonlinear and stochastic aspects thus appears to be a common feature of the different complex systems reported in the conference. A conclusion is that our understanding of complex systems will make use of the methods of the theory of stochastic processes and nonlinear dynamics on the basis of the physico-chemical laws of thermodynamics and statistical mechanics.

Final programme

Wednesday, March 16th 2005

COMPLEXITY

Chair P. Gaspard

8h30-9h15 *Registration*
9h15-9h30 *Welcome and opening address*
9h30-10h00 G. Chaitin (New York, USA)
10h00-10h30 P. Schuster (Wien, Austria)

10h30-11h00 *Coffee break*
11h00-11h30 T. Arecchi (Florence, Italy)
11h30-12h00 E. Mosekilde (Lyngby, Denmark)
12h00-12h30 J.L. Deneubourg (ULB, Belgium)

Irreducible complexity in pure Mathematics
How Nature circumvents low probabilities:
The molecular basis of information and complexity

Feature binding and neuron synchronization: Quantum aspect
Oscillator clustering in a resource distribution chain
Decision-making in group-living organisms

REACTION-DIFFUSION SYSTEMS I

Chair P. Borckmans

14h30-15h00 K. Showalter (Morgantown, U.S.A.)
15h00-15h30 J. Boissonade (Bordeaux, France)

15h30-16h00 J.L. Hudson (Charlottesville, USA)

16h00-16h30 *Coffee break*
16h30-17h00 A. Mikhailov (Berlin, Germany)
17h00-17h30 T. Tél (Budapest, Hungary)
17h30-18h00 K. Seki (Tsukuba, Japan)

Addressable media for modeling collective behavior
Oscillatory dynamics in a chemomechanical system:
a first theoretical approach
Emerging coherence and collective dynamics
in a population of chemical oscillators

Sudden onset of corrosion as a cooperative critical phenomenon
Reactivity in flowing media
Fractional reaction-diffusion equation

Thursday, March 17th 2005

STATISTICAL MECHANICS

Chair M. Mareschal

9h00-9h30 S. A. Rice (Chicago, USA)
9h30-10h00 J. Piasecki (Warsaw, Poland)
10h00-10h30 J.P. Boon (ULB, Belgium)
10h30-11h00 *Coffee break*
11h00-11h30 Y. Pomeau (Paris, France)
11h30-12h00 J. Bricmont (Louvain, Belgium)
12h00-12h30 B. Matkowsky (Evanston, USA)

Confined colloid suspensions
Unusual dynamics in a 2D Lorentz model
Temporal diffusion

Open questions in kinetic theory
On the derivation of Fourier's law
Dynamics in a rod model of solid flame waves

NONLINEAR DYNAMICS

Chair A. Goldbeter

14h30-15h00 M. G. Velarde (Madrid, Spain)
15h00-15h30 C. Baesens (Warwick, UK)
15h30-16h00 Y. Elskens (Marseille, France)

16h00-16h30 *Coffee break*
16h30-17h00 T. Erneux (ULB, Belgium)
17h00-17h30 R. Klages (London, UK)

The surfing of electrons on a nonlinear electrically conducting lattice
Transport properties in Frenkel-Kontorova chains
Derivation of the Fokker-Planck equation
from strongly chaotic Hamiltonian dynamics

Nonlinear dynamics with delay
Active Brownian particles and Nose-Hoover thermostats

Friday, March 18th 2005

REACTION-DIFFUSION SYSTEMS II

9h00-9h30 I. Epstein (Brandeis, USA)
9h30-10h00 R. Kapral (Toronto, Canada)
10h00-10h30 S. K. Scott (Leeds, UK)
10h30-10h45 *Group photo*
10h45-11h15 *Coffee break*
11h15-11h45 J.W. Turner (ULB, Belgium)
11h45-12h15 P. Coulet (Nice, France)

Chair P. De Kepper

Pattern formation in reactive microemulsions
Spiral waves in chaotic systems
Pattern formation and wave propagation in chemical systems

Limit cycles and Riemann surfaces
Poincaré's homoclinic tangle and spatial complexity:
Storing information in cellular patterns

QUANTUM SYSTEMS

14h30-15h00 H. L. Frisch (Albany, U.S.A.)
15h00-15h30 S. Tasaki (Tokyo, Japan)

15h30-16h00 *Coffee break*
16h00-16h30 C. Maes (Leuven, Belgium)
16h30-17h00 D. MacKernan (Dublin, Ireland)

Chair S. A. Rice

Aharonov-Bohm effects in entangled molecules
C*-algebraic approach to nonequilibrium phenomena
in quantum junction systems

Discovering quantum mechanics via the Kac ring model
Quantum classical dynamics: the role of classical chaos

17h00-18h30 *Poster session*

19h30 *Banquet*

Saturday, March 19th 2005

MESOSCOPIC SYSTEMS

9h00-9h30 F. Baras (Dijon, France)

9h30-10h00 A. Provata (Athen, Greece)
10h00-10h30 J. Bentz (Ames, IA, USA)
10h30-11h00 *Coffee break*
11h00-11h30 J. Kozak (Chicago, IL, U.S.A.)
11h30-11h45 *Closing remarks*

Chair A. De Wit

Thermodynamics and reaction kinetics of small particles
in combustion synthesis
Oscillatory dynamics in the ZGB model with surface reconstruction
Reactants in a finite lattice: Non-nearest-neighbor effects

Invariance relations in the $d = 2$ random walk problem