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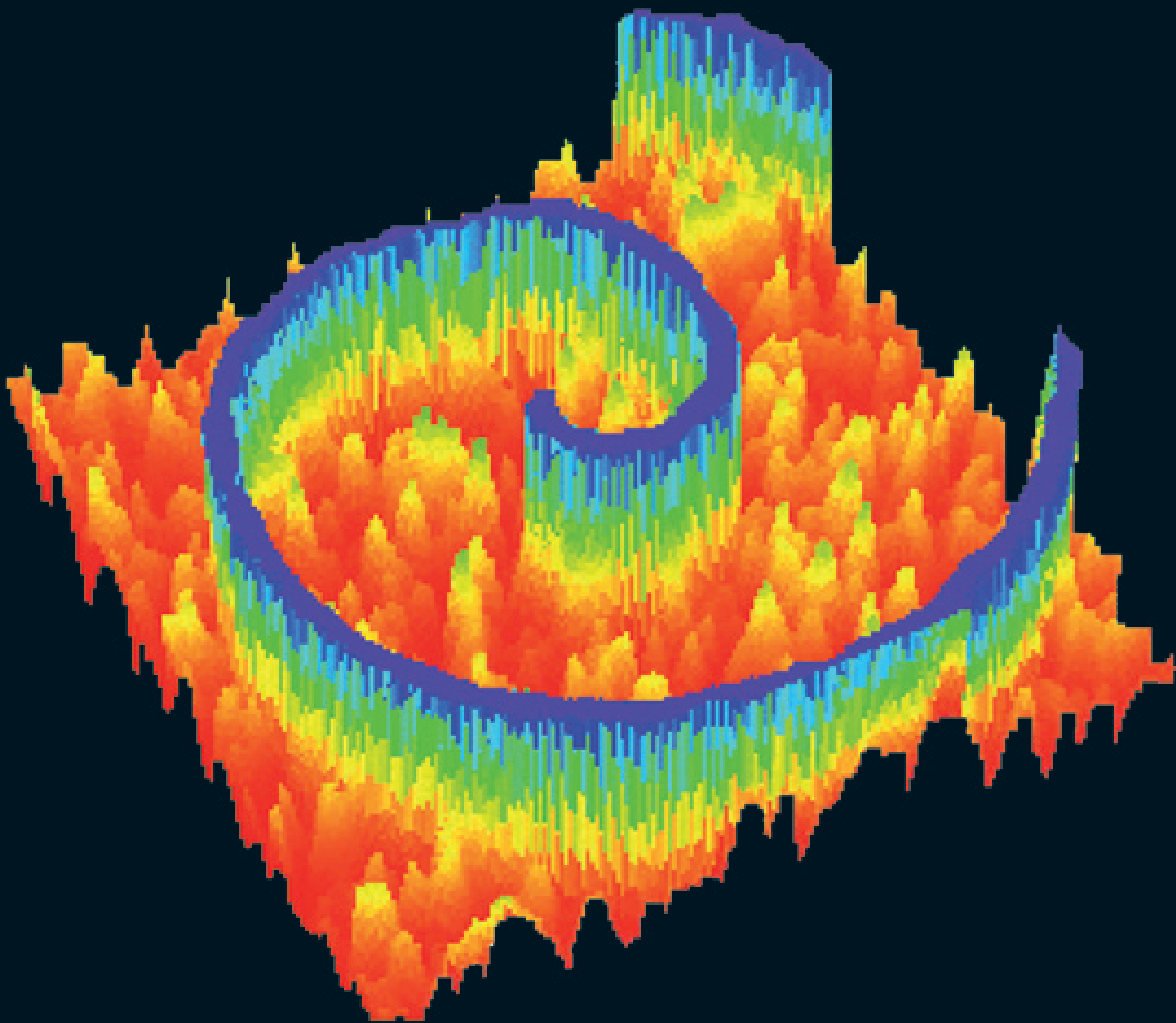
Stochastic Dynamics: Fundamentals and Applications (STOCHDYN)

An ESF Standing Committee for Physical and Engineering Sciences (PESC) Programme



Stochastic tools have been used successfully both for theoretical modelling of complex systems and for the analysis of experimental data, where the stochastic aspects may represent uncontrolled environmental impacts, thermal fluctuations or hidden internal dynamics. These tools provide a versatile interdisciplinary technique for tackling nonlinear dynamics of large systems as encountered in statistical mechanics, solid-state physics, chemical physics, nanotechnology, biophysics and climatology.
In sharp contrast to their effect on linear systems, or systems close to equilibrium, the influence of noise and fluctuations in nonlinear dynamics can often be quite unexpected and counterintuitive. Important phenomena can arise through channelling effects due to nonlinearities and the occurrence of large but rare events. These may give rise to increased order and signal amplification by noise, or to the emergence of directed motion due to the presence of non-equilibrium fluctuations.
The goal of the established network programme is to address the foundations of the different levels of stochastic description in nonlinear systems, to stimulate the further development of analytic and numerical tools, and to investigate specific problems as they arise in different areas of research. The programme intensifies the exchange of ideas between specialists in physics, chemistry and biology, with a particular emphasis on the promotion of an ongoing dialogue between theoreticians and applied scientists. Furthermore, the programme provides a forum for young European scientists where they can learn about this new expanding field of interdisciplinary research.

The running period of the ESF STOCHDYN programme is for five years from May 2003 to May 2008.

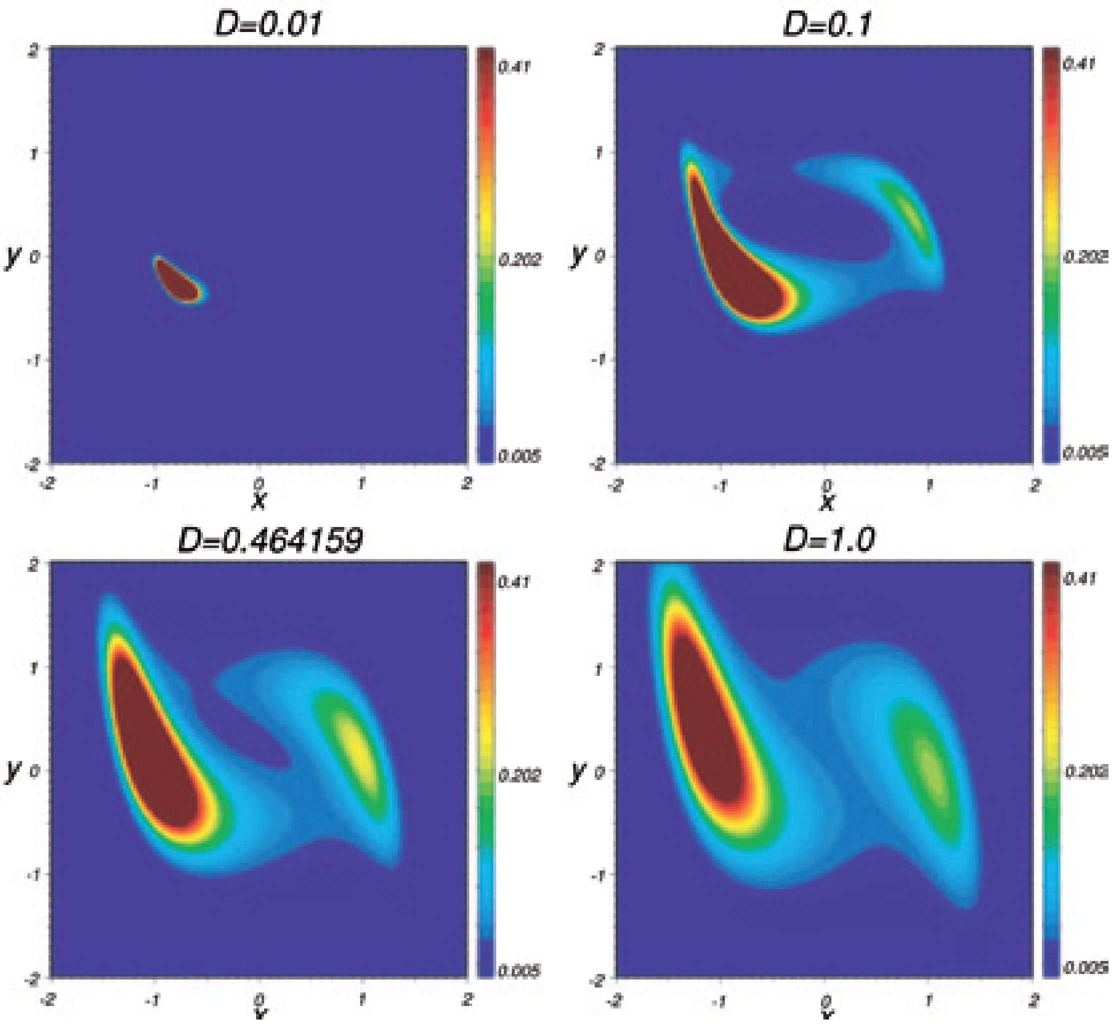
Cover:
Spiral wave under spatio-temporal fluctuations in a two-dimensional excitable medium. Values of the activator field (cold colours corresponding to higher values of the concentration) are superposed on the value of the external stochastic background.
S. Alonso et al., Phys. Rev. E 65, 066107 (2002).

Aims and objectives

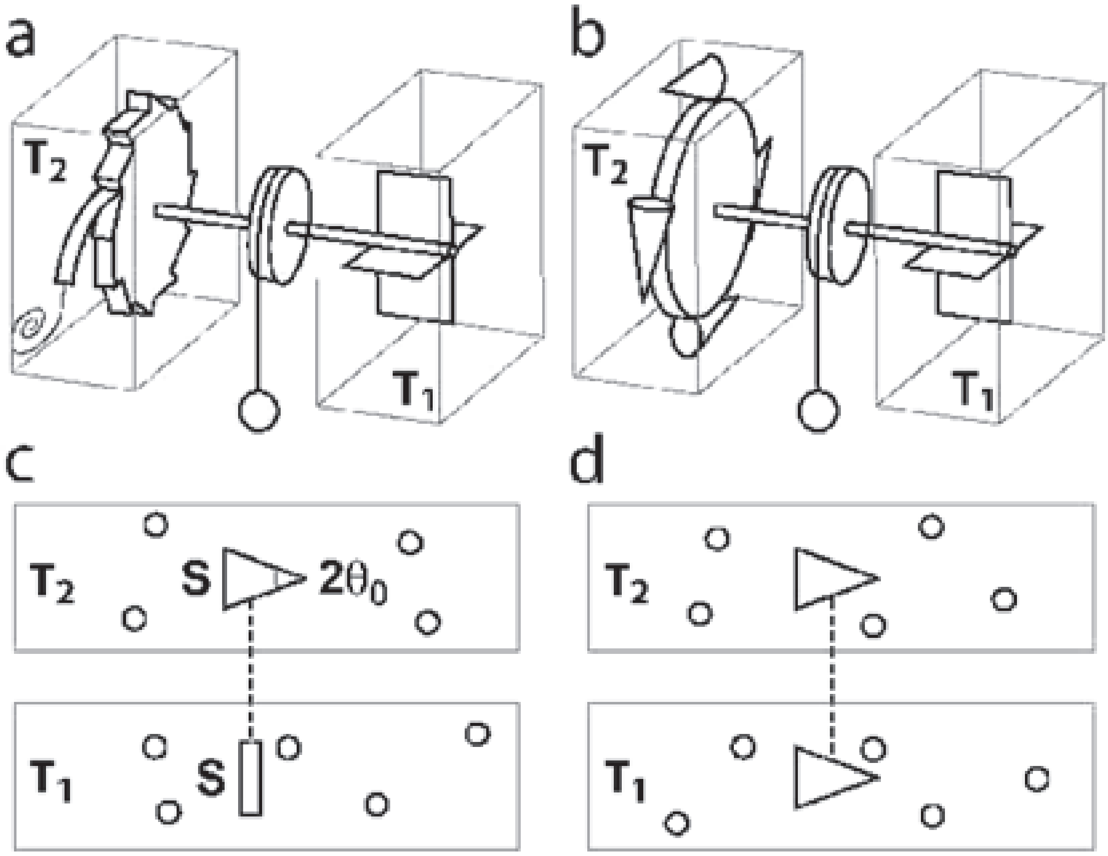
The complex properties of spatially or hierarchically extended non-equilibrium systems, in which nonlinear interactions within or among individual elements play a crucial role, present a major challenge to theoreticians and experimentalists in many fields of science. Despite the apparent diversity of different topics, two common aspects of these systems are of central interest to our interdisciplinary collaboration. First, many of the systems are necessarily subject to noise. It may be imposed either by the rapid dynamics of internal degrees of freedom, or by extrinsic environmental fluctuations. Second, they share a similarity in their mathematical description. One example is the class of systems represented by arrays of coupled stochastic nonlinear elements. Another example is Brownian motion in complex potential landscapes with energy pumps (a prototype model describing inter alia the non-trivial behaviour emerging in chemical reactions involving macromolecules, the motion of interfaces, polymer translocation through membranes, and the operation of molecular motors and pumps.

The traditional view on noise was guided by investigations of the linear dynamics of systems close to equilibrium. In such cases, noise introduces disorder and destroys temporal and spatial patterns. In most applications, therefore, there have been attempts to minimise its effects.

In contrast to this conventional textbook picture, it has recently been shown that noise in nonlinear non-equilibrium systems can act in precisely the opposite way: It can be used constructively, in a controlled



Contour plot of the stationary probability distribution density of the noisy Fitzhugh-Nagumo model, for different intensities D of additive Gaussian white noise. The density has one peak for weak noise, a crater-like shape for moderate noise, and is double peaked for strong noise.
M. Kostur et al., Fluctuation and Noise Letters 3, L155 (2003).



The Feynman ratchet and pawl construction (a) can be simplified to a two-dimensional model, (c) and (d), involving only hard core interactions. When the temperatures are different, the construction operates as a Brownian motor, whose properties can be calculated exactly in the limit of ideal gases.
C. Van den Broeck et al., Phys. Rev. Lett. 93, 090601 (2004).

manner, to enhance nonlinear features leading to ordered behaviour, or to support signal transmission. Investigations of the dynamics of ion channels in biological membranes, of synchronisation and coherent responses in chemical and biological systems, and of the behaviour of social insects (all involving nonlinear evolution in the presence of strong noise) are examples that demonstrate a subtle beneficial synergy between noise and nonlinearities creating ordered patterns in space or time.
Our research collaboration aims to clarify this counterintuitive role of noise and fluctuations in nonlinear systems far from equilibrium. It addresses fundamental questions of statistical physics, such as the breakdown of detailed balance and the channelling of noise in nonlinear dynamics (see Task A). Another goal is to improve the available analytic and numerical techniques to advance model-building ability. These goals will be attained by means of an organised exchange of knowledge between specialists working on fluctuations at various levels, ranging from molecular scales to extended continuous systems (see Task B). Last but not least, the programme focuses on the practical aspects of developing applied tools and providing guidelines for applications. Task C comprises methodological questions such as the determination of escape rates and their higher moments, the comparison of stochastic models with results from molecular dynamics, and time series analysis.

Task A

Breaking detailed balance

Equilibrium situations are restricted by the detailed balance condition, which is the microscopic basis of the second law of thermodynamics. The breakdown of detailed balance is an obvious sign of non-equilibrium. It is responsible for a wealth of important dynamical phenomena such as noise rectification, directed motion and stochastic resonance. Noise-induced oscillations in neuronal models or in excitable chemical dynamics, as well as the higher dimensional motion of Brownian particles in ratchet-like potentials, result from coherent structures in the stationary probability flows.

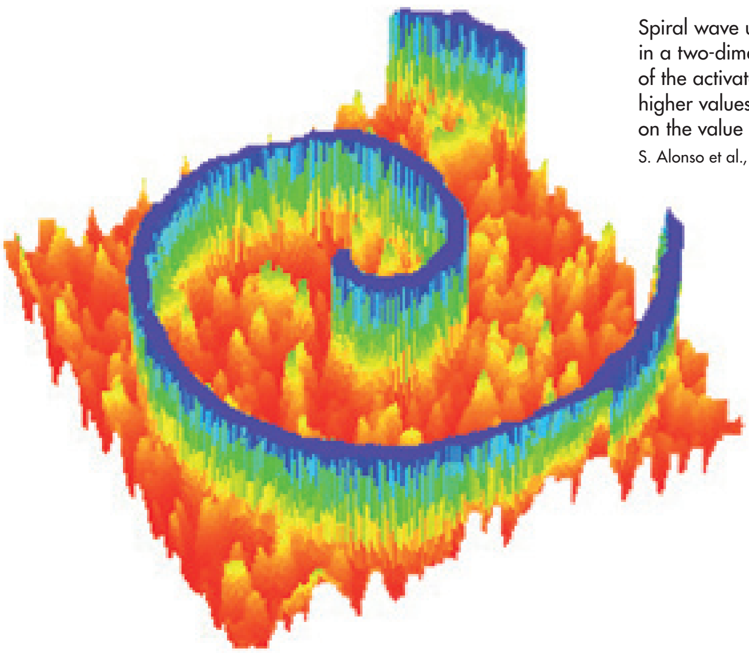
A theoretical appreciation of situations where detailed balance is violated is crucial for the understanding of out-of-equilibrium processes. So far, most solutions of the Fokker-Planck- and master equations are based on vanishing or constant probability fluxes, or on fluxes where stationary densities obey a potential condition. Only a few studies rely on a more complex structure of the probability flux, for example, those with single or multiple rotating vortices.

Because of its special importance, this particular issue is of central interest to the network. Detailed studies of mechanical nonlinear oscillators with inertia, of coupled overdamped oscillators, and of Lotka-Volterra systems, to name just a few examples, foster a deeper understanding of noise-induced dynamical states relying on non-trivial probability flows.

Noise-induced order

Noise-induced phase transitions, noise-induced propagation of waves and noise-induced transmission of signals, stochastic or coherence resonance and synchronisation, or the control of complex dynamical systems by noise, are all intriguing phenomena revealing the generic ability of nonlinear systems to amplify an ordered response by channelling noise to special degrees of freedom. This field of research has found many different applications in diverse areas, ranging from the pure sciences to applications in engineering. However, their detailed understanding, in particular with respect to potential applications, still has a long way to go.

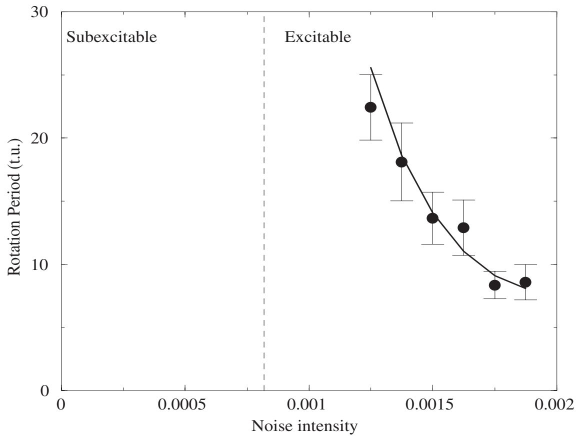
For example, the noise-sustained amplification of signals in bi-stable and in threshold systems, so-called stochastic resonance, has been extensively studied during the last decade. A well-based understanding has now been achieved in the physics, chemistry and biology of periodically or randomly driven stochastic nonlinear systems with few degrees of freedom. However, only a relatively small number of investigations of stochastic resonance in extended or coupled systems have been conducted to date. Their study is especially relevant for a better understanding of the interplay of signals and noise in biological sensors, and in neuronal models where stochastic resonance is expected to be of great importance.



Spiral wave under spatio-temporal fluctuations in a two-dimensional excitable medium. Values of the activator field (cold colours corresponding to higher values of the concentration) are superposed on the value of the external stochastic background.
S. Alonso et al., Phys. Rev. E 65, 066107 (2002).

Coherence resonance, a similar phenomenon in which noise-induced coherent oscillations are promoted in excitable non-forced systems, is another scenario to be investigated in relation to its relevance in neurophysiological systems (spiking or bursting behaviour of neuronal units). Here again, passing from the investigation of single units to that of complex coupled architectures will be an important aim.

Noise may induce transitions from one temporal or static behaviour to another, or it may modify the way in which such transitions take place. Noise may also create ordered spatial patterns. Recently, purely noise-induced phase transitions were discussed theoretically in the case of extended systems that do not generate structure-forming processes in the absence of noise. Moreover, their individual units do not exhibit unusual behaviour in the presence of noise. Remarkably, locally uncorrelated fluctuations of control parameters can induce a phase transition of the macroscopic system to an ordered state.



Theoretical (line) and numerical (points) mean rotation period of noise-sustained spiral waves in subexcitable media versus noise intensity for a reaction-diffusion model of active media. The vertical line shows the transition between subexcitable and excitable media due to noise.

S. Alonso et al., Phys. Rev. E 65, 066107 (2002).

Task B

Many dynamical properties and phenomena in complex systems rely on the specific and sometimes dominant role of fluctuations. Let us name but a few.

Molecular objects

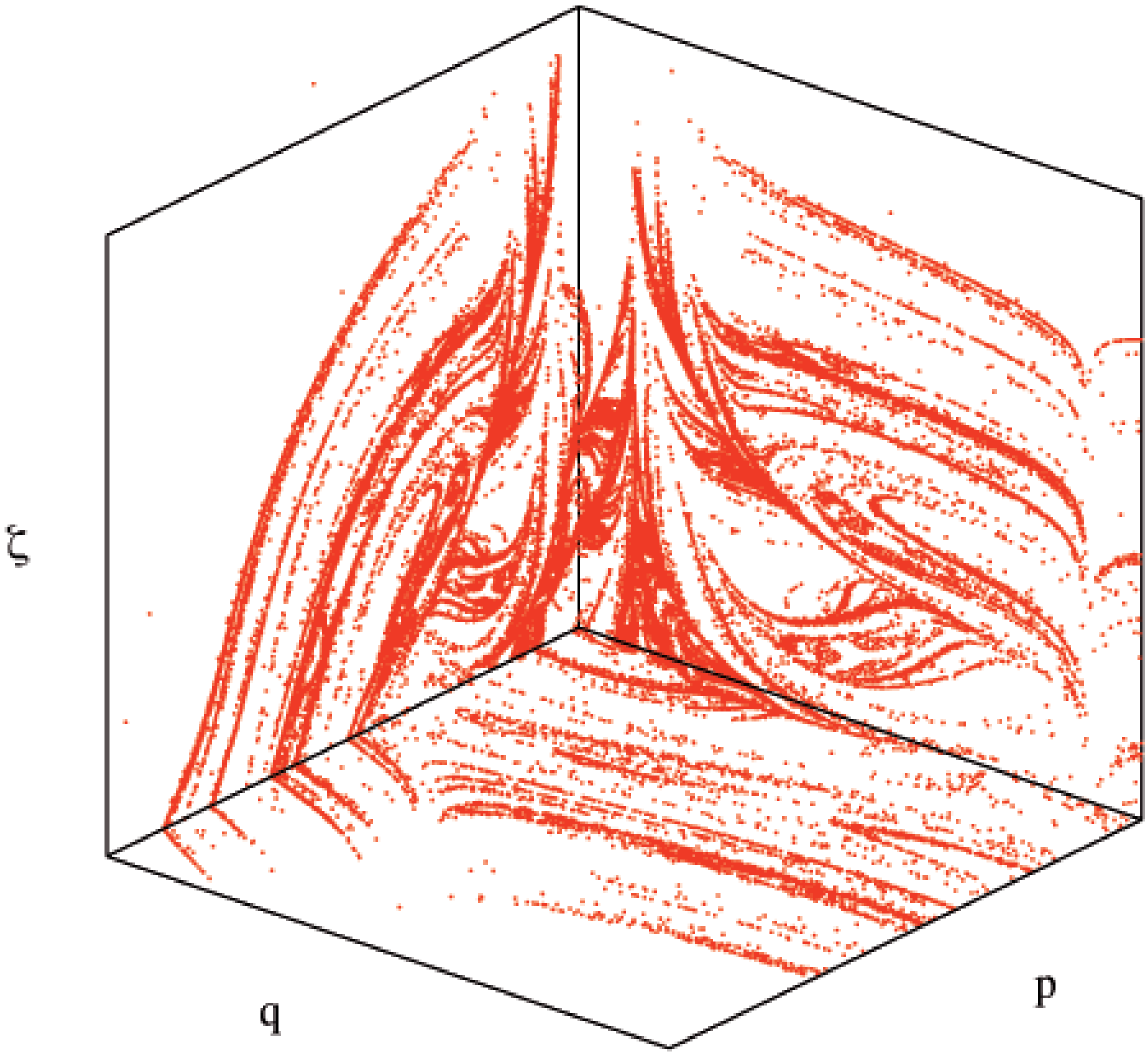
Nanotechnology has provided the means to manipulate molecular-scale objects, and new techniques have emerged that allow the study and control of small-scale biological processes. On these microscopic scales, thermal fluctuations play an important and often constructive role, thus opening a largely unexplored and only recently experimentally accessible territory for the application of stochastic methods.

Ratchet-like devices have demonstrated their ability to separate colloids or DNA by using micro-fabricated structures. Fluctuations dominate the conformational dynamics of proteins and are believed to be decisive for Brownian motors and enzyme reactions. SQUIDs and quantum dots allow one to observe experimentally the intricate interplay between quantum properties and thermal fluctuations. These issues are being investigated by pooling the theoretical and experimental expertise of the network, including in particular biological Brownian motors, self-propelling objects, noise-induced self-organisation of Brownian particles, quantum dots, ‘Maxwell’s demon’ constructions, and micro-pumps.

Internal fluctuations in reaction processes

The hitherto well-accepted description of reactive systems formulated in terms of standard rate constants and mean-field laws, which are the basic ingredient of classical kinetics, has recently been questioned. This applies especially to phenomena in restricted geometries and low dimensional systems. The focus of research is changing from the usual macroscopic and homogenised processes in laboratory-scale samples to those taking place in microscopic or confined reactors typical of cellular environments or supramolecular architectures. Just to mention one example in this context, the dynamics of calcium release by ion channels requires an understanding of the internal fluctuations arising only from the small number of molecules that are involved. Reformulation of the classical kinetic mechanisms for enzymatic reactions will be an important development in the biochemical description of single reactions and complex metabolic networks.

The role of particle fluctuations has also been revealed in recent experiments on heterogeneous



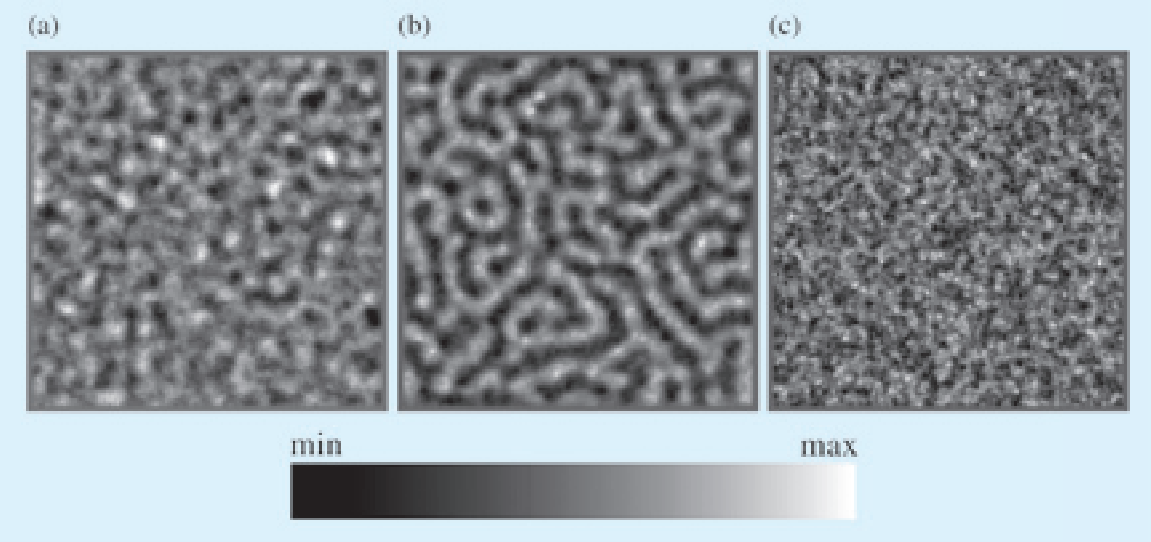
catalysis. In this quite different scenario, sophisticated techniques have allowed real-time and in situ observations of catalytic processes with nanoscale resolution. Clustering of adsorbates, through direct or surface-mediated interactions of variable interaction range, constitutes only one ingredient of the complex dynamics of such processes. Also to be considered are reversible or irreversible steps of adsorption-desorption, together with the diffusion-reaction mechanisms themselves.

Particle systems evolving in non-equilibrium stationary states are characterised by multifractal probability distributions in phase space, if stationarity is maintained by dynamical time-reversible thermostats. The figure shows three orthogonal Poincare surfaces of sections of such a distribution for a simple one-dimensional charge-conductivity model of a particle in a periodic potential. Similar structures are found, if the non-equilibrium stationary state is maintained by stochastic thermostats. This profoundly affects the understanding of transport properties.

H. A. Posch et. al., Physica D 187, 281 (2004).

Influence of external noise on pattern-forming systems

Recent chemical experiments (the photosensitive Belousov-Zhabotinski reaction) provide striking examples of the importance of external noise in extended systems. It was successfully demonstrated



Snapshots of a noise-induced phase transition yielding pattern formation. A scalar field with nonlinear dynamics, multiplicative noise and coupled by a Swift-Hohenberg operator exhibits a labyrinth-like structure in the case of moderate additive noise (b).
A. A. Zaikin and L. Schimansky-Geier, Phys. Rev. E 58, 4355 (1998).

that externally imposed fluctuations can have the effect of organising, supporting, dispersing or even creating autowaves. Similar situations have also been observed in hippocampal slices of rat brains and astrocyte syncytium.

Here, our goal is to go from the two-dimensional and quite ideal experimental and numerical scenarios investigated so far to real three-dimensional situations. In this way one can hope to deal with extended media allowing the propagation of excitations, either in the form of scroll waves or as more complex entangled structures.

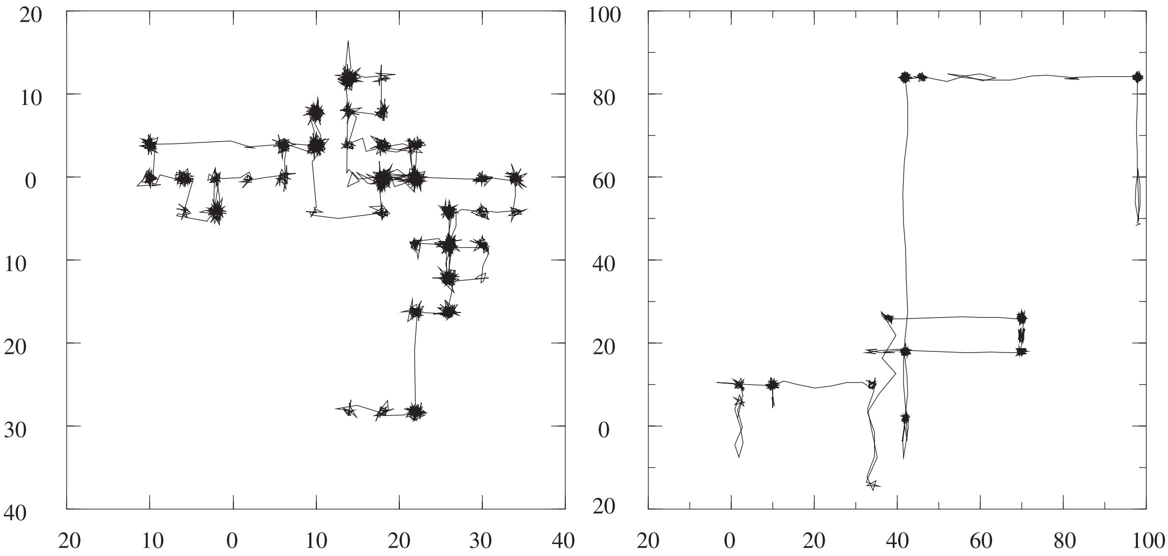
Media such as brain or cardiac tissues are natural objects to be investigated from this perspective. Of central interest are the control or reduction of spatio-temporal chaos (fibrillation) by noise or, in general, noise-induced synchronised patterns of activity to be employed in non-trivial tasks such as coherent signal processing, learning, or adaptation.

Task C

Investigations of basic topics and specific problems face common difficulties related to the modelling, mathematical treatment and, in particular, numerical simulation. Special attention is therefore devoted to the following areas.

Escape processes and rates

In many examples the description relies on an understanding of the noise-driven escape of particles from a metastable state. In equilibrium, these processes are now fairly well understood. Under non-equilibrium conditions, however, with non-Gaussian or strongly correlated noise or with noise combined with temporal signals and in higher dimensional phase spaces, escape still presents significant challenges that need to be tackled on account of their high practical importance. A prominent example is the surmounting of barriers by particles into pockets or active centres of vibrating or excited biomolecules, where the phenomenon of resonant activation may give a clue to the understanding of the mechanisms through which biomolecules catalyse enzymatic reactions.



Simulation of the stochastic motion of clusters on the surface of a solid-state sample with a periodic structure and high (left) and low (right picture) friction. In the case of low friction, the anomalous diffusive transport is realised via long straight jumps.
J. M. Sancho et al., Phys. Rev. Lett 92, 250601 (2004).

Another important field of activity deals with activation processes of molecules (chains, polymers), for example the translocation of molecules through pores in membranes or the motion of interfaces in external potential fields. Successful stochastic approaches describe the structure of the molecules in terms of just a few variables and hence are thus able to map the activation onto a stochastic motion in low-dimensional phase spaces.

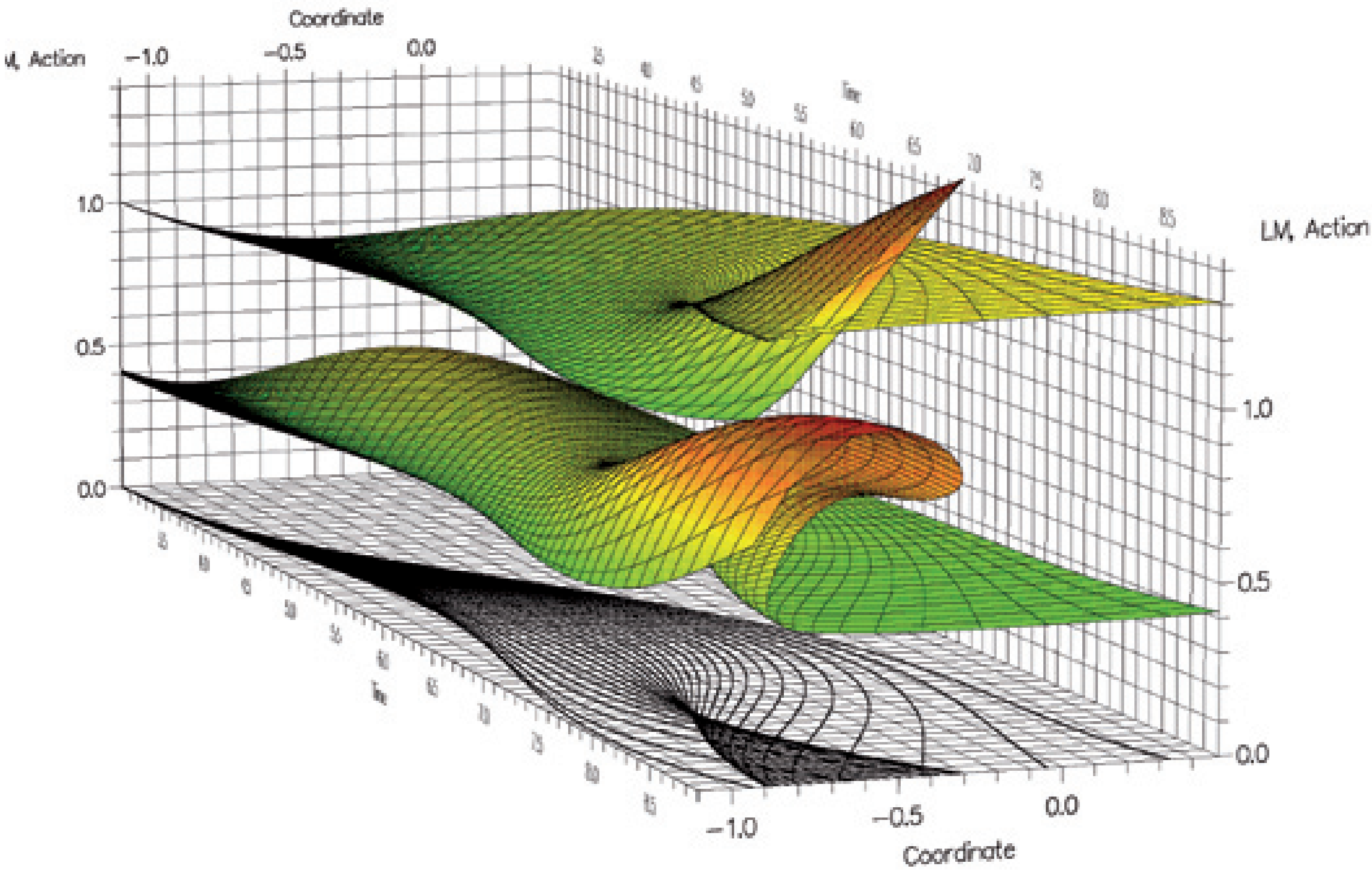
Levels of stochastic description

Relationships between the microscopic, stochastic and macroscopic levels of description for non-equilibrium systems need to be understood in depth. 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 mutual interrelationships and consistency of the various stochastic descriptions have to be clarified, in particular formalisms based on master equations or stochastic differential equations).
Further work is also needed on the formulation of the thermodynamics of stochastic processes including, for example, entropy production by fluctuations. Progress on all these issues can be achieved through the study of simple model systems, such as the adiabatic piston, ideal chemical reactions, the Feynman ratchet, the multi-Baker map, or the asymmetric exclusion process.
Molecular dynamics and direct simulation Monte-Carlo techniques allow for comparison between the different levels of description, leading to verification and refinement of the theoretical apparatus. More realistic models may allow for a closer comparison with experiment, for example in heterogeneous catalysis and pattern-forming instabilities. In particular, the distinctive effects of external noise, parametric perturbation and thermal noise in such systems can be investigated experimentally.

Analysis of stochastic signals

In strongly fluctuating systems the distinction between deterministic behaviour and fluctuations is difficult. Within the network, modern mathematical tools such as the wavelet transform, detrended fluctuation analysis, and generalised entropy are being elaborated to extract relevant information, even from very noisy data. Descriptions in terms of probability densities require more advanced techniques, for example, the consideration of fractional Fokker-Planck equations.

Among many possible applications in science, the network especially supports research on climate dynamics, neuro-informatics and synchronisation phenomena in medicine. In these disciplines,

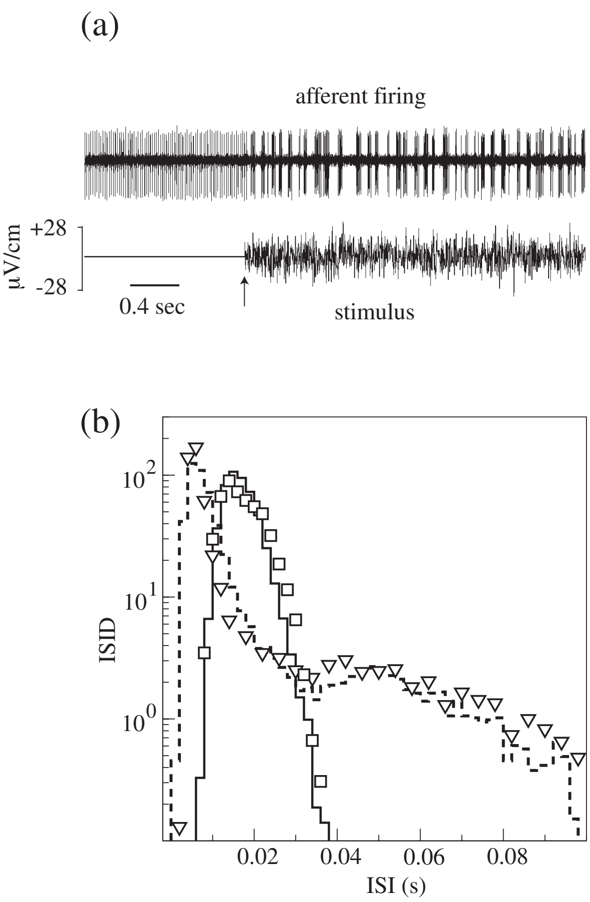


stochastic methods are widely discussed while the modelling of the corresponding dynamical processes has reached a high level of sophistication. The interaction of specialist groups from these fields with the research community of nonlinear stochastic dynamics is thus especially welcome.

Many of the techniques and concepts were originally developed by researchers from the field of statistical physics, or within a chemical or biophysical context. These investigations and their thought-provoking discoveries prompted a surge in the fundamental mathematical research on noisy nonlinear systems. Thus, stochastic resonance, synchronisation and noise-induced transitions from negative to positive Lyapunov exponents recently appeared as new topics in the mathematical literature. Even though mathematical theories per se are not a central issue of the proposed network, the collaboration, advice and participation of mathematicians falls under the permanent scope of the networking programme.

This figure shows the origin of singularities in the pattern of optimal fluctuational paths for a generic non-equilibrium system (a periodically driven double-well Duffing oscillator). The Langrangian manifold (middle sheet) acquires a fold, leading to intersecting action surfaces (upper sheet). The most probable paths are those of least action which, projected down onto the coordinate plane (bottom) lead to a pattern of optimal paths with two caustics emanating from a cusp point. Physically meaningful paths cannot cross the switching line defined by the intersection of the action surfaces.

D. G. Luchinsky, Contemporary Physics 43 (5), 379 (2002).



Noisy stimulus (lower row) and the induced bursting of the firing activity in a paddlefish electroreceptor (upper row). Interspike interval densities for spontaneous activity (squares) and with noisy external stimulus (triangles). Lines denote simulations of a two-variable stochastic burster model.

S. Liepelt et al., Journal on Theoretical Biology, (in print).

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