8th International Conference
Engineering of Chemical Complexity

Abstracts

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1 Plenary Talks

8th Intl. Conference on *Engineering of Chemical Complexity*
22-26 June 2015
Munich, Germany

*Collective dynamics and competition in single and competing bacterial colonies**

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We examine the growth of colonies of a rod-shaped motile bacterium commonly found in soil. The bacteria within a growing colony exhibit collective motion (swarming) and large (non-thermal) fluctuations in the number growing in a given area [1]. When neighboring colonies of the bacteria grow and approach one another, the growth slows and stops. Analysis of the gel between the competing colonies reveals the presence of a lethal protein secreted by the colonies [2]. The immediate question is why doesn't this toxin kill the bacteria secreting it? A mathematical model helps answer this question. Further, sub-lethal concentrations of the toxin are found to induce the rod-shaped bacteria to switch to a spherical shape that is resistant to the toxin and to other antibiotics. Thus the bacteria adapt to adverse environmental conditions by a change in form; this morphological switching is reversed if favorable conditions are encountered [3].

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8th Intl. Conference on *Engineering of Chemical Complexity*
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HYDRODYNAMIC COLLECTIVE EFFECTS OF ACTIVE PROTEINS

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Biological cells contain large numbers of active proteins that repeatedly change their conformations and need a supply of ATP or other substrates to maintain their cyclic operation. While these protein machines have a variety of specific functions, acting as motors, ion pumps, or enzymes, they also induce fluctuating hydrodynamic flows in the cytoplasm and in cellular membranes. Because such fluctuating flows are non-thermal, energy can be extracted from them and work can be performed. We show that these flows can substantially enhance diffusive motions of passive particles. Furthermore, when gradients in concentrations of active proteins or substrate (ATP) are present, a chemotaxis-like drift should take place. Such nonequilibrium effects are universal: they hold for all passive particles and for active proteins themselves.

2 Talks

2.1 Active Particles

Collective Behavior of Self-Powered Single Molecules and Nanoparticles

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One of the more interesting recent discoveries has been the ability to design nano/microparticles which catalytically harness the chemical energy in their environment to move autonomously. These "bots" can be directed by chemical and light gradients. Further, our group has developed systems in which chemical secretions from the translating micro/nanomotors initiate long-range, collective interactions among the particles. This behavior is reminiscent of quorum sensing organisms that swarm in response to a minimum threshold concentration of a signaling chemical. We will discuss recent experimental results, as well as approaches to the modeling of the complex emergent behavior of these particles.

Active Particles near Surfaces

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Abstract:
Both in soft matter and in biology, there are numerous examples of microswimmers and self-propelled particles [1]. With a typical size in the range of micro-meters, both low-Reynolds-number hydrodynamics and internal noise are essential to determine their dynamics.
We focus here on the behavior in systems of biological and artificial microswimmers and self-propelled particles near surfaces [1]. The helical flagella of peritrichous bacteria synchronize and form bundles for propulsion, but also unbundle to induce bacterial tumbling [2,3]. Non-tumbling bacteria display a circular motion near surfaces, due to the counter-rotation of flagella and body, which depends on the fluid boundary conditions (slip or no-slip) at the surface [4]. This behavior can be employed to construct striped surfaces which enforce a directed bacterial motion [4]. Tumbling bacteria also show a large surface excess, which depends on the run-length distribution [5]. The behavior of run-and-tumble particles near surfaces can be compared with that of active Brownian particles [6,7]. The effects of self-propulsion, hydrodynamic interactions, microswimmer shape, and noise on these phenomena will be discussed.

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Engineering Chemically Active Nano- and Micro-motors

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One of the challenges of active transport at low Reynolds numbers is how to enable small objects to develop autonomous, directional motion (so-called self-propulsion) and perform advanced tasks. A promising approach consists on employing chemically powered micro- nano-motors that can extract "chemical" free energy from the surrounding liquid and to transform it into mechanical energy.

Different engineering approaches enable the fbarication of these active particles, with shapes that can vary from nanowires, spherical micro- and nano-particles, or microtubes. Several propulsion mechanisms emerge depending on the type of self-propellers, such as bubble propulsion, self-electrophoresis or self-diffusiophoresis [1].

In this talk, I will present our recent advances in the design of different types of catalytic motors, from the nanoscale [2] to the micrometer regime [3,4] including microtubes and spherical motors. Their motion can be externally controlled by magnetic field [5], by using chemical gradients experiencing chemotaxis [6], or by engineering "smart walls" [4].

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Exploring active particles as a new class of soft-matter systems

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Active particles or microswimmers constitute a new and fascinating class of soft-matter systems the physical principles of which need to be explored both for single swimmers and also for their collective dynamics. Chemical processes are relevant on both levels. In this talk I will review some of our theoretical work in this field.

Emulsion droplets become active with the help of a self-induced Marangoni flow at their interfaces [1]. Hydrodynamic flow fields generated by microswimmers strongly influence their collective motion and the swimmer type determines their phase behavior [2]. Active particles in a harmonic trap can even form fluid pumps through a symmetry breaking transition [3]. Active or self-propelling colloids are able to sense their environment and perform chemotactic motion mimicking bacterial systems [4]. Finally, microswimmers at the surface of a thin liquid film may induce an instability and thereby generate appealing dynamic patterns [5].

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2.2 Fluctuations Far from Equilibrium

Active microrheology in dense crowded systems

Gleb Oshanin
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In this talk I will survey our recent analytical and numerical results obtained for a minimal model, which mimics standard experimental settings of active microrheology and consists of a tracer particle subject to a constant external force in a crowded medium composed of identical hard-core particles performing unbiased random walks constrained by a mutual exclusion. I will show that the tracer particle motion is essentially dependent on the geometry of the system : In case of single files, in which the initial order of particles is preserved at all times since the particles can not bypass each other, all cumulants of the tracer particle displacement show the same sublinear dependence on time. In quasi-one-dimensional systems, such as, e.g., two-dimensional stripes or three-dimensional elongated capillaries, the tracer particle velocity ultimately attains a constant value, but the variance of the tracer particle displacement exhibits a surprising super-diffusive growth at intermediate times, which then crosses over to a giant diffusion at later times. In two-dimensional systems and in slit pores, the variance shows a weakly superdiffusive growth which crosses over to ordinary diffusion. We also analyse the dependence of the terminal velocity on the magnitude of the force, and show that in some cases it may be a non-monotonic function of the latter exhibiting the so-called negative differential mobility. A set of other questions, such as, e.g., convergence of the distribution function to a Gaussian, emerging interactions between biased particles when several such particles are present, will also be discussed.

Hot Brownian motion

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The classical theory of Brownian motion rests on fundamental laws of statistical mechanics, such as the equipartition theorem and the fluctuation-dissipation theorem, which do not hold under non-isothermal conditions. I will discuss the generalized fluctuation-dissipation relations and Langevin equations governing non-isothermal Brownian motion, including some explicit results for the frequency-dependent noise temperature and Brownian thermometry far from equilibrium. The derivation is based on the underlying fluctuating hydrodynamic equations of motion assumed to be in local equilibrium with a spatially varying temperature field. Useful experimental applications comprise "hot" and "cold" Brownian motion, self-thermophoretic nano-swimmers, and photothermal detection.

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Description of diffusion in confined environments placing the coordinate frame at the tube's axis

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We develop a theoretical framework to study the diffusion of Brownian point-like particles in bounded geometries, the main idea of the approach is to place the coordinate frame at the tubes' axis parametric curve. To this end we use the Frenet-Serret moving frame as the coordinate system. To describe the evolution of the probability density of the particles diffusing inside the tube from this frame of reference, we find the transformation that allows us to write the Fick equation in tubular coordinates system. For narrow tubes we use an effective one-dimensional description reducing this diffusion equation to a Fick-Jacobs-like equation. From this last equation we can calculate the effective diffusion coefficient applying Neumann boundary conditions. For 3D tubes, at zeroth and first-order our approximation for this effective coefficient, do not coincides with any reported in the literature previously, moreover their dependence is not only on the tube's normal plane area derivative, but also on its area itself. For 2D channels at first order we recover the effective diffusion coefficient obtained by Kalinay and Percus, and our second-order gives important correction to the previous order. Finally, we validate our analytic predictions for the effective diffusion coefficients for a periodic a tube formed by overlapping spheres (3D) and a periodic channel former by overlapping disks (2D). When comparing the values obtained from Brownian dynamics simulations with our first-order (3D) and second-order (2D), it turns out to be highly accurate.

Stationarity, ergodicity, and fluctuations in simple models of anomalous diffusion.

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We discuss the nature of anomalous diffusion in crowded molecular environments, and try to bring order in a large zoo of corresponding models. One of the ways of classification of the corresponding random processes is discussing such their properties as stationarity or ergodicity. We start from discussion of different mathematical definitions and show how the properties considered, or absence thereof, follow from the microscopic description of the systems on the level of master equations, giving a relatively clear intuitive picture. We moreover discuss in some detail the behavior of simple paradigmatic models, and the corresponding statistical tests [1].

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2.3 Synchronization Phenomena

Optimal Entrainment Control of Electrochemical Oscillations

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Entrainment of oscillations to an external forcing of widely different waveforms is often used to provide means to timing of essential system processes. Different fields of science often use different waveforms that include smooth (e.g., sinusoidal), square, or pulse waveforms. In this contribution, we formulate a unified theoretical framework for optimal entrainment of weakly forced nonlinear oscillators. We show that large locking range for power, magnitude, and area constraints of the forcing waveform corresponds to smooth, square, and pulse waveforms, respectively. The results are demonstrated in laboratory experiments with oscillatory nickel dissolution in sulfuric acid.

Synchronization of rhythmic spatiotemporal patterns and network dynamics

Hiroya Nakao (Tokyo Institute of Technology, Japan)

Rhythmic spatiotemporal patterns in reaction-diffusion systems or rhythmic collective dynamics in networks of coupled dynamical elements can be regarded as macroscopic limit-cycle oscillators as a whole. In this study, we generalize the conventional phase reduction theory for low-dimensional limit-cycle oscillators to such types of high-dimensional oscillatory dynamical systems. Using the generalized theory, we analyze synchronization properties of the macroscopic rhythms in heterogeneous high-dimensional systems, such as the excitable media with pacemakers and network-organized systems consisting of oscillatory and excitable elements.

Synchronization of synthetic gene oscillators

M. Bennett [1], *T. Danino* [2], *J. Hasty* [3], *W. Mather* [4], *O. Mondragon-Palomino* [5], *A. Prindle* [3], *J. Selimkhanov* [6], *J. Stricker* [3], *L. S. Tsimring* [3]

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One of the defining characteristics of life is the ability to keep time, which organisms often achieve by using internal genetic "clocks" to govern fundamental cellular behavior. While the gene networks that produce oscillatory expression signals are typically quite elaborate, certain recurring network motifs are often found at the core of these biological clocks. In this talk I will describe our recent theoretical and experimental work on the oscillatory dynamics of synthetic gene circuits. One common motif which leads to oscillations in many natural biological "clocks" is delayed auto-repression. We designed and constructed synthetic gene circuits based on this design principle, and observed robust and tunable oscillations of gene expression in bacteria [1]. Computational modeling and theoretical analysis show that the key mechanism responsible for oscillations is a small delay in the negative feedback loop. In a strongly nonlinear regime, this time delay leads to long-period oscillations that are characterized by "degrade and fire" dynamics [2]. Using a variant of the same design in which oscillators are coupled chemical signals diffusing through cell membranes, we studied regimes of population-wide synchronization [3,4]. We also observed an interesting regime of intra-cellular synchronization of two different gene oscillators indirectly coupled by a common degradation enzyme [5].

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Permutation symmetries and phase wave synchronization on networks of heterogeneous chemical oscillators

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Synchronization phenomena are observed in a wide variety of systems ranging from synchronizing fireflies through firing neurons to electrical power grids [1,2]. Recently it has been demonstrated that permutation symmetries of the underlying oscillator networks are of fundamental importance for zero-lag synchronization patterns [3]. In this contribution, we address the question: What role do network symmetries play, when the frequency detuning of the individual oscillators is too large to allow for zero-lag synchronization? Experiments and simulations on networks of discrete chemical relaxation oscillators [4] reveal transitions from incoherence through partial synchronization to phase waves following symmetry clusters with increasing coupling strength.

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Scroll Wave Chimeras

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Chimera states occur when an oscillator population splits into two coexisting spatially distinct parts, one synchronized but the other oscillating with incoherent phases. This amazing phenomenon was discovered in 2002 by Kuramoto and Battogtock for non-locally coupled complex Ginzburg-Landau equation and derived in details for respective Kuramoto model [1]. Currently, this is an area of intense theoretical and experimental research including one- and two-dimensional systems from different fields.

In the talk, two principal classes of three-dimensional chimera states are reported for Kuramoto model in 3D grid topology with periodic boundary conditions, both available in wide regions of the parameter space: (I) oscillating without rotation and (II) spirally rotating. They are (I) coherent/incoherent balls, tubes, crosses, and layers in incoherent/coherent surrounding and (II) scroll waves with incoherent rolls of different modality, topology, and large scale dynamics which can be stationary, periodic, or chaotic [2]. Intriguingly, different chimera types can robustly co-exist for the same system parameters when given by different randomly choosen initial conditions. Moreover, these striking patterns co-exist with the fully synchronized and rotating wave solutions. We discuss the scroll chimeras multistability and its possible phenomenological relation to three characteristic regimes in cardiovascular heart disease, namely, normal sinus rhythm, ventricular tachycardia, and ventricular fibrillation. The presentation is illustrated by videos of the 3D chimera dynamics.

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2.4 Contributed Talk Session I

Active particles at and close to fluid-fluid interfaces

Paolo Malgaretti [1,2], *Mihail Popescu* [1,2], *Alvaro Dominguez* [3], *Siegfried Dietrich* [1,2]
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Chemically active swimmers are particles whose surface promotes the catalysis of suspended molecules. When the surface properties of these particles are not homogenous, the asymmetry in the density field generated by the process of catalysis can lead to particle motion [1,2].
In this contribution I will discuss how the presence of a fluid-fluid interface affects the dynamics of chemically active particles. In particular I will focus on two main cases, namely the case in which active particles are already trapped at the interface and the case in which they are close (but not yet trapped) to a fluid-fluid interface.
When the particles are trapped at fluid-fluid interfaces their motion is constrained along the direction parallel to the interface. In such a scenario, the presence of a viscosity contrast generates torques on the particle promoting states for which the torque disappear (not motile states) or it is balanced by the interface (motile states) [3].
In the case in which active particles are suspended close to a fluid-fluid interface, the density field they generate will be distorted by the interface hence leading to various effective interactions when the confining surface is not a hard wall. I will show, via a simplified model, how different dynamics regime can arise and how they can lead to an effective attraction (repulsion) the particle from the interface. Finally I will briefly discuss collective effects [4].

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On the connection between computational and biochemical measurement

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From the literature on computation developed in the 20th century, and particularly in the wake of Maxwell's demon, much is known about the thermodynamics of taking a measurement or copying a system's state into a memory device. If it were possible to perform many measurements using a single bit of memory without putting in work, Maxwell's demon would be able to violate the second law of thermodynamics. It has been argued, however, that this is impossible, and the necessity of work in the measurement cycle has been demonstrated in a range of physical models [1-3]. The Landauer bound of $kT \ln 2$ sets the minimum amount of work that is required to perform a perfectly accurate vopy that has a 50/50 outcome [1,3].

Superficially, many biological processes appear to perform computational copies [1]. Perhaps the most tantalising analogy is in the context of cellular sensing of external ligand concentrations. In 1977, Berg and Purcell suggested the noisy signal from a single receptor could be improved by averaging the receptor signal over time [4]. It has since been argued that downstream signaling networks can achieve this by taking multiple measurements of the same receptor, essentially copying the receptor's state into memory [5-7]. Currently, however, the analogy between computational and biological systems is qualitative, rather than quantitative. How efficient are biological networks at performing copies, and can they reach the Landauer bound? Can the action of biological networks be understood in terms of typical idealized computational protocols? In this work we formally describe a steady-state receptor-readout network as a process that performs copies at a certain rate and with a certain accuracy. We relate the network directly to typical idealized protocols from the computational literature. We find that the biochemical network does not reach the limits of thermodynamic efficiency, with a cost per copy that diverges logarithmically as the system approaches 100% accuracy. This deviation is qualitative as well as quantitative, and optimal behaviour cannot be achieved simply by reducing copying speed. The biochemical network, however, is more adaptive than standard thermodynamically optimal protocols. Biased measurement outcomes (i.e., not 50:50) have a lower minimal cost per measurement [3], but achieving this limit requires a distinct ideal protocol for each bias. By contrast, the biochemical network automatically adapts to dissipate less when the measurement outcome is biased.

Fundamentally, the biochemical network has a constant thermodynamic drive set by the free energy stored in fuel molecules such as ATP, whereas optimally efficient computational protocols involve quasistatic manipulation of biasing potentials. We conclude by demonstrating that this difference can be overcome through exogeneous manipulation of ATP and ADP concentrations, enabling the design of biochemical copying protocols that reach the optimal Landauer bound. Our proposal provides a novel biochemical setting for the experimental investigation of non-equilibrium and information-related thermodynamics.

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Dissipative self-assembly steady states: from batch to open systems

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Living organisms reside in far-from-equilibrium states [1]: they need to consume nutrients, fluids, and oxygen to power the continuous chemical processes occurring in each of their cells, in order to stay alive. When the supply of food or nutrients is stopped for a certain time, the living systems relax to their thermodynamic equilibrium state, that is, death. Up to now, scientists in the field of supramolecular chemistry have managed to fabricate synthetic analogs of many of the intricate structures found in nature [2]. These synthetic supramolecular structures, impressive as they are mostly at thermodynamic equilibrium, or in kinetically trapped states. In sharp contrast with nature, however, we still struggle to keep self-assembled structures in a continuously dissipative—that is, an energy consuming—state. Here, we present different supramolecular systems that change their structure in response to magnetic fields, or by undergoing enzyme-mediated chemical reactions. The key challenge is to create supramolecular systems that can be switched rapidly and in a completely reversible way, so that many assembly/disassembly cycles can be performed in a short time. The structure and dynamics of the assemblies depends on the switching frequency, and thus on the distance from the equilibrium state [3].

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Influence of Time-Delayed Feedback on a Solitary Domain in an Excitable Reaction-Diffusion System

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Solitary localized domains can be observed in many types of dissipative systems, gas-discharge systems, semiconductor devises, nonlinear optical resonator, etc [1]. Since some of these systems are often expressed in nonlinear reaction-diffusion equations, it is worth to investigate the dynamics of solitary domains in a reaction-diffusion system. Especially in an excitable reaction-diffusion system, spontaneous traveling domains are realized by changing the reaction rate.

On the other hand, there are some studies about controlling patterns of dissipative systems by time-delayed feedback. Time-delayed feedback has been used to control a chaotic behavior in nonlinear systems. However, its application has been generalized to control the dynamics of dissipative patterns. Recently, it has been reported that applying the delayed feedback to the Swift-Hohenberg equation makes a stationary solitary domain travel [2].

We have investigated the influence of time-delayed feedback on a solitary domain in a one-dimensional excitable reaction-diffusion system. We have carried out numerical simulations of the modified FitzHugh-Nagumo model, which is one of activator-inhibitor systems, with the term of time-delayed feedback. We have considered two cases, one is that a domain is stably motionless and the other is that a domain is spontaneously traveling. These two cases are realized by changing the reaction rate as mentioned above. To obtain nontrivial results, we have applied a positive feedback in the former case and a negative feedback in the latter case. Increasing the absolute value of the feedback strength or delay time, we have found that a motionless domain begins to move in the former case whereas a traveling domain decreases its velocity and finally stops in the latter case. In addition to it, we have observed some interesting behaviors of a solitary domain such as a rocking motion, oscillatory traveling, etc.

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2.5 Mathematical & Computational Methods

Data mining and fusion for complex/multiscale dynamical systems

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I will discuss some issues that arise in the analysis/mining of dynamic data from complex systems - in particular, the detection of nonlinear intrinsic variables from multiscale dynamic data, and the fusion of different observation ensembles of measurements from the same experiment/computation. Our tool of choice will be Diffusion Maps (including various "twists" and extensions, like Vector Diffusion Maps and the use of the Mahalanobis distance, and various graph metrics for data-mining graphs).
I will also briefly discuss the integration of the resulting "coarse variables" in modeling and in enhancing/accelerating scientific computation.

Sensitivity of chemical reaction networks: A structural approach.

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In living cells a large number of reactions are connected by sharing substrates or product chemicals, forming complex network systems like metabolic network. One experimental approach to the dynamics of such systems examines their *sensitivity*: each enzyme mediating a reaction in the system is increased/decreased or knocked out separately, and the responses in the concentrations of chemicals or their fluxes are observed. However, due to the complexity of the systems, it has been unclear how the network structures influence/determine the responses of the systems. In this study, we present a mathematical method, named *structural sensitivity analysis*, to determine the sensitivity of reaction systems from information on the network alone. We investigate how the sensitivity responses of chemicals in a reaction network depend on the structure of the network, and on the position of the perturbed reaction in the network. We establish and prove a general law which connects the network topology and the sensitivity patterns of metabolite responses directly. Our theorem explains two prominent features of network in sensitivity: localization and hierarchy in response pattern. We apply our method to several hypothetical and real life chemical reaction networks, including the metabolic network of the E. coli TCA cycle. The theorem is useful, practically, when examining real biological networks based on sensitivity experiments.

What is An Amorphous Structure? –Topological View Point-

Yasumasa Nishiura[1], *Yasuaki Hiraoka*[1], *Takenobu Nakamura*[1], *Akihiko Hirata*[1], *Emerson G. Escolar*[2], *Kaname Matsue*[3]

[1]WPI-AIMR, Tohoku University, Japan

[2]Graduate School of Mathematics, Tohoku University, Japan

[3]The Institute of Statistical Mathematics, Japan

The description of amorphous structures has been a long-standing problem [1, 2], and conventional methods are insufficient for revealing intrinsic structures. In this talk, we propose a computational homological approach that provides indicators of amorphous structures. We found curves in the persistence diagram (PD) [3, 4], which describes shapes and scales of medium-range order (MRO). The presence of such curves explicitly indicates geometric constraints on amorphous structures, which have not been observed using conventional methods. Furthermore, the PD reproduces the wavelength of the first sharp diffraction peak (FSDP) observed in the structure factor and clarifies the real space origin of FSDP. These curves are preserved under strain, indicating that PDs also contain information on elastic response.

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Simple kinetics of complex biochemical systems

Stas Shvartsman, Princeton University

I will present recent results from our ongoing work on enzyme kinetics in developing embryos. We are studying the Extracellular Signal Regulated Kinase (ERK), an enzyme that phosphorylates dozens of proteins in cells of organisms from worms to humans, providing essential control of processes such as cell division and differentiation. We are using the early embryo of a fruit fly Drosophila melanogaster to visualize the dynamics of ERK activation and function, aiming to produce high resolution movies of ERK activity in a living tissue. In parallel, we are using genetic approaches and biochemical experiments with purified proteins to study how ERK controls its substrates. Studies at both ends of this spectrum, from individual proteins to whole organisms, are needed to fully appreciate the intrinsic complexity and functional capabilities of biochemical networks that control cells and tissues.

2.6 Control of Chemical Self-Organization

Hierarchical Selforganization: From Nanorods to Microscopic Biomorphs and Macroscopic Tubes

Oliver Steinbock
Florida State University, Department of Chemistry and Biochemistry, Tallahassee, FL 32306-4390, USA

Inorganic precipitation systems can generate a wealth of patterns that extend from the nanoscale into the macroscopic world. We report novel results obtained from selfassembly and selforganization processes in the coprecipitation of barium carbonate and silica. This reaction is known to create biomorphs which are complex micrometer-scale structures built from witherite nanorods. We specifically discuss periodic surface undulations on biomorph sheets that we analyze with atomic force, optical, and electron microscopy. We find nearly concentric stripe patterns as well as disorganized patterns that–based on 2D-FFT analyses–have the same micrometer-scale wavelength. The patterns form directly in the wake of the crystallization front and have a substantial height amplitude. We also present additional results obtained for chemical-garden-like systems and show that the formation of macroscopic tubes does not depend on the presence of polymerizable anions such as silicates, phosphates, or carbonates.

Writing down reaction-diffusion equations with DNA

Anton Zadorin[1], *Adrián Zambrano*[1], *Jean-Christophe Galas*[1], *Yannick Rondelez*[2] *and André Estévez-Torres*[1]

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[2]LIMMS/CNRS-IIS, University of Tokyo, Komaba 4-6-2 Meguro-ku , Tokyo, Japan

For decades, the Belousov-Zhabotinsky reaction and its cousins have been the reference experimental system to investigate the emergence of spatiotemporal complexity in chemistry. They are cheap, produce large color changes and provide suitable nonlinear feedback. They are, however, hard to engineer as it is very difficult to predict the reactivity of small molecules. As a possible solution to this drawback I will introduce a recent approach to engineer non-equilibrium chemical reaction networks using DNA and three enzymes. I will then describe the experimental implementation of various reaction-diffusion patterns with this system: monostable and bistable traveling fronts, predator-prey waves and spirals, and immobile fronts. I will conclude by showing that microfabrication and microfluidics may be interesting techniques to control the behavior of these patterns.

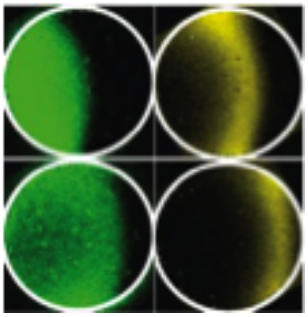

Figure 1: Prey waves (yellow) followed by predator waves (green) for a predator-prey DNA system in an unstirred circular reactor 11 mm in diameter (white line).

Control of Symmetry-breaking Patterns: Oscillation Death and Chimera States

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Symmetry breaking in a complex dynamical system is a universal phenomenon which occurs in diverse fields such as physics, chemistry, and biology. Special attention has recently been paid to oscillation death (inhomogeneous steady state) and chimera states (coexisting incongruous coherent and incoherent domains) both implying the breakup of symmetry. Using a paradigmatic model of coupled Stuart-Landau oscillators we study how these patterns can be controlled by introducing time-delay in the system. In particular, we show that time delay influences the stability of an inhomogeneous steady state, providing the opportunity to modulate the threshold for oscillation death [1]. Moreover, time delay allows to significantly increase the lifetime of transient amplitude chimera states [2].

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Front propagation in channels with spatially modulated cross-section

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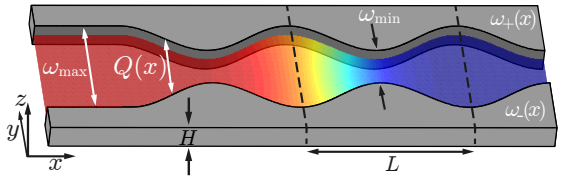
Reaction control is an essential task in biological systems and chemical process industry. A variety of approaches has been developed for the purposeful manipulation of reaction-diffusion (RD) systems, e.g., the application of feedback-mediated control loops with and without delays, external spatiotemporal forcing, or imposing heterogeneities [1]. Here, we focus on the control of RD patterns by designing an "optimal" geometry of reactive domains.



Sketch of a segment of a spatially modulated 3D channel confining the excitable medium. Color-coded is the concentration field $u(\mathbf{r}, t)$ of a front traveling from left to right.

In doing so, the propagation of traveling fronts in three-dimensional channels with spatially modulated cross-section $Q(x)$ is studied using the Schlögl model as a representative example for reaction-diffusion systems. Applying perturbation techniques leads to a reduction of dimensionality in which the spatially dependent Neumann boundary condition translate into a boundary-induced advection term [2]. Treating this advection term as a weak perturbation, an equation of motion for the traveling wave position in weakly corrugated confinements is derived [3]. Comparisons with numerical simulations demonstrate that our analytical results properly predicts the nonlinear dependence of the propagation velocity on ratio of the spatial period of the confinement L to the intrinsic width of the front l; including the peculiarity of propagation failure [2]. Based on the eikonal equation, we obtain an analytical estimate for the finite interval of propagation failure. In particular, we demonstrate that the front velocity is determined by the suppressed diffusivity of the reactants [4] if the intrinsic width of the front is much larger than the spatial variation of the medium, $L/l \ll 1$.

Furthermore, we present a method to control the position $\phi(t)$ of TW solutions to RD systems in modulated channels according to a prespecified protocol of motion. Given this protocol, the boundary function $Q(x)$ is found as the solution of the perturbatively derived equation of motion. Noteworthy, such a boundary control $Q(x)$ can be expressed in terms of the uncontrolled wave profile and its propagation velocity, rendering detailed knowledge of the reaction kinetics unnecessary.

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2.7 Electrochemistry & Surface Reactions

Travelling Vanadium Oxide Islands in a Catalytic Reaction

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Upon evaporation of a submonolayer coverage of vanadium in O_2 onto a Rh(111) surface one obtains well ordered two-dimensional V-oxide islands which we use as model catalysts for the partial oxidation of methanol to formaldehyde[1]. With photoemission electron microscopy (PEEM) we observe that under reaction conditions in the 10^{-4} mbar range the initially homogeneous VO_x film (θ_V=0.2) transforms upon heating at 560 °C into a quasi-stationary macroscopic concentration pattern. This pattern consists of equally spaced parallel stripes of condensed VO_x which are surrounded by nearly bare metal surface. Above 700 °C the stripe pattern changes into a spot pattern of nearly perfectly circular VO_x islands of about 20 - 200 μm diameter. Due to effective attractive interactions these islands approach each other with a velocity which depends on the distance reaches up to a few μm/s. The islands coalesce and afterwards their shape becomes rapidly circular again thus indicating a high line tension at the island boundaries. Remarkably, the islands only move under reaction conditions. A mechanism is proposed which is based on the chemical equilibrium of polymerization of individual VO_x clusters into macroscopic VO_x islands. Since the polymerization / depolymerisation equilibrium is controlled by the oxygen coverage the oxygen gradients surrounding the VO_x islands under reaction conditions can cause a movement of the islands towards each other.

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Noisy CO oxidation on Iridium(111) and Palladium(111) surfaces

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The influence of noise could be described theoretically quite easily, but is hard to measure in an experiment. Reactions on surfaces can be described by nonlinear reaction-diffusion equations. For the CO oxidation on Iridium(111) and Palladium(111) surfaces the influence of noise has been examined directly in ultra high vacuum (UHV) experiments [1,2]. The recorded probability distribution of CO_2 rates around a mean value show directly the influence of the superposed noise. All observations are explained directly with the underlying theoretical description – the Langmuir-Hinshelwood reaction scheme – by solving the equations under realistic assumptions. The averaged CO_2 rate is high in the more reactive state (upper rate, UR, predominantly oxygen covered) and low in the lower rate (LR, predominantly CO covered). The measured effect of colored noise [3], strongly colored noise [4] and large non-Gaussian noise [5] on a bistable surface reaction, such as transitions, bursts and switching is described theoretically. While on Iridium(111) no reversible changes between upper and lower rate are observed for up to medium noise [1,6], on Palladium(111) in addition reversible, short and frequent rate changes between both rates are observed [2,7].

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Electrochemical Regulation and Detection of the Cyanobacterial Circadian Rhythm

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There is growing awareness that circadian clocks are closely related to the intracellular redox state across a range of species. As the redox state is determined by the exchange of the redox species, electrochemically controlled extracellular electron transfer (EC-EET), a process in which intracellular electrons are exchanged with extracellular electrodes, is a promising approach for the external regulation of circadian clocks. Herein, we discuss whether the circadian clock can be regulated by EC-EET using the cyanobacterium *Synechococcus elongatus* PCC7942 as a model system. In vivo monitoring of chlorophyll fluorescence revealed that the redox state of the plastoquionone pool could be controlled with EC-EET by simply changing the electrode potential. As a result, the endogenous circadian clock of *S. elongatus* cells was successfully entrained through periodically modulated EC-EET by emulating the natural light/dark cycle, even under constant illumination conditions. This is the first example of regulating the biological clock by electrochemistry.

Spatial pattern formation in electrochemical dissolution of silicon

Kazuhiro Fukami
Department of Materials Science and Engineering, Kyoto University, Kyoto 606-8501, Japan

In electrochemical reactions, spatiotemporal pattern spontaneously formed on electrode surfaces have often been reported. Of these, the pattern formation on semiconductor electrodes has recently attracted attention. In the present study, we focus our attention to electrochemistry of silicon. Because of the rectification behavior of silicon electrodes, electrodissolution of p-type silicon occurs in the dark. On the contrary, that of n-type proceeds only under illumination. In addition, there are several properties that are different from metal electrodes.

In the present paper, spatial pattern formation on p-type silicon electrodes is discussed in detail. When a p-type silicon electrode is electrochemically anodized in HF solution containing alcohol, a microgroove array is spontaneously formed on the surface [1]. The experimental results suggest that the microgroove is a sort of Turing-type pattern. The characteristic size of the Turing-type pattern is quite small compared with Turing-type pattern reported in electrochemical systems. The reason why the pattern is so small is discussed by considering the semiconductor property of the electrode together with the homogeneous dynamics of the system.

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2.8 Special Symposium on the occasion of the 65th birthday of Alexander Mikhailov

How nonequilibrium conditions influence the dynamics of synthetic motors

Raymond Kapral
University of Toronto

Chemically-powered nanomotors operate by converting the energy supplied in chemical reactions into directed motion. Sustained directed motion is possible
only when the system is constrained to lie out of equilibrium by supplying fuel
and removing product in the system. The dynamics of
nano and Angstrom-scale motors under various nonequilibrium conditions will be described.

Oscillations and waves in the actin system of motile cells

Carsten Beta
Institute of Physics and Astronomy, University of Potsdam.

Actin-driven cell motility plays an essential role in a wide range of biological processes including wound healing, cancer metastasis, and responses of the immune system. In recent years, it became increasingly clear that the dynamics of the actin system show well-known hallmarks of pattern formation in a spatially distributed active medium. For example, we could show that the actin machinery of chemotactic *Dictyostelium* cells operates close to an oscillatory instability. In response to periodic stimuli, we found a clear resonance peak at a period of around 20 s. To explains our experimental findings, we introduced a delayed feedback model that is based on a time-delay in the regulatory network of the actin system. On a sub-cellular scale, dynamic wave patterns can be observed at the substrate-attached side of the actin cortex. Using electro-fused giant cells, we observed that these waves are composite structures consisting of a PIP3-rich band enclosed by an actin-rich border. They show typical properties of an excitable system, like a conserved width, a constant propagation velocity, and annihilation upon collision. To investigate whether localized receptor stimuli can induce the spreading of excitable waves, we delivered spatially confined cAMP stimuli to the cell membrane. We observed that the activity of the signaling pathway remained spatially confined to the stimulated membrane region and no receptor-initiated spatial spreading of excitation waves was observed — a finding that can be explained on the basis of a local excitation/global inhibition (LEGI) mechanism.

Theoretical Study on Clustering near Hopf Bifurcation, Reentrant Transition with Strong Coupling, and Jet lag.

Hiroshi Kori
Department of Information Sciences, Ochanomizu University, Tokyo, Japan

Synchronization often plays a vital role in chemical and biological systems. The theoretical frameworks of synchronization are necessary for the understanding and control of synchronization dynamics. In particular, they have been well developed in two parameter regimes. One is in the vicinity of a Hopf bifurcation, in which complex amplitude equations such as Ginzburg-Landau and Stuart-Landau equations are available. The other one is weak coupling among oscillators, in which phase approximation is applicable. Although those methods are very powerful, they can not treat all the rich dynamics that appear in such and other regimes. One example is clustering behavior, which has been observed near a Hopf bifurcation in an electrochemical system [1]. Another example is a reentrant synchronization transition that occurs in an noisy oscillator strongly coupled to a pacemaker [2]. Conventional theories fail to predict these examples. In this presentation, I will present recent progresses on the development of theoretical frameworks. I will also discuss the mechanism of jet lag [3] in light of such frameworks.

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2.9 Synthetic Molecular Biology

Pattern formation in minimal biological systems

Petra Schwille
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Martinsried, Germany

One of the most distinctive features of living systems is the ability to create order and spatial structures out of seemingly equilibrated systems in the aqueous environment. The relatively simple mathematical conditions for symmetry breaking and pattern formation were formulated in 1952 by Alan Turing, in order to describe biological morphogenesis. However, to date only few self-organizing biological systems have been identified that were indeed simple enough to be quantitatively described on basis of few parameters. One of these systems is the MinCDE protein machinery, wich orchestrates the positioning of the division ring in E.coli bacteria. The Min proteins show a distinct oscillation of protein concentrations between the two cell poles, which are based on self-organization through reaction-diffusion. We have been able to reconstitute these self-organized oscillations of purified proteins in artificial cell-shaped compartments, as well as the faithful downstream positioning of protofilaments of the Z division ring. This could be the first step towards autonomous division of an artificial cell system which we aim to establish in a bottom-up synthetic biology approach.

A minimal system to establish microtubule-based cell polarity in fission yeast

Marileen Dogterom, TU Delft, NL

Establishment of cell polarity is essential for processes such as growth and division. In fission yeast, polarity factors travel at the tips of microtubules to the cell ends where they associate with the membrane and subsequently maintain a polarized pattern. While many molecular components have been shown to play a role in this polarization process, it remains unknown which molecular functionalities are minimally required. We show that a single chimera protein that combines a membrane-binding motif with microtubule tip affinity is able to transiently concentrate at cell ends in wild type fission yeast cells. In addition, we established an in vitro system that allows us to verify the minimal molecular requirements for microtubule-based cell polarity in artificial confinement. First results will be discussed.

Dynamics of synthetic gene circuits in vitro and in vivo

Friedrich C. Simmel

Synthetic biology aims at the design of novel biological “parts” and systems and their technological applications. However, biological systems are complex compared to most technical systems and consist of many multiply interacting (and often poorly characterized) components. Therefore it is often found that a “rationally” designed synthetic system does not behave in the way expected. One way to reduce the complexity of the design task is to study simplified in vitro systems as “toy models”.
As one example, we recently investigated a variety of synthetic in vitro “gene” circuits, which are only based on in vitro transcription reactions (i.e., RNA production). With these, we generated chemical oscullators, studied the influence of load in master-slave circuit configurations, and also investigated the impact of microcompartmentalization on the dynamics of the circuits.
Even though we deal only with a relatively small number of biomolecular species, our synthetic systems already display a considerable degree of complexity and variability.
At the end of the talk, we will also give a short overview over “the real thing”, i.e., our humble attempts to engineer and study real biological systems.

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Driving molecular life with a thermal disequilibrium inside rock pores? Christof Mast, Lorenz Keil, Moritz Kreysing, Simon Lanzmich, Friederike Möller, Matthias Morasch and Dieter Braun, Systems Biophysics, Physics Department, Center for Nanoscience, Ludwig-Maximilians-Universität München, 80799 Munich, Germany, email: dieter.braun@lmu.de

Introduction: The Origin of Life is one of the fundamental, unsolved riddles of modern science. Life as we know it is a stunningly complex non-equilibrium process, keeping its entropy low against the second law of thermodynamics. Therefore it is straightforward to argue that first living systems had to start in a natural non-equilibrium settings. Recent experiments with non-equilibrium microsystems suggest that geological conditions should be able to drive molecular evolution, i.e. the combined replication and selection of genetic molecules towards ever increasing complexity.

Non-Equilibrium Settings: As a start, we explored the non-equilibrium setting of natural thermal gradients. Temperature differences across rock fissures accumulate small monomers more than millionfold [1] by thermophoresis and convection [2]. Longer molecules are exponentially better accumulated, hyperexponentially shifting the polymerization equilibrium towards long RNA strands [3]. The same setting implements convective temperature oscillations which overcome template poisoning and yield length-insensitive, exponential replication kinetics [4]. Accumulation and thermally driven replication was demonstrated in the same chamber, driven by the same temperature gradient [5]. Protein-free, non-ligating replication schemes can be driven by thermal convection. For example, the hairpins of tRNA can be used for reversible codon-sequence replication, bridging from replication of genes to the translation of proteins [6]. Non-templated polymerization and hybridization- dependent degradation leads to replication-like information transmission [7]. Replication and trapping of DNA persist over long time in a constant influx of monomers, closely approaching the criteria for an autonomous Darwin process.

Biotechnology Spinoff: Experiments using non-equilibrium conditions at the microscale are non-trivial. For example, molecules have to be detected selectively with the most sensitive biochemical, optical and microfluidic approaches. Advances of biotechnology in this regime is very fruitful. Our award winning NanoTemper spinoff company, with now more than 70 employees, demonstrated that basic research for the origin of life can lead to cutting edge biotechnology [8][9].

Environments: Besides temperature gradients, many more non-equilibrium settings can be imagined and become increasingly accessible to experimentation. For example, geological pH gradients, geological redox potentials or the optical excitation of geological nanoparticles should drive metabolic reactions in a very peculiar way. To be successful, an effort on the origin of life has to be embedded in a strong and very active interdisciplinary background of biology, biochemistry, chemistry, astrogeology and not the least, theoretical modeling at various levels of abstraction.

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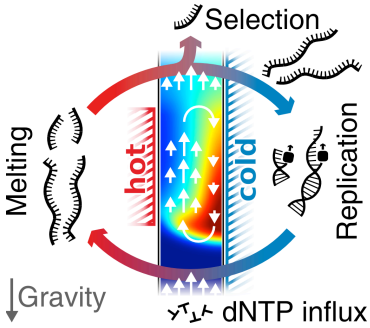

Selection for increasing complexity: The replication of long nucleic acid sequences was required for the evolution of biological complexity during the origin of life; however, short sequences are normally better replicators than long ones. Recently, we showed how a common physical environment provides a simple mechanism to reverse this trend and enables long sequences to flourish [10].

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Duration Robustness of Linear Signaling Cascades

Jon Young [1], *Kunihiko Kaneko* [1], *Tetsuhiro S. Hatakeyama* [1]

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Signal transduction networks are a key component in many cellular processes, and as such their properties have been studied extensively. Recently, the dynamics of these networks have received attention for their ability to process and encode temporal information about their environment. This opens many more avenues of signal processing that cells could take advantage of. However, in order for temporal duration to be used as a source of information, it is necessary that these temporal profiles be robust to changes in the cellular environment. Robustness, insensitivity of a state against perturbations, is one of the most important characteristics in biology, but most studies have focused on the stability of fixed states and not necessarily on the transient dynamics.

We have used mathematical modeling and phase space analysis to investigate whether the temporal profiles of linear signaling cascades can exhibit robustness to changes in phosphatase concentrations. We have found that the response duration against a transient input does indeed have an intrinsic robustness. Furthermore, the response decay can exhibit plateauing behavior. This suggests that storing information as a temporal profile is feasible and that a linear signaling cascade motif may be used as a form of short term memory storage.

2.10 Contributed Talk Session II

Solid/Liquid Interfaces in Ionic Liquids: From Scientific Debates to Electrochemical Energy based Applications

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The efficiency of electrochemical renewable energy devices is largely determined by electrolyte and solid/liquid interface properties. The former facilitate charge density and transport while the latter are responsible for charge transfer or capacitance. Thus, both high charge density and interfacial properties are subjected to intensive studies towards efficiency improvements. Room temperature ionic liquids (RTILs) are attractive for such applications due to their high charge density as well as for their tunable anion/cation design, low vapor pressure and wide electrochemical windows. However, intense investigations of RTILs have triggered scientific debates about spatial ion distributions within the bulk and near the solid/liquid interfaces. While many observations report on an alternating charge layering (i.e., spatially extended decaying charge density oscillations) [1], there are recent conjectures that ionic liquids bare similarity to dilute electrolytes (including a monotonic diffuse layer) [2]. Using a modified Poisson-Nernst-Planck model for ionic liquids, we show that both behaviors appear as fundamental properties of ionic liquids [3]. The transition from non-monotonic (oscillatory) to monotonic structure of electrical diffuse layers appear to non-trivially depend on ionic density in the bulk and affected by the applied voltage, domain size, molecular packing, and short range electrostatic correlations [4]. Consequently, the results not only reconcile between the empirical observations but also provide novel vistas to nonlinear electrochemical aspects of highly concentrated electrolytes.

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Oscillatory behaviour in an array of globally coupled noisy bistable microelectrodes

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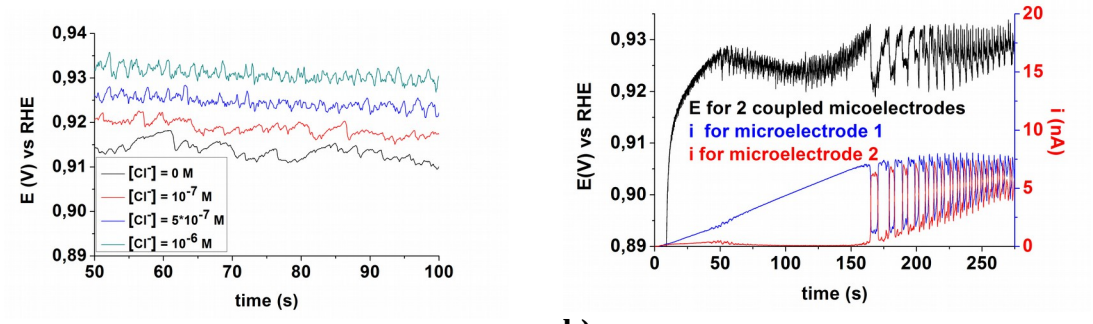
The understanding of the properties of nanostructured electrochemical systems is of utmost importance for many fields of applications, such as batteries, fuel cells, physico-chemical sensors, or corrosion. When reactions with nonlinear kinetics occur in nanostructured systems, new cooperative phenomena, which do not exist at the macroscopic scale, may emerge, depending on the size of the active elements and on the nature and strength of the coupling between them.

The electro-oxidation of CO on Pt electrodes is an archetype of electrochemical bistable reaction kinetics associated with an S-shaped negative differential resistance in the current-potential curve. In this presentation, we will discuss first the potential fluctuations that can be observed with a single Pt microelectrode during the galvanostatic CO oxidation in the presence of a small amount of chloride anions in the electrolyte (cf. Fig. 1a). In a second part, we will focus on the emergence of regular potential oscillations when at least two fluctuating microelectrodes are globally coupled. The individual currents flowing through each microelectrode during the galvanodynamic scan could be measured using a custom-made galvanostat (Figs. 1b). The cooperative behaviour of the electrochemical system will be discussed with the help of a mathematical modelling of CO electrooxidation using finite element simulations. In particular, the influence of the microelectrode size on the oscillatory behaviour will be experimentally and theoretically explored.



a) **b)**

Figure 1: Oscillatory behaviour during the galvanodynamic scan (GDS) of one single (a) and two short-circuited (b) microelectrodes in CO saturated 0.5 mM H_2SO_4 in the presence of different concentration of chlorides.

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Classification of cross-diffusion-driven convection in 2-component double-layer systems: Theory and Experiments.

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Cross-diffusion, whereby a flux of a given species entrains the diffusive transport of another species, can trigger unconventional buoyancy-driven hydrodynamic instabilities at the interface of initially stable stratifications [1,2,3]. Here a cross-diffusion-convection (CDC) model is derived by coupling the fickian diffusion to the Stokes equations [1]. In order to isolate the effect of cross-diffusion in the destabilization of a double-layer system, we impose in the bottom layer a starting concentration gap in one of the species while the other is homogeneously distributed over the spatial domain. We show that, depending upon which species features the initial concentration gap, we can selectively activate different cross-diffusion feedback and promote two possible types of hydrodynamic scenarios (negative cross-diffusion convection, NCC, and positive cross-diffusion convection, PCC) corresponding to the sign of the operational cross-diffusion term. The study of the space-time density profiles along the gravitational axis allows to obtain analytical conditions for the onset of convection in terms of two important parameters: the dominating cross-diffusivity and the buoyancy ratio, giving the relative contribution of the two species to the global density. The general classification of the NCC and PCC scenarios in this restricted parameter space is supported and complemented by numerical simulations of the fully nonlinear CDC problem. The resulting spatio-temporal convective dynamics excellently compare with experiments performed with AOT water-in-oil reverse microemulsions (ME) [2], in which initially stable stratifications between two ME are studied in a Hele-Shaw cell by just imposing a gradient in water or AOT concentration. ME are shown to be a convenient model system for inducing both convective modes predicted and, while PCC scenarios have been already identified experimentally in previous works [3], NCC modes are isolated, for the first time, with ME. Our approach constitutes a reference framework for future studies on pattern formation arising from the interplay between cross-diffusion convection and chemical reactions.

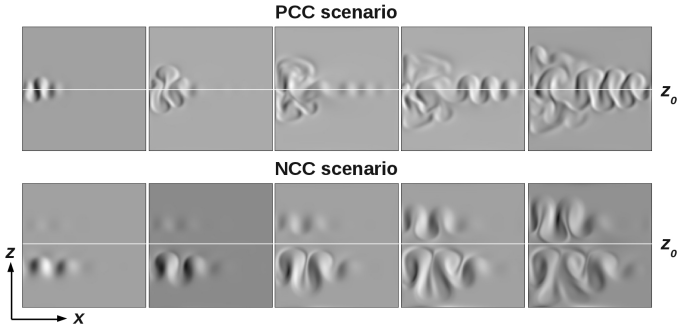

Figure 1: Typical spatio-temporal evolution of a PCC (top) and a NCC (bottom) instability.

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Unusually simple way to create spiral wave in an excitable medium

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Spiral waves are generic spatio-temporal patterns, which have been observed in a broad spectrum of excitable media in chemistry, biology and medicine. While during the aggregation of Dictyostelium discoideum spiral chemotactic waves play a decisive role in the colony self-organization, the appearance of spiral electrophysiological waves in the heart muscle is known to completely disorganize rhythmic activity resulting in cardiac arrhythmia and sudden death. One very important problem is to identify mechanisms of spiral wave initiation that can help to predict and/or to prevent the appearance of this life-threatening self-sustained activity. To date the paradigm for spiral wave initiation requires at least two excitation stimuli. Here we show that, under quite natural conditions, spiral waves can be created after application of one stimulus only. The discovered unusually simple scenario is based on a counterintuitive fact that in an inhomogeneous excitable medium a rapid spatial increase in wave propagation velocity can result in a propagation block. We present quantitative conditions for the propagation block in a one-dimensional medium and demonstrate that the inhomogeneity can be easily modified to create a unidirectional propagation block that is known to result in reentry in the cardiac tissue. The proposed natural scenario gives new insights into deleterious spiral waves generation and has to be taken into account in the theoretical and experimental investigations especially in context of cardiac arrhythmias.

2.11 Waves and Patterns in Active Media

Self-organisation and Patter Formation in Carcinomas and their Microenvironment

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When cancer cells are mixed with normal cell they self-organize in a tumour spheroid surrounded by normal cells. This cell aggregation in tumours is not driven by differential adhesion. Cell jamming is a key factor that stabilizes the tumour boundary. The epithelial mesenchymal transition (EMT) can be described as an unjamming transition alike a solid to fluid transition in glasses. Cell softening in rigid tumours triggers the formation of channels for cellular streaming. The mechanical alterations to a tumour's microenvironment are a measure for the barrier strength and spatial sharpness of a tumour boundary.

Patterns in Polarisable Elastic Active Layers

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We explore a class of macroscopic continuous models with feedback interactions inducing spontaneous vector or nematic polarisation and mechanical deformation of elastic active media. Linear stability analysis predicts, depending on the sign of feedback interaction coefficients, either monotonic or oscillatory instability of the homogeneous isotropic state. In the former case, the emerging pattern undergoes a slow coarsening process but permanent polarity may emerge when the system is topologically constrained. Oscillatory instabilities arise in active systems on a finite wavelength, and lead to complex wave patterns. Transition to a deformed polarised state may be frustrated in constrained geometry but leads to boundary undulations in free-boundary settings.

Migratory behaviour of Physarum polycephalum microplasmodia

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The motility of amoeboid cells of the plasmodial slime mould *Physarum polycephalum* was studied experimentally. Analysis of their trajectories and of their mean square displacements reveal two characteristic types of behaviour that depend on the time interval τ between any pair of points along the trajectory. Whereas free migration of cells is observed for time intervals $\tau > 300$ s, at short time intervals (of up to $\tau \approx 100$ s) the motility is due to changes in the cell shape induced by the peristaltic pumping of protoplasm though the cell [1]. Freely migrating cells display persistent random motion with very long persistence times of up to $\approx$ 1.5 h. Superdiffusive motion typically lasts for ≈ 5 h, while at longer times the dynamics becomes diffusive. Whereas symmetric velocity distributions are found for short time intervals τ, the typical velocity distributions from freely migrating cells show an asymmetric component, which reflects the long-lasting persistent motions. We observed that high propagation velocities are correlated with both, episodes of straight motion and an elongated cell shape [1]. Furthermore, the patterns of cell thickness oscillations (that provide for theintracellular peristaltic pumping of protoplama) also changed as a function of the propagation velocity of the cell [2].

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Modeling crawling cell motility

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Self-propelled motion, emerging spontaneously or in response to external cues, is a hallmark of living organisms. Self-propulsion relies on the force transfer to the surrounding. While self-propelled swimming in the bulk of liquids is fairly well characterized, many open questions remain in our understanding of self-propelled motion of cells along substrates. Here we present a phenomenological model for crawling cells based on an advected phase field model and other reaction-diffusion equations. The force transfer from the cell to the substrate is explicitly taken into account, giving rise to complex modes of cell movement such as bipedal motion and stick-slip motion. The model captures the generic structure of the traction force distribution and faithfully reproduces experimental observations, like the response of a cell on a gradient in substrate elasticity (durotaxis). Collective states of motion such as concerted rotation arises for multiple interacting cells on patterned substrates [1,2].

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2.12 Self-Organization in Biological Cells

Active mechanics of epithelia during morphogenesis

Guillaume Salbreux, The Francis Crick Institute,London, UK

Epithelial tissues are dynamically remodeled during development due to forces generated in the cells, cellular rearrangements, and cell division and extrusion. Such remodeling leads over long timescales to reorganization of the tissue, allowing to establish the shape of the organism. In this work, we introduce a physical description of the slow timescale behavior of an epithelium. We obtain hydrodynamic constitutive equations describing the continuum mechanics of an epithelium on spatial scales larger than a cell. Within this framework, topological rearrangements relax elastic stresses in the tissue and can be actively triggered by internal cell processes. Using segmentation of the wing disc cell packing at pupal stage of the fly, we analyze experimental coarse-grained patterns of flow field and tissue shear within the continuum theory framework. We show that topological transitions respond to cell elongation with a delay, and are autonomously polarised in the tissue.

Fundamental limits to sensing

P. ten Wolde[1]
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Chemical and chiral oscillations in simple polymerization models

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[3]Centro de Astrobiologia (CSIC-INTA), Torrejon de Ardoz (Madrid), Spain

Some fundamental building blocks of living matter, such as amino acids and sugars show the preference of one of the two chiral states of an otherwise chemically identical molecule. The origin of this so-called biological homochirality is still a matter of debate, even after decades of intense theoretical and experimental work. At the heart of many theoretical approaches lies a mechanism responsible for spontaneous mirror symmetry breaking, leading finally to stable stationary states of given chirality, i.e., states with nonvanishing enantiomeric excess. In this talk, we discuss a model purporting to describe general chiral polymerization processes, devised for explaining the appearance of homochirality. We observe the onset of stable chemical oscillations in this model which are in fact related to the appearance of oscillations in the enantiomeric excess, the so-called chiral oscillations. We compare this to the phenomenon of chiral excursions, found in similar systems, but which do not show permanent symmetry breaking. We discuss the importance of the results in light of recent experiments on amino acids reporting chiral oscillations.

Cell fate decisions using a simple multi-cell model with inhibitory cell-cell interaction and noise

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Cell differentiation is one of the most fundamental ability of biological cells. Although biological system includes both of internal and external noises, the differentiating system seems to be robust to these fluctuations. For example, the differentiation ratio (the ratio between different types of cells) in a cell population is well maintained in a biological system. In the differentiation process, cell states are governed by the expression levels of certain genes. Recent experiments revealed that a inhibitory interaction between cells has crucial importance for the differentiations process in a cell population. However, the basic mechanisms of cell differentiation process is still under debate.

To understand the basic mechanisms of binary cell fate decisions, we introduce a simple multiple cell model with a lateral inhibitory cell-cell interaction. The state of cell i, which is supposed to determine its fate, obeys a dynamical equation of following form:

$$\dot{s_i} \quad = \quad -\frac{\partial \phi_0(s_i)}{\partial s_i} - k\langle s \rangle_i,$$

where s_i $(i = 1, \ldots, n)$ and k denote the state variable of cell i and the interaction intensity, respectively. The $\phi_0(s) = f_0(1 - s^2)^2$ is a basic potential of this differentiation process and it is affected by average state of other cells $\langle s \rangle_i (= \sum_{j \neq i} s_j / n_i)$. During the differentiation process, the temporal gradient of the potential landscape for each cell changes depending on its surrounding situation.

Starting from the initial condition in which all the cells are in an undifferentiated state (*i.e.*, averaged state variable of all the cells $\langle s \rangle \sim 0$), the state of cell i evolves according to the dynamical equation given above and the system finally reaches an equilibrium state in which all cells differentiate into two different states.

In this model, cell fate of the entire system (the range of proportion R of the number of cells in one state to the total number of cells) is bounded by the reciprocal of the interaction intensity k of as $\mid R - 1/2 \mid \propto k^{-1}$ for $n \to \infty$. In another front, the reliability of the differentiation ratio has an optimal interaction range (number) to gain the reliability of the proportion R. In cases where cells distribute randomly in a two dimensional space, the reliability decreases within a scale of a few cells, because probability of cell-cell interactions increases depending on the interaction range. On the other hand, the reliability increases in the larger scale and converges to a finite variable in a finite size system. Crossover between these two trends gives an optimal range of the differentiation reliability.

2.13 Collective Cell Migration and Chemotaxis

Role of chemotaxis in surface attachment and self-aggregation of *Escherichia coli*

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Bacterial chemotaxis is typically viewed as a single-cell phenomenon, and the importance of motility and chemotaxis in the collective behaviors of bacterial populations remains largely unclear. We investigated the role of motility and its regulation for the two types of collective behavior observed for E. coli, biofilm formation at the surface and formation of multicellular aggregates in cell suspension. We observe that chemotaxis plays an important role for both processes, emphasizing that it might be equally important for individual bacteria and for their populations.

Physical guidance of Cell Migration

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[1]University of Maryland, USA

Formation of Microcolonies in *Neisseria gonorrhoeae* bacteria

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[2]Department of Biology, Brooklyn College, New York, USA

Neisseria gonorrhoeae is the causative agent of the second most common sexually transmitted disease gonorrhea. The bacteria use type IV pili, thin and μm-long filaments protruding out of the cell membrane, to move over a substrate by a process called twitching motility [1]. While the motility of single has been extensively studied during the past years [2,3] the processes that drive the formation of microcolonies are poorly understood.

Bundling of two pili causes attractive cell-cell-interactions that are sufficient to induce the formation of microcolonies consisting of a few hundreds to thousands of cells [4]. One fundamental process during the formation of colonies is coalescence, the merging of two microcolonies into a single larger colony.

We show experimentally that the merging can be characterized by a fast initial approach of the colonies within a few minutes that is followed by a slow relaxation to the spherical shape with a characteristic time of a few hours. A simulation model of cells interacting solely via pili is sufficient to reproduce these experiments.

In order to explain this behavior, we suggest that microcolonies consist of a bulk of cells with a weak mobility and a layer of highly motile cells. Measurements of the mean square displacements of cells in of the bulk and on the surface in both experiments and simulations corroborate this idea.

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Theory on chemotactic migration of eukaryotic cells

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Eukaryotic chemotactic migration is a ubiquitous kind of cell motility, which plays key roles for the immunological response and developmental processes. Cells perform chemotaxis by intracellular signals that tend to localize at the front or back of the cell according to the guidance cues. It is known that such localization occurs even without extracellular cues, which suggests that isotropy is spontaneously violated in the cellular signal network. In light of this, we established the theoretical model for chemotactic migration of a eukaryotic cell with intrinsic polarity, and studied statistics in cell migration [1,2].
In this presentation, I will explain our model and share with you several theoretical results. Our model simulates migration of a chemotactic cell in a chemoattractant solution with the following assumptions:
• The cell spontaneously maintains intrinsic polarity.
• The cell infers the gradient direction by reference to binding states of chemoattractants to receptors on the cell surface.
• The cell tends to reorient the polarity toward the inferred gradient direction. The polarity is also subjected to noise in the intracellular signal process.
• The cell migrates to the polarity direction with a constant speed, so that chemotaxis is realized by the bias of the polarity direction due to the chemical gradient.
Based on this model, firstly I will discuss statistics in spontaneous migrations of a chemotacting cell in a uniform chemoattractant solution. The chamoattractant-concentration dependence of the correlation time of migration directions is derived from our model, and the result agrees with the experimental data for *Dictyostelium discoideum*. We also derived the probability distribution of migration directions in a chemical gradient and the chemotaxis index, which quantifies the accuracy of chemotaxis. We found that the accuracy is improved by introducing the spontaneous intracellular polarity, that optimally accurate chemotaxis is achieved at an intermediate responsiveness of the polarity to chemical gradient, and that polarized *Dictyostelium* cells adopt such optimal responsiveness [1].
Furthermore, I would like to shortly talk about the theory on chemotaxis of an elliptically deformable cell [2,3] and application of our theoretical model to the collective chemotactic migration. Further details will be provided in the presentation.

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3 Posters

3.1 Active Particles

Kramers Escape Problem for Self-Propelled Particles

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In the poster presentation, the dynamics of a self-propelled Brownian particle in an attractive harmonic potential is investigated. Within a 1D constant speed modeling of the particle's dynamics we consider the stationary probability distribution using both numerical and analytical approaches. By means of the results obtained hereby, subsequently the escape problem of a self-propelled particle from a metastable potential well is considered, which is discussed in detail in Ref. [1] for the case of a vanishing self-propulsion.

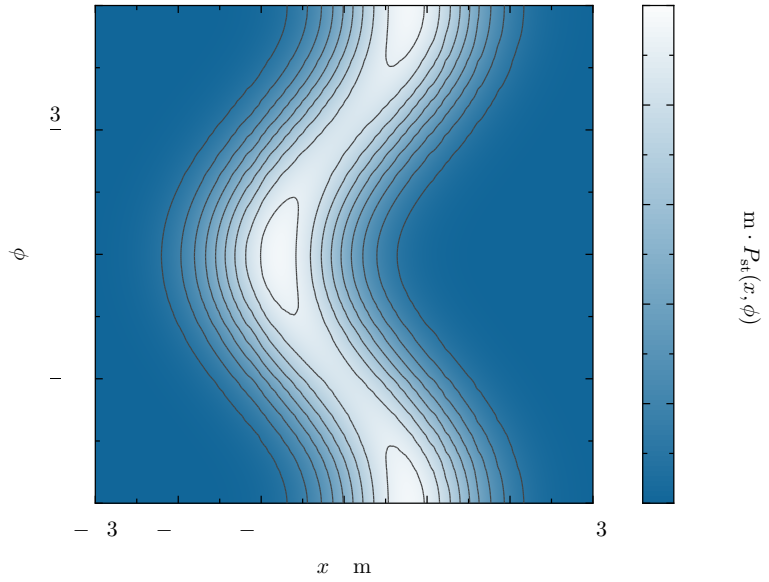

Figure 1: Graphical representation of the stationary probability distribution $P_{\mathrm{st}}(x,\phi)$ of a self-propelled particle's state (x,ϕ) in a harmonic potential, where x denotes the position and ϕ the orientation of the particle.

Regarding the properties of the stationary state in a harmonic potential, two major timescales are found, governing each the translational and the rotational dynamics of the particle. Here, the particle radius is identified to be the essential quantity regulating the ratio between those timescales. For very small and very large particle radii, as well as for weak propulsion forces, approximate analytic expressions for the stationary probability distribution of the particle are derived. These analytic results compare favorably with exact numeric outcomes. Moreover, with respect to Kramers' escape problem, the analytical approximations prove to be quite beneficial, since—within their respective range of validity—the thereby obtained expressions for the escape rate coincide well with numerical findings.

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Numerical Modeling of Collective Dynamics of Self-Propelled Particles -Phonon Like Behavior-

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Understanding the dynamics of self-propelled particles (SPP) is very important for medical engineering applications, for example to achieve targeted drug delivery. In SPP dispersion systems, hydrodynamic interactions play an important role, however, only few studies have succeeded in calculating the dynamics of these systems taking into account the full hydrodynamic effects.

In this work, we conducted direct numerical simulations of 3D SPP dispersion systems with full hydrodynamics. To achieve this, we employed a simple model for SPP, which is called the Squirmer Model[1]. In this model, we treat the SPP as spherical particles with a specified slip velocity on their surface. This surface velocity is responsible for the self propulsion, and can distinguish between different types of swimming: "pushers", or swimmers which generate an extensile flow field, and "pullers", which generate a contractile flow field. This model can be easily incorporated into an efficient calculation method for the dynamics of solid/fluid two phase systems, called the Smoothed Profile Method(SPM)[2]. Using this model and method, we could calculate the dynamics of SPP swimming in a viscous fluid with full hydrodynamics.

Calculating the dynamic structure factor, we found that such systems can have pseudo-phonon-mode dynamics in the absence of any external force. As shown in Fig. 1, we see pseudo sound waves with a velocity equivalent to that of the average SPP swimming velocity. In addition, we confirmed that "pushers" and "pullers" show quite different phonon-mode dynamics. "Pullers" exhibit much larger density fluctuation than "pushers".

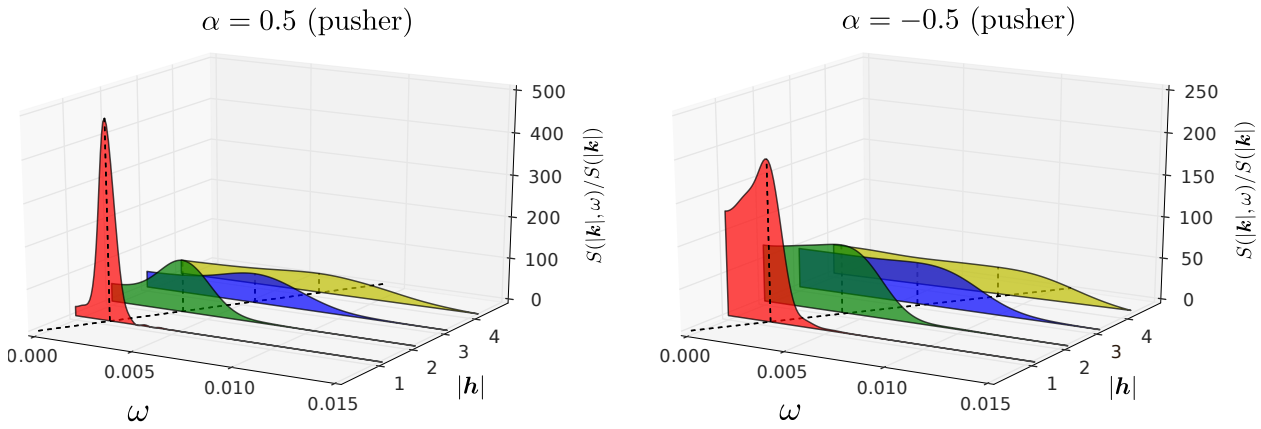

Figure 1: The simulation results for the Dynamic Structure Factor. The vector $\boldsymbol{h}$ is defined in terms of the wave vector $\boldsymbol{k}$ as $\boldsymbol{k} = \frac{2\pi}{L}\boldsymbol{h}$. Dashed lines show the position of peaks. Peaks for both pushers and pullers systems show good dispersion relations, but pullers present significantly higher peaks than pushers, especially at small wave vectors.

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Oscillatory motion of active deformable particles

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Active particle is an object that possesses mechanism to convert potential energy, e.g. chemical potential, into kinetic energy and consequently exhibits spontaneous movements by breaking symmetry. Therefore it has attracted much attention from the viewpoint of various new orders far from equilibrium. Examples include many synthetic active particles such as self-propelled Janus colloids and camphor boats. These active particles are usually rigid and have a time-independent shape. In contrast, there also exist soft active particles, which does change its shape during its dynamical motion. Indeed the shape deformation is of great importance for many biological living cells and microorganisms like protozoa. To understand such biological active systems, simpler artificial active deformable particles have also been realized including active liquid droplets that undergo chemical reactions on the interface.

In order to clarify the mechanisms and properties of each specific active particle, specific modeling is required by taking into considerations the details of complicated chemical reactions. Besides, since the examples of active particles include both biological and artificial systems, it is also necessary to develop general descriptions to elucidate universal features of miscellaneous active particles. What we are interested in is the latter general aspect of the dynamics of active deformable particles. To this end, we have pushed forward theoretical studies in the framework of nonlinear dynamics. In this presentation, we would introduce our recent study concerning the oscillatory motion of active deformable particles.

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3.2 Fluctuations Far from Equilibrium

Length selection and replication in a thermal flow chamber

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The replication of long nucleic acids is central to life. On the early Earth, suitable non-equilibrium boundary conditions would have been required to surmount the effects of thermodynamic equilibrium such as dilution and degradation of oligonucleotides. One particularly intractable experimental finding is that short genetic polymers replicate faster and outcompete longer ones, leading to ever shorter sequences and the loss of genetic information. We show in theory and experiment that heat flux across an open chamber in submerged rock concentrates replicating oligonucleotides from a constant feeding flow and selects for longer strands. The thermal gradient triggers a complex interplay of molecular thermophoresis, external flow and laminar convection, where the latter drives strand separation and exponential replication. The experimental results are understood quantitatively based on the calculation of stochastic trajectories inside the chamber using a two-dimensional random walk model. It allowed to calculate lifetimes and thermal oscillation frequencies of the nucleic acids. In an intermediate range of external velocities, the superposition of flow fields retains strands of 75 nucleotides, while strands half as long die out, inverting above dilemma of the survival of the shortest. In a thermal cycler, the short strands outcompete the long ones. The combined feeding, thermal cycling and positive length selection opens the door for stable molecular evolution in the long-term micro-habitat of an asymmetrically heated porous rock.

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Replica symmetry breaking in trajectories of a driven Brownian particle

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It has been known that equilibrium states of mean-field spin glass models freeze into some irregular patterns at low temperatures. The low temperature phase is characterized by a concept of replica symmetry breaking (RSB) [1]. RSB is a phenomenon reflecting localization of the state in a rugged free energy landscape and is detected by a physical quantity called overlap, which expresses how much two independent identical systems (replicas) are similar to each other. In RSB phase, an overlap takes a non-trivial value. These systems are one example which exhibits stable and diverse states.
In nature, there are many systems which exhibit stable and diverse dynamics. A typical example of such dynamical behavior is cell differentiation. In these systems, an observed time series is stable against perturbation like limit cycle, while a variety of trajectories are observed like chaos and Brownian motion. Behaviors of these systems are characterized by a rugged probability landscape of the trajectory. A natural question is whether there are any dynamical behaviors in which the concept of RSB in path probability appears.
Here, we present a non-equilibrium phenomenon where RSB plays an important role [2]. Concretely, we consider a passive Brownian particle driven by a random velocity field, and study whether RSB in path ensemble occurs when we focus on trajectories of the particle. As a result, we numerically find that, in case of a velocity field driven by the noisy Burgers equation [3], an overlap between two independent particles becomes non-zero. Furthermore, by changing a boundary condition of the model, we theoretically prove that the model can be mapped exactly to directed polymers in random potentials [4], which exhibit RSB. In addition, by comparing the modified system with the original system numerically, we conclude that the original system also exhibits RSB in the path ensemble. This result provides one example where the concept of RSB is useful even in non-equilibrium situation.

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Emergence of chaos in a low-dimensional reactive system

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Nanosystems offer a wide range of applications in materials science, biology, medicine or catalysis. The chemical dynamics of such systems emerges from the interplay between several effects [1]. In spatially restricted media like catalytic surfaces, the lateral interactions between adjacent particles and the local fluctuations of particles density can lead to important deviations from the mean-field (MF) behaviour [2-4]. In this context, several representative nonlinear reactive dynamics have been studied on small low-dimensional lattices. The low dimensionality of the substrate can lead to a displacement of stationary states [5-7] or altogether to the disappearance of dynamical behaviours predicted by the MF description (such as bistability [6] and oscillations [7]).

In this work, we investigated how the low dimensionality of such substrates could affect the emergence of deterministic chaos. We developed to this end an amended version of the classical Willamowski-Rössler model [8], where we account for the impenetrability of the reactive species. We first analyzed the kinetics of this confined system in the macroscopic limit, which included the determination and the linear stability analysis of the stationary states. Then, we studied the influence of the fluctuations and the particles mobility on chaos, by using stochastic simulations (Gillespie and spatial kinetic Monte Carlo simulations).

A low mobility of the particles induces the formation of clusters acting like reservoirs and preventing the complete consumption of species (*i.e.* absorbing states). For intermediate particles mobility, chaos can be observed in large systems. On the contrary, when the particles mobility is higher, the system becomes more homogeneous, the coverages evolve in a synchronized way over the whole lattice, tending to the MF behaviour. Fluctuations may then result in the collision between the chaotic trajectory and an absorbing state, leading to the disappearance of chaos. In conclusion, the emergence of chaotic behaviour in this low-dimensional system is limited by fluctuations, but this effect can be counterbalanced by reducing the mobility of the particles. The sensitivity to fluctuations and mobility effects might however depend on the system considered and it would be interesting to assess other types of chaotic dynamics. Moreover, other potentially compensating effects should be investigated, like the geometry of the system or the number of first-neighbours.

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3.3 Synchronization Phenomena

Edge to edge synchronization of electrochemical oscillations in microfluidic flow cells

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Electrochemical systems often exhibit nonlinear dynamics, resulting from the interplay of the local electrode kinetics and transport processes [1,2]. Recent studies show that in microfluidic flow cells, a large variation of the local resistance along the flow channel can give rise to spatio-temporal patterns with peculiar properties [3,4]. We used an iron electrodissolution model in a microfluidic flow cell geometry to explore the synchronization features [5] of oscillatory patterns localized on the edges of the working electrode. These synchronization features depend mainly on the symmetry properties of the cell. We found a variety of spatio-temporal patterns, like simple in phase or antiphase synchronization of periodic oscillations, complex periodic or quasiperiodic oscillations, as well as coexistence of unsynchronized states. A cell geometry with a more symmetric configuration provides the possibility to control the synchronization properties of the localized oscillations.

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Robust pattern recognition with oscillatory neural networks

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A physical system can be used for pattern recognition if all possible input patterns can be mapped to system states and attractors of the system correspond to desired output patterns. Networks of phase oscillators are especially useful: Synchronisation and antisynchronisation can be used to encode binary patterns and specific sets of attractors can be created by choosing the oscillators' coupling appropriately. Our new architecture surpasses previous ones by reducing the number of physical connections and enabling long-term storage of recognized patterns. Additionally, we provide a simple criterion for recognition success.

Quantification of Precision of Collective Oscillations in Complex Dynamical Systems with Noise

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We have derived general formula for variance in periods of a large number of oscillation cycles in noisy complex dynamical systems. Our systems generate collective oscillations; however, individual elements are not required to be oscillators. We have found that the variance is independent of check point, which is defined as a beginning or end point for a cycle, while variance in one-cycle periods is generally dependent [1]. Thus, the variance mentioned first is useful to quantify precision of collective oscillations. Gene expression model with internal noise [2] have been numerically investigated and the simulation results have agreed with the values predicted by the formula.

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Maximizing coherence of oscillations by external locking

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Dynamical Regimes of Four Almost Identical Chemical Oscillators Circularly Coupled Via Pulse Inhibitory Coupling with Time Delay

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Pulse inhibitory coupling of two identical chemical (BZ) oscillators revealed four main rhythms [1]: anti-phase oscillations at small coupling strength C_{inh} and small time delay τ, in-phase oscillations at larger C_{inh} and τ, complex oscillations at intermediate C_{inh}, and OS regime (when one oscillator is dead and the neighboring one oscillates) at rather large C_{inh}. In case of four identical chemical oscillators circularly coupled via pulse mutual inhibitory coupling, the boundaries between above mentioned regimes are shifted to the direction of smaller C_{inh} and τ. In addition, a new regular simple regime is found, when two neighboring oscillators, let say, oscillators 1 and 2 (pair I), as well as oscillators 3 and 4 (pair II), oscillate in phase, while these two pairs I and II oscillate anti-phase. We call this rhythm IPAP. In anti-phase regime (AP), oscillators 1 and 3 (as well as 2 and 4) oscillate in-phase, while oscillators 1 and 2 (as well as 3 and 4) oscillate anti-phase. Varying parameters C_{inh} and τ between different pairs of oscillators, we have found a lot of more complex regimes. Some of these regimes resemble heteroclinic switching between phase clusters. Multistability (bi- and tri-rhythmisity) has been found for some regions of the parameter space. We discuss a possible application of these regimes to explanation of animal and robot locomotion and to a memory and computational ability of a network of coupled oscillators.

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3.4 Mathematical & Computational Methods

Induced Coherence Resonance in Electrochemical System using a Reference Model

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Some excitable electrochemical systems present complex nonlinearities, which can be induced with the addition of a random signal, providing consistent behavior change. An electrochemical system exhibiting this behavior is H_2SO_4-Fe [1], where noise amplitude works as control variable in order to obtain uniform statistics response. A new strategy integrating Neural Networks (ANN) empirical modeling and the modulating capability of Kalman Filter (KF) is used to achieve this maximum uniformity point. The combination possesses adaption capabilities [2, 3] in order to track the Normalized Variance (NV) curve and reaching and maintaining t maximum coherence behavior. An equivalent derivative curve as error reference for the Proportional Integral (PI) controller was used. This strategy is robust enough to handle the intrinsic noise and deviations caused by working electrode undermining presented in the system. Furthermore, only a short time series bursts are enough to detect the direction that should be taken to reach the minimum point in the Coherent Resonance (CR) curve.

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3.5 Control of Chemical Self-Organization

Continuous, sequence dependent gelation of nucleic acids driven by a thermal gradient.

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Under equilibrium conditions, the phase transition of bio-polymers like DNA toward a compacted state requires mutual binding forces from high polymer concentrations or multivalent ions. We demonstrate that the physical non-equilibrium of a thermal gradient across an elongated chamber accomplishes this task from dilute DNA solutions without the help of multivalent ions, proteins, evaporation or encapsulation. The gelation process is governed by the base pair interactions between respective DNA strands, leading to a highly nonlinear sequence dependency of the gelation process. DNA of different sequences are compacted at distinct sites, yielding a sequence-based physical sorting mechanism. DNA strands with low hybridization energies do not form a gel within the measurement time. The DNA gel is continuously rebuilt inside the thermal gradient in a dynamic turn-over fashion and remains stable for days under dilute equilibrium conditions. The process implements a basic prebiotic machine that selects and stores sticky sequence motifs out of a random sequence pool.

1. Christof B. Mast, Severin Schink, Ulrich Gerland and Dieter Braun

PNAS 110, 8030-8035 (2013)

Turning Spirals into Fingers with Advection

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Inspired by experimentally observed solitary waves with non-curling open ends in an electrochemical flow cell, we present simulations in a two dimensional excitable reaction-diffusion-advection system. Depending on the advection strength, the tip of spiral waves can be pushed toward the flow outlet, leaving a uniform system, or driven against the advective flow, resulting in a stable, finger-shaped wave fragment traveling perpendicularly to the flow that is pinned at the inlet. Thus, the peculiar experimental traveling 'fingers' can be attributed to the advective flow. Moreover, a gradient of the excitability can limit the length of the fingers such that they do not touch the inlet.

Population dynamics on the nanoscale

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Evolution is driven by three main aspects: Replication, mutation and selection [1]. Our experiments allow to test all three in the same experiment. PCR allows to replicate DNA sequences, which are designed in a way that allows cooperative mixing of sequences to enhance the efficiency. Serial dilution transfers into fresh resources mimick the degradation of the molecules, a selection pressure that leads to extinction of inefficient sequences and thus selection for the mutants. Despite the extinction, the sequence information is conserved in the mutant strands, which can be described as cooperative behavior.

We aim to extend the interaction of replicators by using three DNA strains, which suppress each other in a cyclical fashion. To this end we use the DNA-Toolbox [2], in which poylmerase and nickase replicate the DNA species. The latter produce oligos, which suppress the replication of other species. The modularity of the DNA-Toolbox allows to arrange this replicators in a rock-paper-scissor fashion [3]. Due to an exonuclease which degrades the DNA continously, the system is expected to show cyclic oscillations. Simulations confirm this and show spiral waves if the system is observed in 2D.

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3.6 Electrochemistry & Surface Reactions

Stochastic Simulations of Potential Oscillations on Nanoelectrodes

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At nanoelectrodes, the electrode potential changes whenever a stochastic electron-transfer event takes place, and thus it becomes a fluctuating variable. Since the reaction constant depends exponentially on the electrode potential, it becomes a fluctuating quantity as well. This is the crucial difference between chemical and electrochemical reactions at the nanoscale. Employing the electrochemical Master equation, we studied the impact of the time-dependent reaction constant on the quality of oscillations as a function of system size and distance to Hopf and saddle-loop bifurcations and compared the results to nanoscale chemical oscillators. The example system considered is the H_2O_2 reduction on Pt in the presence of halide ions. In contrast to chemical systems, it exhibits a stron size dependence of the oscillation period. In addition, the interspike distances show an asymmetric distribution.

Potential fluctuations on Pt microelectrodes during the galvanostatic electro-oxidation of CO

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Spatially extended dynamical systems can be considered as an ensemble of a large number of individual subsystems. Decreasing the size of the system to micro- or nanoscopic dimensions, i.e. to a considerably smaller number of subunits, may lead to deviations on the behavior predicted for the macroscopic case, e.g. changes on the stability of steady states, synchronization of subsystems, etc. This is known as a finite-size effect.

We studied the influence of the electrode size on an electrochemical reaction. The chosen reaction, CO bulk electrooxidation on Pt, exhibits bistability of the current under potential control; this is associated with an S-shaped negative differential resistance (S-NDR) current-potential curve. In macroelectrodes the S-NDR cannot be observed due to a spatial instability that leads to the formation of stationary domains [1]. Previous studies showed that on a 10um diameter Pt microelectrode the S-NDR can be seen during a galvanodynamic experiment. Furthermore, if several microelectrodes are globally coupled, by short-circuiting them and operating under current control conditions, cooperative phenomena such as complex switching and sequential activation were observed. The present work reports the emergence of potential fluctuations on the galvanodynamic curves when the pH of the electrolyte was set at higher values. These fluctuations are dependent on the concentration of CO in the solution and the size of the electrodes. Coupling two of such electrodes together rendered the fluctuations to cooperative oscillations [3].

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Silicon electrodissolution as a model system for self-organized pattern formation

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The photo-assisted anodic electrodissolution of n-doped silicon shows a wide range of dynamical phenomena, most remarkably self-organized pattern formation. We investigate these patterns which form in the anodically grown oxide layer by spatially resolved ellipsometric imaging. The patterns are often comprised of several regions on the electrode surface, each showing a distinct dynamical behavior, the most prominent among these being the so-called 'chimera state', i.e. the coexistence of synchrony and incoherence. All these patterns could be reproduced in theoretical simulations using a modified version of the complex Ginzburg-Landau equation as a generic ansatz. With this theoretical model a more detailed analysis of the patterns becomes possible. Using the normal form approach for the theoretical modeling then also allows us to interpret the silicon electrodissolution as a model system for a broader class of oscillatory media.

3.7 Synthetic Molecular Biology

Reconstitution of contractile actomyosin cortex inside a cell-sized lipid interface

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Most eukaryotic cells have a cortex structure, which is composed of actin filaments and type II myosin, underlying the cell membrane. The complex of actin and myosin, i.e., actomyosin, actively generates contractile forces to sustain many kinds of biological processes, such as cell motility, cell division, embryotic development, and so on. To understand the native properties of actomyosin and its cortex structure, bottom-up or reconstituted systems have been adopted by using only small number of components involved in the contractile property [1,2]. These studies have successfully verified the active contractile property of purified actomyosin and actomyosin cortex.
In the present study, we focused on the deformation of the membrane that is coupled with the contractile force exerted by the actomyosin cortex. Here, we have developed a reconstituted water-in-oil droplet system with a cell-sized soft interface that encapsulates actin and myosin, which are extracted from *Amoeba proteus* as previously reported [3], to investigate the fundamental contribution of the contractile force to the deformation of the interface. We observed the dynamic wrinkling of the surface of the water-in-oil droplet induced by the contraction of the emergent cortex structure. The power spectra of the observed wrinkled shapes exhibited droplet-size dependence. The size-dependence was explained by a theoretical description of the deformation by taking into account the cortex elasticity and contractility [4].

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3.8 Waves and Patterns in Active Media

Self-organized Alternating Chimera States in Oscillatory Media

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Oscillatory media can exhibit the coexistence of synchronized and desynchronized regions, so-called chimera states, for uniform parameters and symmetrical coupling. In a phase-balanced chimera state, where the totals of synchronized and desynchronized regions, respectively, are of the same size, the symmetry of the system predicts that interchanging both phases still gives a solution to the underlying equations. Through simulations of an oscillatory medium governed by a complex Ginzburg-Landau equation with nonlinear global coupling, we observe this kind of interchange as a self-emergent phenomenon, occurring repeatedly for an apparently indefinite amount of time [1].

Simulations also corroborate the hypothesis that a steady expansion of the turbulent phase is favoured, whereas a global constraint restricts its overall size. In contrast to the case of the non-alternating chimera states also found in our model system, the phase balanced state is not stable for alternating chimera states, leading to diffusional growth slightly beyond phase balance and a subsequent interchange of phases. The existence of self-emergent, self-sustaining alternating chimera states broadens the scope of future research into chimera states in general, and may help improve our understanding of chimera-like phenomena observed in biology.

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Theoretical and Experimental Investigations of Multiple-period Oscillations in Arrays of Oscillators undergoing the Belousov-Zhabotinsky Reaction

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Spatio-temporal dynamics of many biological and chemical systems depend on coupling of individual oscillators e.g. catalyst particles, the heart cells during atrial fibrillation or neuronal networks. In these systems, irregular patterns and bifurcations of frequency are most often observed in regions of critical coupling strength. To elucidate the influence of local coupling of individual oscillators we perform on one hand experiments of the Ferroin-catalyzed Belousov-Zhabotinsky reaction in silica gels and on the other hand numerical calculations of the FitzHugh-Nagumo (FHN) model, both with a catalyst distribution in form of a micro spot pattern. We observe transitions to multiple period oscillations and amplitude oscillations in dependence of spot distance and size. Its dependence on spot size, spot distance, spot shape and parameter variations will be discussed. The importance of gradients of spot distance or spot size for the appearance of bifurcations will be shown. Furthermore, we study the influence of the dimensionality of the oscillator arrays and the introduction of defects in the oscillator arrays for arisal of burst and other special patterns. Deviations between experimental results and numerical analysis can be understood from calculations of the Rovinsky model [1].

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Induction and Control of Luminescent Spatiotemporal Patterns in the Hydrogen Peroxide-Thiocyanate-Copper(II) Homogeneous Oscillator

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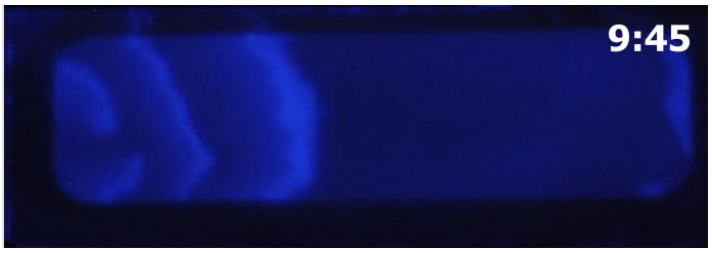
It was originally suggested that the homogeneous H_2O_2-SCN^- - OH^- - Cu(II) oscillator [1] cannot be a source of any kind of spatial or spatiotemporal patterns. However, we found the conditions, under which, in the presence of luminol as an indicator, the luminescent travelling patterns in this system develop. In our very recent work [2], involving both experiments in reactors of different geometries and numerical simulations of the complex kinetic mechanism, we recognized these waves as phase ones, for the induction and controlled progress of which the non-uniform temperature distribution in the solution is required.



The spatial temperature distribution induces the spatial distribution of the oscillatory frequency, thus making the impression of the travelling fronts while the chemical system is permanently oscillating. The speed of the wavefront propagation correlates well with the thermal diffusivity coefficient in water, and not with the remarkably slower molecular diffusion of reacting particles. Thus, the explanation of the formation and propagation of these luminescent fronts is based on an interplay of nonlinear chemical kinetics and physical heat transport phenomena. The appropriate numerical model explains this mechanism semiquantitatively. The origin of those patterns means in fact an operation of a special case of *thermokinetic coupling* between the oscillatory kinetics and spatial progress of the warmed zone of the solution [2]), being a rather unique mechanism of spatiotemporal instabilities in aqueous media.

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Bi-dimensional Study of the Liesegang Pattern Formation in a Gaseous System

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Liesegang pattern formations are widely spread in nature. In spite of a comparably simple experimental setup in laboratory conditions a variety of beautiful spatio-temporal structures may arise [1-3]. Due to easy control of the experimental conditions, Liesegang pattern formation has been mainly studied in gel medium. Here we consider pattern formation in a gas phase [3], and using a special laser technique a complex reaction-diffusion-convection dynamics is uncovered. A qualitative image analysis reveals that two different, apparently independent processes, both highly synchronized across the extension of the reaction cloud, act on different time scales. Each of them and the occurrence of both are responsible of the structure of salt precipitation at the tube walls.

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3.9 Self-Organization in Biological Cells

Self-organized ordering in skin tissue

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Epithelial tissue can be found all over the body, lining inner organs and acting as our skin. It provides essential functions for us and protects us.
The structure of tissues is typically very relevant to their function. As a key example we concentrate on the upper layer of skin, a layer of cells that sits on top of the stroma, a layer made mainly of collagen and fibers. Simply speaking, stem cells sitting on the interface between these layers continually divide into daughter cells which then get pushed upwards over time. As they move up towards the surface they flatten and arrange into a highly regular, columnar arrangement, see fig. 1.

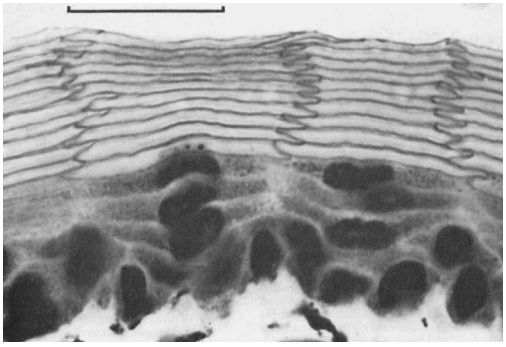

Figure 1: Epithelial tissue sample from a mouse ear in cross section, from ref. [1]. The columnar ordering of cells at the top of the sample can be clearly seen.

Attempts to explain the emergence of this ordering have been made with simple schematic models, e.g. ref. [2], but the mechanisms still remain poorly understood.
Here, we present preliminary results of our investigation of a meso-scale model which relies on classical mechanics and self-organization to explain the ordering of epithelial skin tissue.

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Role of oscillation in periodic pettern formation in a noisy system

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Somites are spatially periodic blocks that form along the head to tail axis of the developing embryo in segmented animals (Fig.1). Somite are formed from the head to tail periodically in time (somite formation). It is believed that the segmentation clock, which is a molecular clock system in each cell, controls the periodicity of somitogenesis. As a model of the somite formation in mammals, a clock and wavefront model is well known [1]. In this model, both the segmentation clock and propagating waves are responsible for determining the somite number, somite sizes, and somite axiality. However, it has recently been reported that somite formation is possible without the aid of the segmentation clock [2]. Besides, it is known that some species including flies do not need segmentation clock for somite formation.

Then, what is the role of segmentation clock? In somite formation, the somite number, somite size, and somite axiality are accurately controlled, and their variations cause a fatal problem. Although the embryo in a developmental stage is subjected to noise, the spatial pattern including the somite number and somite size is kept fixed. It can thus be speculated that oscillations may enhance the robustness of the somite formation.

In this study, to examine whether temporal oscillation may contribute to the robustness of periodic pattern formation, we consider a reaction-diffusion system subjected to periodic forcing and noise:

$$\begin{aligned} \frac{\partial u}{\partial t} &= f(u,v) + D_u \nabla^2 u + \xi_u + C\sin(\Omega t - kx) \\ \frac{\partial v}{\partial t} &= g(u,v) + D_v \nabla^2 v + \xi_v, \end{aligned} \tag{1}$$

where ξ_u and ξ_v are noise and the parameter C is the strength of periodic forcing. We mainly focus on the effect of periodic forcing on spatial periodicity.

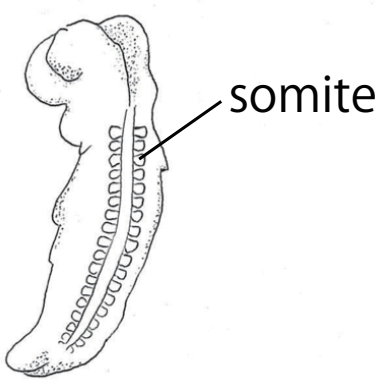

Figure 1: somite of mouse embryo

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