ENGINEERING OF CHEMICAL COMPLEXITY

10th International Conference
June 03-06, 2019, Potsdam, Germany.

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ECC Organisation

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Welcome to ECC 2019

Welcome to the 10th International Conference "Engineering of Chemical Complexity" in Potsdam, Germany. The aim of this conference is to review and discuss the most recent scientific breakthroughs and findings in complex systems research with a particular emphasis on complex chemical systems and their relation to self-organization in biology and active matter physics.

After several editions at different national and international sites, it is a great pleasure to see this conference returning to the Berlin-Brandenburg area for its tenth anniversary. The city of Potsdam, capital of the Brandenburg region, offers one of the oldest and richest scientific sites in Germany. Centered around the University of Potsdam, numerous Max Planck Institutes, Fraunhofer Institutes, and institutions of the Leibniz and the Helmholtz Association build on a scientific tradition that dates back to the 19th century, when the first observatories were established on the Telegrafenberg. Surrounded by a landscape of lakes, forests, and parks with castles from the times of the Prussian kings, the Potsdam cultural landscape - UNESCO World Heritage Site since 1990 - provides a unique experience for our conference.

The conference is organized by the Berlin Center for Studies of Complex Chemical Systems (BCSCCS) in collaboration with the University of Potsdam.

The BCSCCS is a registered non-profit organization that promotes fundamental research, exchange of information, and international contacts in experimental and theoretical studies of complex systems. Furthermore, our conference is kindly supported by the German Research Foundation (DFG, BE 3978/12-1), by the Research Center of Plant Genomics and Systems Biology of the University of Potsdam, and by the Collaborative Research Centers SFB 910 and SFB 1294.

I am looking forward to interesting and stimulating days and hope that we can continue our tradition to offer a forum for interdisciplinary exchange, where expert leaders as well as junior scientists meet and discuss the latest developments in this field. Again, a warm welcome to all and my best wishes for a memorable stay in Potsdam.

Carsten Beta, Conference Chair,
Potsdam University

This conference series was originally initiated in Berlin, where a long-standing tradition of research on complexity and self-organization in various fields of science exists. Cooperation between both parts of the city started already before the fall of the Wall, eventually leading to the establishment of the Collaborative Research Center SFB 555 with Werner Ebeling as its chairman.

In 2000 the first symposium "Engineering of Chemical Complexity" took place with about 50 participants. Its success prompted continuation every two years until 2008. After the SFB 555 program ended, a new organizational framework for the ongoing activities was created by the foundation of the Berlin Center for Studies of Complex Chemical Systems. From 2011 onwards, the "Engineering of Chemical Complexity" conference grew considerably in size and moved to different national and inter-national sites.

After meetings in Warnemünde, Munich, and Barcelona, the conference will now return to the Berlin-Brandenburg area for its 10th edition. We are delighted to welcome all participants to our lakeside conference venue at the Templiner See in Potsdam and we are looking forward to interesting and stimulating presentations and discussions.

Honorary Conference Chairman
Gerhard Ertl, Nobel Laureate

Monday, June 3, 2019

8:00 am	**Registration**		
8:45 am	**Opening and Welcome**		
1	**Active particles and swimmers**		H. Stark, S. Santer
9:00 am	**R. Golestanian**	*Enhanced diffusion and chemotaxis at the nanoscale*	
9.30 am	**S. Santer**	*Light driven diffusioosmosis: manipulation of small particles at solid surfaces*	
10:00 am	**M. Mazza**	*Hydrodynamics and heterogeneous distribution of microswimmers*	
10:30 am	**O. Vinogradova**	*Continuous electroosmotic sorting of particles in grooved microchannels*	
11:00 am	***Coffee Break/Discussion***		
11:30 am	**I. Kiss**	*Controlling electrochemical oscillator networks with local feedback techniques*	
11:50 am	**R. Großmann**	*Chemotaxis strategies for bacterial swimmers with multi-mode motility*	
12:10 am	**P. Arya**	*Motion of porous particles*	
12:30 pm	***Lunch***		
6	**Synchronization phenomena**		H. Engel, M. Hauser
2:00 pm	**A. Pikovsky**	*Common noise vs coupling in oscillator populations*	
2:35 pm	**E. Macau**	*Detecting causal relations from real data experiments by using recurrence*	
3:10 pm	**J. Totz**	*Synchronization transitions in a large network of chemical oscillators*	
3:45 pm	**V. Vanag**	*"Cognitive" modes in small networks of almost identical chemical oscillators with pulsatile inhibitory coupling"*	
4 pm	***Coffee Break/Discussion***		
4:30 pm Plenary talk	**E. Bodenschatz**	*Chemotaxis, cell migration and pattern formation of Dictyostelium discoideum*	

Tuesday, June 4, 2019

5	**Active and self-organizing materials**		O. Steinbock, F. Sagues
9:00 am	**A. Bausch**	*Pattern formation in active biomolecular and cellular systems*	
9.30 am	**A.F. de las Nieves**	*Topological active matter*	
10:00 am	**P. Knoll**	*Life-like Microscale Structures From Nonlinear Reaction-diffusion Processes*	
10:15 am	**P. Malgaretti**	*Dynamics of active polymers*	
10:30 am	**M. A. Budroni**	*Pulsatory behaviours in simple A+B→C reactions: a chemohydrodynamic pathway toward self-organization.*	
10:45 am	**J. Nambisan**	*Orientation of defects in 2D active nematics*	
11:00 am	***Coffee Break/Discussion***		
2	**Cell motility and collective dynamics**		C. Beta, M. Bär
11:30 am	**G. Ariel**	*A phase diagram for bacterial swarming*	
12:00 am	**S. Alonso**	*Interplay among bistability, excitability and fluctuations determines locomotion strategy of crawling cells*	
Group picture at the terrace			
12:30 pm	***Lunch***		
4	**Control of self-organization**		S. Klapp, E. Schöll
2:00 pm	**S. Gurevich**	*Spatio-temporal control of self-organized patterns in dynamic self-assembly systems*	
2:40 pm	**R. Andrzejak**	*Control of chimera states with a pacemaker*	
3:20 pm	**R. Berner**	*Multi-layer structures in slowly adapting networks of coupled oscillators*	
3:40 pm	**H. Reinken**	*Self-organization of microswimmers in arrays of obstacles*	
4:00 pm	***Coffee Break/Discussion***		
4:30 pm	**Poster Session** with discussions, snacks and finger food		

Wednesday, June 5, 2019

7	**Nanoscale patterns and molecular machines**		A. Mikhailov, R. Kapral
9:00 am	**P. Gaspard**	*The nonequilibrium statistical mechanics of self-phoretic active particles*	
9.40 am	**J. Noel**	*Mesoscopic modeling of active and passive membrane deformation created by dynamin oligomers*	
10:00 am	**I. Guido**	*3D wave instabilities of confined active networks*	
10:20 am	**M. Sokolowski**	*Light driven self-sustained motion of spherical polymer brushes*	
10:40 pm	**M. Tarama**	*Mechanochemical modelling of crawling cells*	
11:00 pm	***Coffee Break/Discussion***		
2	**Cell motility and collective dynamics**		C. Beta, M. Bär
11:30 am	**S. Heidenreich**	*Emergence and control of patterns in active fluids*	
12:00 am	**L. Schimansky-Geier**	*Aligning active searchers wheel around their common home position*	
12:30 pm	***Lunch***		
3	**Fluctuations far from equilibrium**		I. Sokolov, R. Metzler
2:00 pm	**R. Metzler**	*Brownian motion and beyond*	
2:40 pm	**K. Kroy**	*How thermodynamic notions fare and fail far from equilibrium*	
3:20 pm	**A. Chechkin**	*Brownian yet non-Gaussian diffusion in heterogeneous environment*	
4:00 pm	*End day 2*		
5:00 pm - 8:00 pm	***Boat trip and dinner*** *(only for registered participants)*		

For all who booked the conference dinner please notice that the dinner will take place on the MS Stadt Potsdam. The meeting point for the scenic boat trip is 5 pm (sharp) at the landing stage "*Potsdam Seminaris Seehotel"* at the lakeside of the venue. The tour will finish by going back to the hotel at 8 pm. Participants who did not book the boat trip will have dinner at the hotel.

Thursday, June 6, 2019

9	**Applications to nonlinear chemical and physical systems**		K. Krischer, H. H. Rotermund
9:00 am	**S. Morris**	*Riddles of a rippled icicle*	
9:40 am	**R. Imbihl**	*Dynamics of V-oxide catalysts from UHV to 0,1mbar*	
10:20 am	**A. Tosolini**	*Bichaoticity induced by inherent birhythmicity during the oscillatory electrodissolution of silicon*	
10:40 am	**M. Stich**	*Oscillations, travelling fronts and patterns in a supramolecular system*	
11:00 am	***Coffee Break/Discussion***		
11:30 am	**R. Klages**	*Asymmetric anomalous diffusion in cell chemotaxis: experiments and stochastic modeling*	
11:50 am	**F. Rühle**	*Dynamics of bottom-heavy squirmer microswimmers*	
12:10 pm	**A. Gholami**	*Spatial heterogeneities shape collective behavior of signaling amoeboid cells*	
12:30 pm	***Lunch***		
8	**Biological self-organization**		M. Falcke, B. Lindner
2:00 pm	**K. John**	*Spreading strategies and morphology of bacterial colonies: interplay between passive physico-chemical effects and bioactive growth*	
2:30 pm	**S. Reber**	*Mitotic spindle scaling: how complexity arises from molecular interaction*	
3:00 pm	**P. Gross**	*Guiding self-organized pattern formation in cell polarity establishment*	
3:30 pm	**K. Alim**	*Self-organization by fluid flows*	
4:00 pm	***Coffee Break/Discussion***		
4:30 pm plenary talk	**Y. Kevrekidis**	*No equations, no variables, no parameters, no space, no time: data and the modeling of complex systems*	
5:30 pm	**Closing remarks**		

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S. Santer		2	*Invited talk*	Mon	2
M. Mazza		3	*Invited talk*	Mon	3
O. Vinogradova		4	*Invited talk*	Mon	4
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S. Alonso		20	*Invited talk*	Tue	20
S. Heidenreich		30	*Invited talk*	Wed	30
L. Schimansky-Geier		31	*Invited talk*	Wed	31
R. Metzler	**3** - Fluctuations far from equilibrium	32	*Invited talk*	Wed	32
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P. Knoll		15	*Contributed talk*	Tue	15
P. Malgaretti		16	*Contributed talk*	Tue	16
M. A. Budroni		17	*Contributed talk*	Tue	17
J. Nambisan		18	*Contributed talk*	Tue	18
A. Pikovsky	**6** - Synchronization phenomena	8	*Invited talk*	Mon	8
E. Macau		9	*Invited talk*	Mon	9
J. Totz		10	*Invited talk*	Mon	10
V. Vanag		11	*Contributed talk*	Mon	11
P. Gaspard	**7** - Nanoscale patterns and molecular machines	25	*Invited talk*	Wed	25
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S. Reber		43	*Invited talk*	Thu	43
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Symposium 1: Active particles and swimmers

H. Stark, S. Santer

Enhanced diffusion and chemotaxis at the nanoscale | 1

Ramin Golestanian, Jaime Agudo-Canalejo, Tunrayo Adeleke-Larodo, Pierre Illien

Department of Living Matter Physics, Max Planck Institute for Dynamics and Self-Organization

Enzymes have been recently proposed to have mechanical activity associated with their chemical activity. In a number of recent studies, it has been reported that enzymes undergo enhanced diffusion in the presence of their corresponding substrate, when this substrate is uniformly distributed in solution. Moreover, if the concentration of the substrate is non-uniform, enzymes and other small molecules have been reported to show chemotaxis - biased stochastic movement in the direction of the substrate gradient - typically towards higher concentrations of this substrate, with a few exceptions. The underlying physical mechanisms responsible for enhanced diffusion and chemotaxis at the nanoscale, however, are still not well understood. I will review the available experimental observations of both enhanced diffusion and chemotaxis, and discuss critically the different theories that have been proposed to explain the two. I put particular emphasis on an equilibrium model recently introduced by us, which describes how the diffusion of dumbbell-like modular enzymes can be enhanced in the presence of substrate, thanks to a binding-induced reduction of the internal fluctuations of the enzyme. We then turn to chemotaxis, beginning with an overview of the chemotaxis-like diffusiophoretic behaviour of micron-sized colloids in solute gradients, followed by a discussion of why chemotaxis at the nanoscale requires special consideration. Next, I review the experimental evidence of nanoscale chemotaxis, and describe a number of shortcomings and pitfalls in the phenomenological models for chemotaxis introduced in some of those works. Finally, we discuss a microscopic model for chemotaxis including both non-specific interactions and binding between enzyme and substrate recently developed by us, which overcomes many of these shortcomings, and is consistent with the experimental observations of chemotaxis

Light driven diffusioosmosis: manipulation of small particles at solid surfaces

2

Svetlana Santer

Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany

Azobenzene molecules undergoing reversible photo-isomerization from a trans- to a cis- state under UV illumination are considered as molecular actuators that can convert optical energy into mechanical work. Here I will show several interesting examples where azobenzenes can be used in order to actuate matter on large time and length scales. Using azobenzene containing surfactant consisting of a charged head and a hydrophobic tail into which an azobenzene group is incorporated [1], I will show how one can manipulate microparticles and even render them self-propelled when trapped at a solid/liquid interface. Depending on the applied wave length one can either disperse/remove or gather particles. The physical origin of this genuine behavior is related to the phenomenon of light driven diffusioosmosis (LDDO) [2]. During irradiation of a solution containing azobenzene surfactant with focused light local fluid flow at the solid-liquid interface is generated. The corresponding forces are sufficiently strong to swiftly clean the illuminated area from particles trapped at the interface. When the colloids are turned into Janus particles, their self-propulsion can be initiated in the solution of azobenzene containing surfactant even under global/homogeneous illumination with blue light (λ=455nm). We will discuss how to establish light-driven flow pattern as a useful and versatile tool for investigating the collective motion and aggregation of active particles. We also show how this flow can be manipulated to remove, gather, or structure assemblies of micro-objects located on a solid-liquid interface.

[1] Santer, S. J Phys D: Applied Physics, 51 (2017) 013002
[2] Feldmann, D.; Maduar S.R.; Santer, M.; Lomadze, N.; Vinogradova O.I.; Santer, S. Scientific Reports, 6 (2016) 36443

Hydrodynamics and heterogeneous distribution of micro-swimmers

3

Marco G. Mazza

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Max Planck Institute for Dynamics and Self-Organization, Dynamics of Complex Fluids Am Faßberg 17, D-37077 Göttingen, Germany

Sailors have known for millennia that periodically the seas appear of unusual color and can even turn red. These large swaths of colors stretching for tens or hundreds of km are caused by countless microscopic organisms called phytoplankton. These are microscopic algae that use sunlight to produce energy. They are the base of the marine food chain, and produce 50% or more of the oxygen in the atmosphere. Phytoplankton often encounter turbulence in their habitat. The spatial distribution of motile phytoplankton cells exhibits patchiness also at distances of decimeter to millimeter scale for numerous species with different motility strategies. The explanation of this general phenomenon remains challenging. We combine particle simulations and continuum theory to study the emergence of patchiness in motile microorganisms in three dimensions, by including hydrodynamic cell-cell interactions, which grow more relevant as the density in the patches increases. By addressing the combined effects of motility, cell-cell interaction and turbulent flow conditions, we uncover a general mechanism: the coupling of cell-cell interactions to the turbulent dynamics favors the formation of dense patches. [R. E. Breier, et al., Proc. Natl. Acad. Sci. USA 115, 12112 (2018)]. We will also discuss the elements of a theory for heterogeneous distributions, and numerical results on the pair distribution function.

Manipulation of particles in microfluidic devices using lubricant-infused unidirectional surfaces

4

Olga I. Vinogradova[1,2*]

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[2]*DWI - Leibniz Institute for Interactive Materials, RWTH Aachen, Forckenbeckstrasse 50, 52056 Aachen, Germany*

Lubricant-infused surfaces have opened a whole new field of investigation, with both fundamental and practical perspectives. In my talk, I will first discuss the enhanced slip properties for a liquid flow over lubricant-infused unidirectional surfaces. This situation reflects many practical settings involving liquid flows past superhydrophobic grooves filled with gas, or past grooves infused with another, immiscible, liquid of smaller or equal viscosity. I will then discuss principles of a generation of secondary transverse shear flow near such slippery lubricant-infused surfaces and its possible applications for manipulation of particles in microfluidic devices. The examples include 1) a generation of an advective superdiffusion of Brownian particles, which could be used for boosting their dispersion at smaller Péclet numbers compared to known concepts of passive microfluidic mixing; 2) a lateral fractionation of sedimented microparticles at low Reynolds number; 3) an inertial migration of neutrally-buoyant particles at finite Reynolds number.

This research was partly supported by the Russian Foundation for Basic Research (grant No. 18-01-00729).

Controlling electrochemical oscillator networks with local feedback techniques

5 *Contributed talk*

Istvan Z. Kiss

Department of Chemistry, Saint Louis University, St. Louis, MO, USA

The spatiotemporal organization of networks of dynamical units can break down resulting in diseases (e.g., in the brain) or large-scale malfunctions (e.g., power grid blackouts). Re- establishment of function then requires identification of optimal intervention site from which the network behaviour is most efficiently re-stabilized. Through a theoretical analysis (by deriving stability hyperbolas), it was found that in many networks, the most influential site can relocate as the coupling strength changes. We discovered such degenerate cases in real-world networks, such as social and power grid networks. Moreover, a computationally efficient method was developed to identify the global optimal and the candidate optimal pinning sites for stabilization of a nondegenerate and a degenerate complex network, respectively. The theoretical development was confirmed in experiments with networks of chemical reactions, where oscillations in the networks were effectively suppressed through pinning of a single reaction site determined by the computational method.

Chemotaxis strategies for bacterial swimmers with multi-mode motility

6 *Contributed talk*

Zahra Alirezaeizanjani, **Robert Großmann**, Veronika Waljor and Carsten Beta

Institut für Physik und Astronomie, Universität Potsdam, Potsdam-Golm, Germany

Active navigation in chemical concentration gradients is key for bacteria to find sources of food or to flee from poisons. The soil bacterium *Pseudomonas putida* self-propels its motion with a polar bundle of rotating, helical flagella. It senses changes in its environment via a chemosensory system and responds to it by adapting the flagellar rotation. Our earlier research demonstrated that the motion pattern of *P. putida* is characterized by persistent runs which are interrupted by sharp reversals [1]. Recently, we showed that the flagella of *P. putida* may operate in three different modes during swimming: the bundle can push, pull, or wrap around the cell body, corresponding to certain swimming modes [2]; changes in the direction of motion are induced by transitions of the flagellar configuration. Based on a novel experimental setup, we are now able to acquire a large number of trajectories together with information on the bundle configuration for each run. We used this data to study the statistics of transitions between the different swimming modes and to elucidate *P. putidas'* swimming strategy when navigating in the direction of a nutrition gradient. Our results reveal that the wrapped mode plays the most prominent role for directional navigation: the run time in the wrapped mode depends on the swimming direction with respect to the gradient orientation. We interpret and discuss these experimental findings in the light of efficiency and robustness of bacterial chemotaxis strategies within a coarse-grained theoretical model.

[1] M. Theves, J. Taktikos, V. Zaburdaev, H. Stark and C. Beta, Biophys. J., 105, 1915 (2013).
[2] M. Hintsche, V. Waljor, R. Großmann, M. J. Kühn, K. M. Thormann, F. Peruani and C. Beta , Sci. Rep., 7, 16771 (2017).

Motion of porous particles

7 *Contributed talk*

Pooja Arya, David Feldmann, Svetlana Santer

Institute of Physics and Astronomy, University of Potsdam, 14476Potsdam, Germany

We report on light driven aggregation and separation of colloidal particles at solid/liquid interface). This is possible to achieve when porous silica colloids are dispersed in a solution containing photosensitive surfactant, in which azobenzene group is integrated in a hydrophobic tail [1]. Upon illumination with light of different wavelength, surfactant undergoes a reversible trans –cis isomerization accompanied by change in physical properties like dipole moment, shape and size. In UV light most of the surfactant molecules are in cis- state, while in blue light there is a ratio of 2 to 1 of trans- and cis-states, respectively. Porous particles dispersed in a water solution containing photosensitive surfactant in trans-state absorb most of the molecules, so that ca. 70% of the surfactant is stored in the particles. During illumination with blue light (λ=491nm) porous particles start to repeal each other and separate within few seconds forming a 2D crystalline pattern. The physical origin of this process is based on generation of local light driven diffusioosmotic flow (LDDO) at each porous colloid. The LDDO phenomenon was discovered during irradiation of a solution of photosensitive surfactant with focused light. In this way global LDDO flow is generated at the irradiated area near the solid/liquid interface. The direction of the LDDO flow depends on the isomerization state of the surfactant [2]. Here we discuss how combinations of irradiation with different wavelengths influence the collective motion and aggregation of particle assembly. We show that the particle assembly can undergo phase separation between aggregated and well separated states even at constant irradiation conditions.

[1] S. Santer J Phys D: Appl Phys 51 (2017) 013002.
[2] D. Feldmann, S. R. Maduar, M. Santer, N. Lomadze, O. I. Vinogradova, S. Santer, "Scientific Reports 6 (2016) 36443.

Common noise vs coupling in oscillator populations | 8

Arkady Pikovsky

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Coupling and common noise are two known mechanisms to synchronize oscillators. Here we discuss an interplay of these two effects, which is especially nontrivial if they counteract each other, i.e. if the coupling is repulsive. We show that in this case, phase locking (i.e. phases of oscillators stay together) with frequency anti-entrainment (i.e. frequencies become more different) can be observed.

Detecting causal relations from real data experiments by using recurrence

Elbert E. N. Macau[1,2,*], Antônio Mario T. Ramos [1], Juergen Kurths[3], Norbert Marwan[3]

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[3]*Potsdam Institute for Climate Impact Research, Potsdam 14473, Germany.*

In this work, we present the Recurrence Measure of Conditional Dependence (RMCD), arecent data-driven causality inference method using the framework of recurrence plots. The RMCD incorporates the recurrence behavior into the transfer entropy theory. We apply this methodology to some paradigmatic models and to investigate the possible influence of the Pacific Ocean temperatures on the South West Amazon for the 2010 and 2005 droughts. The results reveal that for the 2005 drought there is not a significant signal of dependence from the Pacific Ocean and that for 2010 there is a signal of dependence of around 200 days. These outcomes are confirmed by the traditional climatological analysis of these episodes available in the literature and show the accuracy of RMCD inferring causal relations in climate systems.

Keywords: Synchronization, Recurrence Plot, Extremes in Chaotic Systems, Network dynamics, nonlinear dynamics, climate.

Physical Review E, v. 95, n 5, May 11 2017,
https://journals.aps.org/pre/abstract/10.1103/PhysRevE.95.052206

**Email: elbert.macau@inpe.br*.

Synchronization transitions in a large network of chemical oscillators

10

Jan F. Totz[1], Dumitru Calugaru[2], Erik Martens[3], Harald Engel[1]

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Synchronization is a ubiquitous phenomenon in nature. Examples range from flashing fireflies, chirping crickets, firing neurons, beating heart cells, and circadian rhythms in biology to pendula, lasers, Josephson junctions, computer chips, power grids, and bridge-crossing pedestrians in engineered systems and beyond [1]. It is well known that synchronization in an ensemble of oscillators occurs once the interaction between them is sufficiently strong [2,3]. However, the character of the synchronization transition is determined by the network topology and frequency distribution [3].

Here we will show our latest experimental results on synchronization transitions utilizing a versatile setup based on optically coupled chemical micro-particles, that allows for the study of synchronization dynamics in very large networks of relaxation oscillators. In the past we employed this setup to experimentally verify the elusive spiral wave chimera [5] that was predicted theoretically by Kuramoto in 2002 [6]. Furthermore, the setup allows for reproducible experiments under laboratory conditions on networks with N>2000 oscillators. It facilitates the free choice of network topology, coupling function, coupling strength, range, and time delay, all of which can even be chosen as time-dependent. These experimental capabilities open the door to a broad range of future experimental inquiries into pattern formation and synchronization on large networks, which were previously out of reach.

[1] A. Pikovsky, M. Rosenblum, and J. Kurths. "Synchronization: A Universal Concept in Nonlinear Sciences" Cambridge University Press (2001)
[2] Y. Kuramoto. "Chemical Oscillations, Waves, and Turbulence" Springer (1984)
[3] I. Z. Kiss, Y. Zhai, and J. L. Hudson. "Emerging Coherence in a Population of Chemical Oscillators" Science 296, 16761678 (2002)
[4] E. A. Martens et al. "Exact results for the Kuramoto model with a bimodal frequency distribution" Phys. Rev. E 79, 026204 (2009)
[5] J. F. Totz et al. "Spiral wave chimera states in large populations of coupled chemical oscillators" Nat. Phys. 14, 282285 (2018)
[6] Y. Kuramoto. "Reduction methods applied to non-locally coupled oscillator systems" in "Nonlinear Dynamics and Chaos: Where do we go from here?" CRC Press, 209-227 (2002)

"Cognitive" modes in small networks of almost identical chemical oscillators with pulsatile inhibitory coupling

Contributed talk **11**

Vladimir K. Vanag

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The Lavrova-Vanag (LV) model of the pulsed-coupled oscillatory Belousov-Zhabotinsky (BZ) reaction has been investigated. For such coupling, a sharp spike of the BZ reaction in one oscillator induces a short inhibitory pulse that perturbs the BZ reaction after some time delay τ in other oscillators. The dynamics of this BZ system is strongly dependent on the amplitude C_{inh} of the perturbing pulses. At $C_{inh} > C_{cr}$, a new pseudo steady state (SS) emerges far away from the limit cycle of the unperturbed BZ oscillator. The perturbed BZ system spends rather long time in the vicinity of this pseudo SS, which serves as a trap for phase trajectories. As a result, the dynamics of the BZ system changes qualitatively. We observe new modes with packed spikes separated by long either "silent" dynamics or small-amplitude oscillations around pseudo SS, depending on C_{inh}. Networks of five or four identical LV-BZ oscillators are able to generate so-called "cognitive" modes which are very sensitive to small changes in C_{inh} and to initial conditions [1]. At the same time, these modes are well reproducible. We demonstrate that networks of even two or three LV-BZ oscillators with self-inhibition are able to generate the same "cognitive" modes if a strong pulse coupling is organized in an appropriate way [2]. These modes emerge only at rather strong periodic pulse perturbation when even a single BZ oscillator, which is far from the limit cycle of the unperturbed oscillator, demonstrates qualitatively new dynamics.

[1] V. K. Vanag and V. O. Yasuk, Chaos, 28(3), 033105; (2018)
[2] V. K. Vanag, Chaos, 29(3), 033106 (2019).

PLENARY TALK

Chemotaxis, cell migration and pattern formation of *Dictyostelium discoideum*

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In my talk I shall review our work on Dicty staring from new results on pattern formation, then transitioning to the statistics of chemotaxis and ending with an analysis of acto-myosin oscillations in single cells.

I thank my many collaborators over the past 20years who made this research possible.

Pattern formation in cytoskeletal and cellular systems | 13

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Living cells rely on the self-organization mechanisms of cytoskeleton to adapt to their requirements. In processes such as cell division, or cellular motility rely on the controlled self-assembly and disassembly of well-defined active cytoskeletal structures interacting with lipid membranes. One important and promising strategy to identify the underlying governing principles is to quantify the underlying physical processes in model systems mimicking functional units of living cell. Here I'll present in vitro minimal model systems consisting of active microtubule and actin filament systems which show pattern formation resulting from active transport processes. I will discuss how small variations in local interactions results in nematic or polar patterns in high density motility essays. On the supra-cellular level I will discuss how collective motion of epithelial cells in 3D networks lead to a tension feedback mechanism, ultimately leading to the formation of higher order structures in organoids.

Topological active matter

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We will discuss our recent results with active nematics confined to toroidal surfaces. Topology enters via the global properties of the confining surface, which enforces global constraints that must be fulfilled, and via the presence of topological defects in the nematic liquid crystal, which cannot be removed locally from the material. Activity, however, spices things up highlighting the role of the local geometry in how defects segregate within regions of positive and negative Gaussian curvature and bringing about large numbers of defects that both create and annihilate in time. Overall, our results illustrate how topology, geometry, order and activity all conspire to result in novel phenomena without analogue in equilibrium systems.

Life-like microscale structures from nonlinear reaction-diffusion processes

Contributed talk **15**

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Biomorphs are polycrystalline aggregates that self-assemble during inorganic precipitation reactions. They are composed of thousands of nanocrystals that form microstructures resembling life-like shapes such as helices, funnels, leaf-shaped sheets, and complicated hemispherical objects such as corals. This nano-to-microscale self-organization occurs from simple reactants in aqueous solution and suggests new engineering methods as well as insights into biomineralization. The underlying mechanisms that give rise to the growth of these structures are still widely unclear. Here we describe a reaction-diffusion model for two-dimensional sheet growth that reproduces the experimentally observed biomorph shapes. The sheet edges are logarithmic spirals caused by the propagation failure of the crystallization front with a resulting defect motion that is dynamically related to nonlinear wave dynamics in subexcitable media such as the photo-inhibited Belousov-Zhabotinsky reaction. We further developed a model to describe the three-dimensional hemispherical architectures ranging from radial spikes and stemmed cones to folded sheets reminiscent of coral shapes.

P. Knoll, E. Nakouzi, and O. Steinbock, “Mesoscopic Reaction-diffusion Fronts Control Biomorph Growth”, *J. Phys. Chem. C* **121**, 26133-26138 (2017).
A.-K. Malchow, A. Azhand, P. Knoll, H. Engel, and O. Steinbock, "From Nonlinear Reaction-diffusion Processes to Permanent Microscale Structures" *Chaos* (2019)

Dynamics of active polymers

Contributed talk **16**

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Active systems show very surprising dynamics due to the local breaking of the equilibrium that allow active systems to form collective structures that their equilibrium counterparts cannot attain. This coupling between microscopic local equilibrium breaking and the meso/macroscopic structure formation is a general feature that have been observed for diverse systems including bacteria and, synthetic swimmers. In this contribution I will show that the coupling between the microscopic equilibrium breaking and the onset of mesoscopic structures holds also in the case of active polymers, i.e. polymers made of active monomers. By means of numerical simulations and approximated analytical analysis I will discuss the novel features that active polymers display [1]. First I will show that increasing the activity leads active polymers to undergo a coil-to-globule transition, i.e. active polymers are more compact than their equilibrium counterparts. This phenomenon is interesting since typically activity has been regarded as an "enhanced" effective temperature whereas in the present case this analogy breaks down. Second, I will show that the diffusion coefficient of active polymers eventually becomes independent on polymer size, in contrast to their linear dependence at equilibrium. Finally I will briefly discuss the relevance of these results in the context of biological scenarios such as DNA transcription and chromosome separation as well as for the design of novel smart, active materials.

[1] V. Bianco, E. Locatelli, P. Malgaretti: Phys. Rev. Lett. 121, 217802 (2018)

Pulsatory behaviours in simple A+B→C reactions: a chemohydrodynamic path-way toward self-organization.

Contributed talk **17**

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We present a new mechanism through which self-organized chemical oscillations and waves can be induced in batch conditions with a simple A+B→C reaction, in the absence of any nonlinear chemical feedback or external trigger. Two reactants A and B, initially separated in space, react upon diffusive contact [1] and the product actively fuels *in-situ* convective Marangoni flows by locally increasing the surface tension at the mixing interface. These combine in turn with the reaction-diffusion dynamics, inducing damped spatio-temporal oscillations of the chemical concentrations and the velocity field. By means of numerical simulations, we single out the detailed mechanism and minimal conditions for the onset of this periodic behavior. We show how the antagonistic coupling with buoyancy convection, due to concurrent chemically-induced density changes, can control the oscillation properties, sustaining or suppressing this phenomenon depending on the relative strength of buoyancy- and surface-tension-driven forces. The oscillatory instability is characterized in the relevant parametric space spanned by the reactor height, the Marangoni (Ma_i) and the Rayleigh (Ra_i) numbers of the *i*-th chemical species, the latter ruling the surface tension and buoyancy contributions to convection, respectively. This study suggests possible scenarios where emergent phenomena can develop even in the absence of nonlinear kinetics, which is commonly assumed as a minimal requirement for complex behaviours in chemical systems.

[1] L. Gálfi and Z. Rácz, Phys. Rev. A 38, 3151 (1988).
[2] M.A. Budroni, V. Upadhyay, L. Rongy, submitted (2019).

Orientation of defects in 2D active nematics

Contributed talk **18**

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Topological defects are regions in an ordered material where the characteristic order is un- defined. These defects are of significant interest in understanding the dynamics of active nematics, which are intrinsically out of equilibrium [1]. We are interested in the orientation of defects in curved geometries, and this initially calls for a thorough analysis of how the defects behave in at space. Following previous studies on defect hydrodynamics, we treat these defects as self-propelled particles that move under an active stress [2,3]. In our case, this active ow is generated by the turbulent motion of microtubule filaments, which form an extensile nematic at an oil-water interface. In this talk, we explain how we prepare and image this system and identify the defects using image analysis techniques. We focus on their orientation calculated directly from the divergence of the nematic tensor order parameter [4]. We then use the defect positions and orientations to define relevant order parameters – polar and nematic order for the +1/2 defects, and a 3-fold bond angle order for the -1/2 defects. These quantities give us insights on the orientational ordering in our system. We also look at orientational correlations of the detected defects, and connect it to theoretical results.

[1] P.W. Ellis, D. J. G. Pearce, Y. W. Chang et. al., Nat. Phys. 14, 85 - 90 (2018).
[2] M. C. Marchetti, J. F. Joanny, S. Ramaswamy et. al., Rev. Mod. Phys. 85, 1143-1189 (2013).
[3] L. Giomi, M. J. Bowick, P. Mishra et. al., Phil. Trans. R. Soc. A 372: 20130365 (2014).
[4] A. J. Vromans and L. Giomi, Soft Matter 30, 6490-6495 (2016).

A phase diagram for bacterial swarming | 19

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Bacterial swarming is a mode of motion in which dense collectives of rod-shaped flagellated cells migrate rapidly on surfaces. The transition into swarming involves several cellular processes, including changes in cell aspect ratio, suggesting that bacteria manipulate these properties in order to promote physical conditions that are favorable for swarming. New results with monolayer swarms of Bacillus subtilis with different aspect ratios – ranging from 5.5 to 19, were analyzed at different cell-densities. Tracking of individual cell trajectories allows a comprehensive analysis of both the individual and collective dynamics of bacteria in a swarm. These are used to compose a phase diagram, showing sharp transitions between phases corresponding to qualitatively different swarm statistics.

Comparing with theories of active particles, we find some successful theoretical predictions, but mostly in the large aspect ratio regime. Several aspects (e.g. bimodal cluster-size distributions and giant number fluctuations) are found to some extent, while other prominent experimental features cannot be explained by current theories.

From a biological perspective, we find that under standard conditions bacteria inhabit a region of phase space in which the swarm dynamics is highly robust and insensitive to fluctuations. In this regime, bacteria do not form very large clusters and lack global orientational order, properties which may reduce the colony's ability to expand rapidly in the absence of external directional cues.

Joint work with Avraham Be'er (BGU), Bella Ilkanaiv (BGU), Renan Gross (Weizmann), Daniel Kearns (Indiana U), Sebastian Heidenreich (PTB) and Markus Bär (PTB).

[1] Avraham Be'er and Gil Ariel, A statistical physics view of swarming bacteria. Movement Ecology 7, 9 (2019).

Interplay among bistability, excitability and fluctuations determines locomotion strategy of crawling cells

20

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Cells polarize spontaneously due to internal biochemical reaction-diffusion processes. After polarization, cell motion is generated by the push on the membrane of the actin microfilament network. The attachment of the filaments at the membrane is controlled by proteins involved in the polarization process. Therefore, the changes on biochemical concentrations produce differences in the stress on the membrane and different strategies of cell motion can be selected.

We model cellular motion by the coupling of a stochastic biochemical reaction-diffusion model inside of the cell with the deformation of the membrane by the use of an additional phase field for the cellular area. Such additional field accounts for the deformation and displacement of the cell membrane.

We employ a single simple model to study amoeboid and keratocyte-like motions, which are compared with experiments on individual *Dictyostelium discoideum* cells under different conditions. We can, furthermore, easily evaluate numerically the effect of confinement of the spatio-temporal patterns inside the cells by changing the simulation domain. The obtained results are employed to interpret experiments with giant *Dictyostelium discoideum* cells generated by electrically-induced cell fusion.

Symposium 4: Control of self-organization

S. Klapp, E. Schöll

Spatio-temporal control of self-organized patterns in dynamic self-assembly systems

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The control and engineering of the dynamical behavior of spatio-temporal patterns in complex systems is one of the key issues of recent research. A variety of different control methods has been developed within the last decades. In particular, external periodic forcing methods as well as feedback loops have been widely used to influence the dynamics of patterns. In this talk, using a combination of theoretical, numerical and path-continuation methods we discuss how these control strategies can be applied to surface coating problems. In particular, we focus on a theoretical description of experimental techniques such as dip-coating or vapor deposition of molecules that are often used for the coating of surfaces with a precise density and structure. We shall show how the basic properties of different systems lead to the formation of specific self-organized patterns. This enables the development of methods to control structure formation, e.g. by pre-structured substrates or external time-dependent fields.

Control of chimera states with a pacemaker

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Chimera states are phenomena in networks of oscillators in which synchronisation coexists with incoherent behaviour. In finite-size networks chimera states are not stable, they collapse to a fully synchronous state at some random moment in time. Furthermore, the coherent and incoherent groups that form the chimera drift across the network. I will review a recent proposal of ours to control chimera states in ring-networks of non-locally coupled phase oscillators [1]. We break the rotational symmetry of the network by turning one network node into a pacemaker, i.e. an oscillator which does not receive any input from other oscillators and therefore rotates at a constant frequency. Accordingly, this method acts exclusively on the connectivity structure of the network. We find that the pacemaker attracts the incoherent part of the chimera, thus preventing its drifting. Moreover, a pacemaker can generate a chimera state for initial conditions for which it would not form spontaneously and can also prevent the chimera from collapsing to the synchronous state. Exploiting the symmetry breaking idea behind the pacemaker, we show that even minimal modifications of the network's connectivity allow one to control chimeras. In closing, I will discuss how our control mechanism can be extended to multilayer networks.

[1] G Ruzzene, I Omelchenko, E Schöll, A Zakharova, RG Andrzejak. Controlling chimera states via minimal coupling modification, Chaos, in press.

Multi-layer structures in slowly adapting networks of coupled oscillators

Contributed talk **23**

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Dynamical systems on networks with adaptive couplings appear naturally in real-world systems such as power grid networks, social networks as well as neuronal networks. We investigate collective behaviour in a paradigmatic network of adaptively coupled phase oscillators. The coupling topology of the network changes slowly depending on the dynamics of the oscillators on an all-to-all coupled background. We show that such a system gives rise to numerous complex dynamics, including relative equilibria and hierarchical multi-cluster states. Parameter regimes of high multi-stability are found. An analytic treatment for equilibria as well as multi-cluster solutions reveals that existence and stability are significantly influenced by the slow-fast time separation. Interactions between different clusters are further studied numerically and analytically in the framework of multiplex networks. Our results allow for the interpretation of equilibria as functional units in multi-cluster structures. The results contribute to the understanding of mechanisms for self-organized pattern formation in adaptive networks, such as the emergence of multi-layer structure in neural systems and their interaction.

Self-organization of microswimmers in arrays of obstacles

Contributed talk **24**

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Bacterial suspensions, a paradigmatic example of an active fluid, are known to exhibit a state denoted as mesoscale turbulence which is characterized by chaotic dynamics of vortices of a characteristic size. In a recent experiment, these vortices have been stabilized into a square lattice with antiferromagnetic order by geometrically constraining the bacterial suspension using periodic arrays of obstacles with a spacing in the range of the unconstrained vortex size [1]. Interestingly, the vortices are consistently located in the gaps between the obstacles rather than forming around them [1]. We aim to reproduce the patterns observed in the experiment using a recently derived fourth order field theory for a vectorial order parameter representing an effective microswimmer velocity [2]. In this continuum-theoretical framework, we propose a set of boundary conditions that implicitly favors negatively charged topological defects located in the centers of the pillars. By tuning the pillar size we can influence the topological charge already for a single pillar in otherwise unconstrained mesoscale turbulence and, in particular, stabilize an antiferromagnetic vortex lattice in a large configuration of pillars.

[1] D. Nishiguchi, I. S. Aranson, A. Snezhko and A. Sokolov, Nat. Comm., 9, 4486 (2018).
[2] H. Reinken, S. H. L. Klapp, M. Bär, and S. Heidenreich, Phys. Rev. E, 97, 022613 (2018).

The nonequilibrium statistical mechanics of self-phoretic active particles

25

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Micrometric active particles can be driven away from equilibrium by self-diffusiophoresis, if catalytic reactions generate concentration gradients along the surface of the particles. Because of their micrometric size, their orientation and position undergo stochastic movements. To be consistent with microreversibility and Onsager reciprocal relations, the fluctuations in the reaction rate should also be included in the description. In this way, coupled overdamped Langevin equations are obtained satisfying a mechanochemical fluctuation theorem in consistency with microreversibility and the entropy production expected for systems driven by mechanochemical coupling. Similar considerations apply to particles propelled by self-thermophoresis. The consequences of these results for the single-particle and many-particle dynamics will be presented.

[1] P. Gaspard and R. Kapral, Mechanochemical fluctuation theorem and thermodynamics of self-phoretic motors, J. Chem. Phys. 147 (2017) 211101.
[2] P. Gaspard and R. Kapral, Fluctuating chemohydrodynamics and the stochastic motion of self-diffusiophoretic particles, J. Chem. Phys. 148 (2018) 134104.
[3] M.-J. Huang, J. Schofield, P. Gaspard, and R. Kapral, Dynamics of Janus motors with microscopically reversible kinetics, J. Chem. Phys. 149 (2018) 024904.
[4] P. Gaspard and R. Kapral, Thermodynamics and statistical mechanics of chemically-powered synthetic motors, to be published in Adv. Phys. X (arXiv :1810.04543).

Mesoscopic modeling of active and passive membrane deformation created by dynamin oligomers

Contributed talk **26**

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Dynamin builds long filaments wrapped around membrane tubes, and, in the presence of GTP, it is able to cut membrane tubes. Even in the absence of motor activity, the intrinsic helical shape of dynamin allows it to constrict the tube, balancing deformations of the filament and the membrane. First, a continuum elastic-theory description for dynamin filaments on deformable membrane tubes is developed. Then, a discrete polymer-like model with the dynamin dimer as the building block is constructed and applied. Explicit solvent simulations and structurally-resolved coarse-grained simulations for dynamin were performed to determine elastic parameters of its filaments, indicating that the stiffness of dynamin is effectively comparable to that of the membrane. The results explain the experimentally observed weak dependence of the coated tube radius on the tension and bending parameters of the membrane, and additionally predict a strong dependence of the pitch of the helical filament. Introduction into the model of cross-dimerization and nucleotide-dependent conformational changes between dynamin dimers in neighboring turns provides a detailed picture of dynamin scission activity.

3D wave instabilities of confined active networks

Contributed talk **27**

Tobias Strübing, Andrej Vilfan, Eberhard Bodenschatz, Ramin Golestanian, **Isabella Guido**

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Networks of biofilaments and motor proteins are important model systems for the understanding of the out-of-equilibrium behavior of the cellular cytoskeleton. In the last years the active nematic behavior of microtubules with kinesin motors confined on a 2D substrate was reported [1]. In this study we present experimental and theoretical results on a 3D active nematic system. In our setup the solution used for the assembly of the active system contained polymerized microtubules, multi-headed kinesin-1 motor proteins, poly(ethylene glycol) or PEG and ATP as reported in [2]. The non-equilibrium nature of the system was due to kinesin-1 that in the presence of ATP moves along the microtubules. By adding the nonadsorbing polymer PEG, attractive interactions between microtubules are induced through depletion force that leads to bundle formation [3, 4]. These bundles were subjected to the force exerted by the motors that crosslinked the microtubules and let them slide against each other, depending of their polarity. By confining the network into a PDMS channel we could observe the formation of 3D wrinkling instabilities resulting from the contraction and the extension of the network. Indeed, it contracted in a sheet along the z-direction, which represents the height of the channel, and extended along the longitudinal axis of the channel. As the system is confined in the volume of the microfluidic device the extension due to the polarity sorting of the molecular motors induced a network buckling that generated 3D wrinkles in the z-direction. We believe that the requirements for the wrinkle instabilities are the bundle formation and their anisotropic orientation within the network, e.g. the nematic order we observed in the direction of the extensile force.

[1] T. Sanchez, D. T. N. Chen, S. J. DeCamp, M. Heymann and Z. Dogic, Nature, 491, (2012).
[2] T. Sanchez, D. Welch, D. Nicastro and Z. Dogic, Science, 333, 6041 (2011).
[3] S. Asakura and F. Oosawa, The Journal of Chemical Physics 22, 7 (1954).
[4] D. Needleman, M. A. Ojeda-Lopez, U. Raviv, K. Ewert, J. B. Jones, H. P. Miller, L. Wilson and C. R. Safinya, Phys. Rev. Lett., 93, 19 (2004).

Light driven self-sustained motion of spherical polymer brushes

Contributed talk **28**

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For manipulating nano- and micro sized objects at interfaces there is no immediate concept to gently move an ensemble of objects within a selected, possibly very small area. Atomic Force Microscope (AFM) has been the only method allowing a controlled motion of micro/nano- objects by mechanical pushing of single particles adsorbed at a surface.1 With that approach the reordering and manipulation is only possible on few particles, where on a macroscopic scale this approach is very time consuming and thus not beneficial. Recently Feldmann et al. reported a method of particle manipulation at liquid/solid interface by using light as external stimuli. The mechanism of particle manipulation is based on light induced generation of local hydrodynamic flow in the solution containing photosensitive molecules. These molecules are cationic surfactant in hydrophobic tail of which azobenzene group is incorporated to. Under illumination the photosensitive surfactant photo-isomerizes from trans- to cis- state resulting in changing of the hydrophobicity of the whole molecule.3 By local illumination with light of appropriate wavelength, the particles trapped at the solid interface can be collected or removed at the desired area of choice.2 So far, another attractive application is a near perfect particle separation at interface. Here we report on light induced manipulation and active motion of particles decorated by polymer brushes. The driving force of motion is a reversible release of brush interior surfactant molecules into the bulk solution by a controlled illumination of the macroscopic area. The release of surfactant molecules creates a hydrodynamic flow around each particle. On a macroscopic scale the lateral hydrodynamic flow around each particle separates all brush modified particles uniformly at the interface. In this study we systematically studied how the extend of particle motion depends on different parameters such as brush thickness, the surfactant concentration, the degree of ionization of polyelectrolyte brush.

[1] Y. Sun, X. Liu. Micro- and Nanomanipulation Tools (Wiley-VCH: Weinheim, 2015).
[2] D. Feldmann, S. R Maduar, M. Santer, N. Lomadze, O. I. Vinogradova, S. Santer, Scientific Reports, 6, 36443 (2016).
[3] S. Santer, «Remote control of soft nano-objects by light using azobenzene containing surfactants» Journal of Physics D: Applied Physics, 51, 013002 (2017)

Mechanochemical modelling of crawling cells

Contributed talk **29**

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Despite the diversity of cell types, biological cells, which are the basic unit of living creatures, share common structures. They are composed of a number of proteins, lipids, and sugars, which form stable structures such as cellular membranes. At the same time, a living cell is at a far-from-equilibrium state. Complex chemical reactions take place inside a cell, the information of which is converted to mechanical forces by molecular motors. Consequently, a cell exhibits various dynamics spontaneously.

Spontaneous motion is a key property of active matter, which generates force in itself by consuming potential energy. Such force vanishes in total because of the law of action and reaction. To achieve a net directional motion under the force-free condition, symmetry breaking plays a fundamental role.

Typical mechanism of cell crawling is thought of as a cycle of four processes: 1) protrusion of the leading edge, 2) adhesion of the leading edge to the substrate, 3) deadhesion of the trailing edge from the substrate, and 4) contraction of the trailing edge. In our previous study [1], we clarified the importance of the order of these four basic processes by introducing a simple model crawling cell composed of two elements connected by a viscoelastic spring. The spring contains a linear actuator that elongates and shrinks in time, represent in the protrusion and contraction. Since the force generated by the actuator acts on the two elements symmetrically, the force-free condition is satisfied. In addition, the substrate friction characteristics switches between the adhered stick state and the deadhered slip state, modelling the adhesion and deadhesion processes. The phase shift between the stick-slip transitions in the substrate friction of the two elements breaks the symmetry, which enables the cell to achieve a net migration.

In this presentation, we consider an extension of the model to two dimensions where the cell is modelled by many of such subcellular elements connected by viscoelastic springs [2]. In order to control the actuator elongation and the stick-slip transition of the substrate friction of each subcellular element, we couple the mechanical model with reaction-diffusion equations that represent intracellular chemical reactions. By introducing mechanical and chemical dependence of the substrate friction, we show that the cell changes migration behavior depending on the intracellular chemical state.

[1] M. Tarama and R. Yamamoto, J. Phys. Soc. Jpn., 87, 044803 (2018).
[2] M. Tarama, K. Mori, and R. Yamamoto, (preprint).Mitsusuke Tarama [1], Kenji Mori [2], Ryoichi Yamamoto [2;3]

Emergence and control of patterns in active fluids | 30

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Active fluids like suspensions of bacteria, microtubule bundles and artificial microswimmers consist of individuals that are able to transform internal energy into a directed motion. As a result, the system is always out of equilibrium even without external forces and driving boundaries which yields fascinating collective phenomena and unexpected pattern. Many efforts have been made to understand the influence of individual's properties onto the emergence of pattern on the meso- or macroscale. In the talk, I first introduce a simple model for a microswimmer that generates a flow of the surrounding fluid and then formulate "microscopic" equations of motion representing a collection of these swimmers including alignment interaction, rotational and translational noise. Secondly, I sketch the derivation of "mesoscale" continuum equations from the collection of model swimmers. Depending on the symmetry of the interaction between swimmers the continuum equations obtained lead to polar or nematic order parameter equations coupled to the hydrodynamic equation of the surrounding fluid. As a result, the different symmetries lead to the emergence of different topological defect as well as different forms of collective motion and patterns. I will give a brief overview about these patterns and finally I select mesoscale turbulence to present and discuss that phenomenon in detail. Finally, I will briefly address the topic of control of the emerging mesoscale by means of external fields and obstacles.

Aligning active searchers wheel around their common home position

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I will discuss an ensemble of active searchers which are connected to a common home which is the central position of their search and return. The single searcher explores actively the space around this home and returns permanently to its home position due to an internal stochastic path integrating search and return mechanism. The dynamics of a deterministic searcher is integrable but the stochastic active searcher becomes dissipative whereby the relaxation of its angular and spatial variables scale differently with the noise. These scalings causes an optimal noise for a successful finding of a new food sources near to the home. An aligning interaction of the velocity directions between searchers models the avoidance of collisions between neighboring units. With overcritical interaction strength, we find a transition to a cooperative behavior wherein the active searchers wheel around their common home position. Numeric findings are supported analytically by the formulation of transport equations outgoing from the nonlinear mean field Fokker-Planck equation. In the asymptotic stationary limit after decoupling the higher angular moments using a von Mises distribution we find expressions for the mean radial and orbital velocity and for their variances. We also derive expressions for the marginal spatial and angular particle densities in the under- and in the over-critical regime.

Brownian motion and beyond | 32

Ralf Metzler

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Roughly 190 years ago Robert Brown reported the "rapid oscillatory motion" of microscopic particles, the first systematic study of what we now call Brownian motion. At the beginning of the 20th century Albert Einstein, Marian Smoluchowski, and Pierre Langevin formulated the mathematical laws of diffusion. Jean Perrin's experiments 110 years ago then prompted a very active field of ever refined diffusion experiments.

Despite the long-standing history of Brownian motion, after an historic introduction I will report several new developments in the field of diffusion and stochastic processes. This new research has been fuelled mainly by novel insights into complex microscopic systems such as living biological cells, made possible by Nobel-Prize winning techniques in laser physics, superresolution microscopy, or through supercomputing studies. Topics covered in-clude Brownian yet non-Gaussian diffusion [1], the geometry-control of chemical reactions [2], and anomalous diffusion with a power-law time dependence of the mean squared dis-placement [3,4].

[1] A. V. Chechkin, F. Seno, R. Metzler, and I. M. Sokolov, Phys. Rev. X 7, 021002 (2017).
[2] D. Grebenkov, R. Metzler, and G. Oshanin, Comm. Chem. 1, 96 (2018).
[3] K. Nørregaard, R. Metzler, C. M. Ritter, K. Berg-Sørensen, and L. B. Oddershede, Chem. Rev.117, 4342 (2017).
[4] R. Metzler, J.-H. Jeon, A. G. Cherstvy, and E. Barkai, Phys. Chem. Chem. Phys. 16, 24128 (2014).

How thermodynamic notions fare and fail far from equilibrium

33

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Far from equilibrium, conventional coarse-grained descriptions of interacting many-body systems in terms of pressure and temperature, say, are not guaranteed to work consistently anymore. Often, they are jeopardized by unwieldy fluctuations and (e.g. non-reciprocal or inelastic) interactions. I will discuss several toy models, which allow some of the problems to be elucidated, and which provide hints at useful generalisations of classical thermodynamic notions and their limits. Examples comprise non-isothermal and active Brownian particles, retarded interactions, and active heat engines.

Brownian yet non-Gaussian diffusion in heterogeneous environment

34

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We discuss the situations under which Brownian yet non-Gaussian (BnG) diffusion can be observed in the model of a particle's motion in a random landscape of diffusion coefficients slowly varying in space. Our conclusion is that such behavior is extremely unlikely in the situations when the particles, introduced into the system at random at t = 0, are observed from the preparation of the system on. However, it indeed may arise in the case when the diffusion (as described in Ito interpretation) is observed under equilibrated conditions. This paradigmatic situation can be translated into the model of the diffusion coefficient fluctuating in time along a trajectory, i.e. into a kind of the "diffusing diffusivity" model.

Symposium 9: Applications to nonlinear chemical and physical systems

K. Krischer, H. H. Rotermund

Riddles of a rippled icicle

35

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Many natural icicles have very regular ripples or ribs around their circumference. Why? We delved into the subtle physics of icicle morphology by studying laboratory-grown icicles. The first surprise is that the ripples only form when small amounts of impurity are present [1]. Ripples travel up or down the icicle, depending on the impurity concentration. Similar ripples are observed on stalactites, but the detailed mechanism of their growth is only partly analogous. So far, linear stability theory fails to account for icicle ripples, but not for lack of trying.

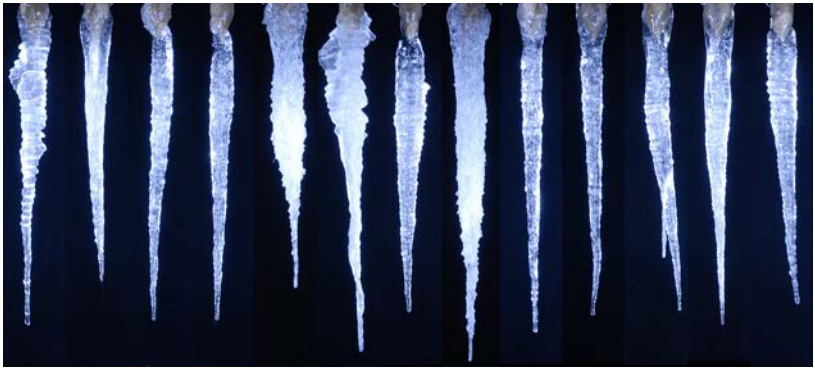

Figure 1: See the Icicle Atlas at https://www.physics.utoronto.ca/Icicle Atlas/

[1] Antony S-H. Chen and Stephen W. Morris, New Journal of Physics, 15, 103012 (2013).

Dynamics of V-oxide catalysts from UHV to 0.1 mbar | 36

Ronald Imbihl[1], Bernhard von Boehn[1], Helder Marchetto[2, 3], Thorsten Franz[3], Gerhard Lilienkamp[4]

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The dynamics of ultrathin vanadium oxide layers on a Rh(111) surface during catalytic methanol oxidation have been studied in situ with spatially resolving imaging techniques from ultra-high vacuum (UHV) to the 10^{-2} mbar range. At 10^{-6} - 10^{-4} mbar VO_x condenses into macroscopic circular islands that exhibit a substructure. This substructure arises due to an oxygen gradient inside the VO_x islands, resulting in different coexisting 2D-phases of VO_x on Rh(111). This substructure is also responsible for a "breathing-like" oscillatory expansion and contraction that the islands undergo under stationary conditions. On the basis of a 2D-phase diagram calculated with density functional theory, the oscillatory behavior can be understood as a periodic phase transition between two 2D phases of VO_x. With a newly developed near ambient pressure – low energy electron microscope (NAP-LEEM) it was shown that VO_x islands disintegrate at 10^{-2} mbar generating turbulent dynamics.

Bichaoticity induced by inherent birhythmicity during the oscillatory electrodissolution of Silicon[1]

Contributed talk **37**

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The electrodissolution of p-type silicon in a fluoride-containing electrolyte is a prominent electrochemical oscillator with a still unknown oscillation mechanism. In this talk dynamical states within a wide range of the applied voltage - external resistance parameter plane are presented. Thereby the focus lies on the bistability of two prominent routes to deterministic chaos, induced by the inherent birhythmicity of the system. We provide evidence of two coexisting limit cycles each linked to a distinct feedback loop sharing a common variable. The interplay of these two mechanisms gives rise to a large variety of dynamical states.

[1] A. Tosolini, M. Patzauer, K. Krischer Bichaoticity Induced by Inherent Birhythmicity during the Oscillatory Electrodissolution of Silicon, 29, 043127 Chaos (2019).

Oscillations, travelling fronts and patterns in a supramolecular system

Contributed talk **38**

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Supramolecular polymers, such as microtubules, operate under non-equilibrium conditions to drive crucial functions in cells, such as motility, division and organelle transport. In vivo and in vitro size oscillations of individual microtubules and collective oscillations have been observed. In addition, dynamic spatiotemporal structures can form in non-stirred systems. Here [1] we describe an artificial supramolecular polymer made of a perylene diimide derivative that displays oscillations, travelling fronts and centimetre-scale self-organized patterns when pushed far from equilibrium by chemical fuels. Oscillations arise from a positive feedback due to nucleationelongationfragmentation, and a negative feedback due to size-dependent depolymerization. Travelling fronts and patterns form due to self-assembly induced density differences that cause system-wide convection. In our system, the species responsible for the nonlinear dynamics and those that self-assemble are one and the same. In contrast, other reported oscillating assemblies formed by vesicles, micelles or particles rely on the combination of a known chemical oscillator and a stimuli-responsive system, either by communication through the solvent (for example, by changing pH), or by anchoring one of the species covalently (for example, a Belousov-Zhabotinsky catalyst). The design of self- oscillating supramolecular polymers and large-scale dissipative structures contributes to the creation of more life-like materials that respond to external stimuli similarly to living cells.

[1] Jorge Leira-Iglesias, Alessandra Tassoni, Takuji Adachi, Michael Stich and Thomas M. Hermans, Nature Nanotech., 13, 1021-1027 (2018).

Asymmetric anomalous diffusion in cell chemotaxis: experiments and stochastic modeling

Contributed talk **39**

[1]Peter Dieterich[1], Otto Lindemann[2], Mats Leif Moskoppa[1], Sebastien Tauzin[3], Anna Huttenlocher[4], **Rainer Klages**[5,6,] Aleksei Chechkin[7,8,] and Albrecht Schwab[2]

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We study the diffusive motion of neutrophil granulocytes under chemotaxis [1]. First we report experimental results of different cell types in vitro and in vivo by extracting the mean position, the mean square displacement and velocity autocorrelation functions. We find that chemotacting neutrophils exhibit asymmetric anomalous dynamics with temporal long-range correlations superimposed on a constant drift, which guides efficient chemotactic behavior. These experimental results are reproduced consistently by an asymmetric overdamped Langevin equation with power-law correlated noise. On this basis we also study the validity of work fluctuation relations for which we find characteristic deviations from the conventional form [2].

[1] P.Dieterich et al., submitted
[2] A.V.Chechkin, F.Lenz, R.Klages, J.Stat.Mech. L11001 (2012)

Dynamics of bottom-heavy squirmer microswimmers

Contributed talk **40**

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The self-propulsion of active biological or synthetic microswimmers is often influenced by a gravitational field [1,2], where a density mismatch leads to sedimentation, and an off-set center of mass triggers reorientation antiparallel to the direction of the external force [2]. Combining these passive effects with swimmer self-propulsion and hydrodynamics, incorporated by the squirmer model [3,4], a variety of collective dynamics is observed: While a system of roughly 1000 neutral squirmers exhibits a conventional sedimentation profile for strong external forces, it favors an inverted profile for weaker forces and finite gravitational torques. Additionally, we find continuous convective plumes, induced by the top wall, and convective rolls at the bottom wall for some parameters. If the sedimentation velocity is so strong that it approaches the self-propulsion velocity, we observe long-lived spawning clusters with vertically oriented swimmers close to the bottom wall. Pusher- and puller-type squirmers also show conventional and inverted sedimentation, however clusters and plumes remain transient, due to disturbing swimmer-swimmer hydrodynamic interactions.

[1] J. Palacci et al., Phys. Rev. Lett., 105, 088304 (2010).
[2] K. Drescher et al., Phys. Rev. Lett. 102, 168101 (2009).
[3] M. J. Lighthill, Commun. Pure Appl. Math. 5, 109 (1952).
[4] J.-T. Kuhr et al., Soft Matter 13, 7548 (2017).

Spatial heterogeneities shape collective behavior of signaling amoeboid cells

Contributed talk **41**

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We present novel experimental results on pattern formation of signaling Dictyostelium discoideum amoeba in the presence of a periodic array of millimeter-sized pillars. In our experiments with caffeine treated cells, we observe concentric cAMP waves that initiate almost synchronously at the pillars and propagate outwards. These waves have a higher frequency than the other firing centers and dominate the system dynamics. The cells respond chemotactically to these circular waves and stream towards the pillars, forming periodic domains that reflect the periodicity of the underlying lattice. We performed comprehensive numerical simulations of a reaction-diffusion model to study the role of caffeine and characteristics of the boundary conditions given by the obstacles. Our simulations show that a critical minimum accumulation of cAMP around the obstacles is required for the pillars to act as the wave source. This critical value depends on the cAMP production rate, a variable which we can experimentally decrease by adding caffeine. Moreover, our simulations reveal that caffeine reduces the excitability threshold of the cells and increases the sensitivity to cAMP accumulation around the obstacles. In the absence of caffeine, non-treated cells are less sensitive to cAMP accumulation around the pillars and ignore them, as observed in our experiments. Our results suggest that in nature the excitability threshold of the cells is tuned by an adaptation process that optimizes the sensitivity to waves while ignoring the cAMP accumulations around spatial heterogeneities which can interrupt the development process of the cells in complex environments.

Spreading strategies and morphology of bacterial colonies: interplay between passive physico-chemical effects and bioactive growth

42

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The spreading of bacterial colonies at solid–air interfaces is determined by the physico-chemical properties of the involved interfaces and bioactive growth processes. The production of surfactant molecules by bacteria is a widespread strategy that allows the colony to efficiently expand over the substrate. On the one hand, surfactant molecules lower the surface tension of the colony, effectively increasing the wettability of the substrate, which facilitates spreading. On the other hand, gradients in the surface concentration of surfactant molecules result in Marangoni flows that drive spreading. These flows may cause an instability of the circular colony shape and the subsequent formation of fingers. In this work, we study the effect of bacterial surfactant production and substrate wettability on colony growth and shape within the framework of a hydrodynamic thin film model. We show that variations in the wettability and surfactant production are sufficient to reproduce four different types of colony growth, which have been described in the literature, namely, arrested and continuous spreading of circular colonies, slightly modulated front lines and the formation of pronounced fingers.

Mitotic spindle scaling & size control: how complexity arises from molecular interactions

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The mitotic spindle is a molecular machine, which assembles once every cell division to align and segregate the genetic material. The spindle is an evident example why size of intracellular organelles matters: The spindle must be large enough to span sufficient distance to physically separate chromosomes into two opposite halves of the cell. While approaching a near to complete proteomic parts lists of the metaphase spindle, mechanisms that control its defined shape and size remain poorly understood. One reason why this question has been hard to answer is that the size of an organelle is generally not simply set by a "ruler" but is an emergent property of molecular collectives. We have shown that mass balance together with a "liquid crystal" analogy is a useful working hypothesis to account for the dynamic properties of spindles and link these to spindle length. Cytoplasmic extracts prepared from eggs of the African clawed frog Xenopus laevis have proven valuable for studying spindle assembly and organization. More recently, comparison with extracts of the related but smaller frog Xenopus tropicalis allowed the identification of spindle scaling factors. We are interested in how the biochemistry of the basic building block of the spindle, αβ-tubulin, contributes to differences in spindle morphology. We combine in vitro reconstitution assays, state-of-the art imaging and simulations to show how biochemical adaptation on the molecular scale can create physiological structures in the µm-scale that enable faithful chromosome segregation.

Guiding self-organized pattern formation in cell polarity establishment

44

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Spontaneous pattern formation in Turing systems relies on feedback. But patterns in cells and tissues seldom form spontaneously—instead they are controlled by regulatory biochemical interactions that provide molecular guiding cues. The relationship between these guiding cues and feedback in controlled biological pattern formation remains unclear. Here, we explore this relationship during cell-polarity establishment in the one-cell-stage Caenorhabditis elegans embryo. We quantify the strength of two feedback systems that operate during polarity establishment: feedback between polarity proteins and the actomyosin cortex, and mutual antagonism among polarity proteins. We characterize how these feedback systems are modulated by guiding cues from the centrosome, an organelle regulating cell cycle progression. By coupling a mass-conserved Turing-like reaction–diffusion system for polarity proteins to an active-gel description of the actomyosin cortex, we reveal a transition point beyond which feedback ensures self-organized polarization, even when cues are removed. Notably, the system switches from a guide-dominated to a feedback-dominated regime well beyond this transition point, which ensures robustness. Together, these results reveal a general criterion for controlling biological pattern-forming systems: feedback remains subcritical to avoid unstable behaviour, and molecular guiding cues drive the system beyond a transition point for pattern formation.

Self-organization by fluid flows

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Long-ranged dynamic patterns are important for development and functioning of large-scale organisms. In the tubular networks of plasmodial slime molds the tubes' periodic contractions organize in a traveling wave on scales of up to several centimeters. What drives communication across the network? What drives the self-organization of the tube's cortex to form long-wavelength patterns? Searching for the mechanism of signal propagation we find that flows are hijacked by signals to propagate through the network. Signals promote their own transport by invoking a propagating front of increased flow. This mechanism is sufficient to explain complex dynamics of the organism like finding the shortest path through a maze. Importantly, we find that distant parts within the tubular network communicate by fluid flow. We investigate the mechanism behind the self-sustained contractile waves by developing a minimal model, coupling the mechanics of a cell's cortex to a contraction-triggering chemical. The chemical itself is spread with the fluid flows that arise due to the cortex contractions. Through theoretical and numerical analysis, we find that the oscillatory component of the flows can give rise to robust scaling of contraction waves with system size—much beyond predicted length scales.

No equations, no variables, no parameters, no space, no time: Data and the modeling of complex systems

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Obtaining predictive dynamical equations from data lies at the heart of science and engineering modeling, and is the linchpin of our technology. In mathematical modeling one typically progresses from observations of the world (and some serious thinking!) first to equations for a model, and then to the analysis of the model to make predictions. Good mathematical models give good predictions (and inaccurate ones do not) - but the computational tools for analyzing them are the same: algorithms that are typically based on closed form equations.

While the skeleton of the process remains the same, today we witness the development of mathematical techniques that operate directly on observations -data-, and appear to circumvent the serious thinking that goes into selecting variables and parameters and deriving accurate equations. The process then may appear to the user a little like making predictions by "looking in a crystal ball". Yet the "serious thinking" is still there and uses the same -and some new- mathematics: it goes into building algorithms that jump directly from data to the analysis of the model (which is now not available in closed form) so as to make predictions. Our work here presents a couple of efforts that illustrate this ``new" path from data to predictions. It really is the same old path, but it is travelled by new means.

PLENARY TALK

POSTER

Chemical reaction-diffusion phenomena in a two-channel fluidic device

P1

Brigitta Duzs, Istvan Szalai

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Pattern formation in living systems often relies on reaction-diffusion mechanisms, hence it is straightforward to construct simplified experimental setups in order to mimic and understand the dynamics leading to complex spatiotemporal behavior far from thermodynamic equilibrium. Inorganic chemical oscillatory reaction networks are excellent candidates to provide the required nonlinearities in chemical kinetics by using common initial reagents. [1] These reactions consist of coupled positive and negative feedbacks and are known for the versatile nonlinear phenomena shown under well-mixed conditions, e.g. bistability, excitability, sustained temporal oscillations or chaos. The application of spatial gel reactors extends the observations towards spatial instabilities. Typically, a piece of hydrogel, fed from one or two outer reservoir(s), is applied as a non-convective medium where the reaction-diffusion phenomena occur. The pattern formation due to chemical gradients is a prototype of spatial information coding in biological systems. Patterns generated at antagonistic gradients of reactants have raised attention, because the appropriate separation of the initial chemicals locates spatial instabilities in a well-defined zone. [2] In this work we develop a two-channel fluidic de- vice shaped from an agarose cuboid, where the reaction-diffusion patterns form between two continuously owing channels. We apply autocatalytic and oscillatory chemical reactions to generate three-zoned patterns, waves and stationary structures. As a great advantage of this geometry, compared to a classical two-side-fed gel reactor, the patterning zone and the feeding channels are made of the same piece of gel. In the future, this one-block construction may allow us to detect volume changes due to the emerging chemo-mechanical structures when a responsive gel material is applied.

[1] I. R. Epstein and J. A. Pojman, An Introduction to Nonlinear Chemical Dynamics: Oscillations, Waves, Patterns and Chaos (Oxford University Press, USA, 1998).
[2] B. Duzs and I. Szalai, RSC Adv., 8, 41756 (2018).

Movement of DNA within microporous materials in an electric field

P2

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Directed movement of DNA fragments in organic and inorganic networks could be successfully implemented and monitored, using a fiber-based chip with imprinted electrodes. Investigation regarding molecular interaction of biopolymers under electrical force and differences in mobility of DNA samples in fiber-based test setups will influence the present DNA detection and verification methods in low-cost disposable bioanalytical devices.

Self-entrainment of an inherent birhythmic system

P3

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Si electrodissolution in fluoride-containing electrolytes is one of the rare experimental systems which exhibits birhythmicity, i.e. the coexistence of two stable limit cycles. In this contribution, we present data of the dynamics in the birhythmic region of n-type Si electrodes as a function of two parameters, the applied voltage and the illumination strength. It is demonstrated that the interaction of the two coexisting limit cycles can lead to different modes of self-entrainment. Moreover, at low illumination strength, the locking of the two inherent oscillatory modes might go along with spatial symmetry breaking, giving rise to cluster patterns. Our results indicate that a system with two co-existing inherent limit cycles might exhibit dynamics as rich as those of coupled oscillators or periodically forced oscillatory active media.

Photosensitive surfactants at hydrophilic and hydrophobic surfaces

P4

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Here we report on study of adsorption kinetics of photosensitive azobenzene containing surfactants on different substrates under illumination with UV (λ=355nm) and green (λ=532nm) light. The work is motivated by the newly discovered phenomenon so-called light driven diffusioosmosis (LDDO): local liquid flow is generated at solid/liquid interface under irradiation with focused UV or green light [1]. Colloidal particles trapped at solid/liquid interface move passively within this LDDO flow, and can be arranged in different pattern, removed selectively or gathered on demand. The main ingredient of this process is photosensitive azobenzene containing surfactant which undergoes photo-isomerization reaction from trans- to cis- state with corresponding changes in physical properties such as dipole moment, shape and size [5]. In trans-state the molecule is hydrophobic, while in cis- state hydrophilic. The generation of LDDO flow depends strongly on the interaction of surfactant molecules with a solid surface. Therefore, it is important to understand the adsorption of surfactant molecules as a function of isomerization state, surfactant concentration and properties of surfaces. Here we perform analysis of the surfactant adsorption on a hydrophilic glass and a hydrophobic Teflon surfaces using Zeta potential and quartz crystal microbalance (QCM-D) measurements. We analyses the adsorption isotherms in terms of four and five step models [2-4]. It has been shown that the adsorption of trans- and cis-isomers differs significantly on each type of surfaces. In-situ measurements, i.e. under illumination with different wavelength, of the adsorption isotherms has been performed and analyzed as well.

[1] D. Feldmann, S. S. Maduar, N. Lomadze, O. Vinogradova and S. Santer, Scientific Reports, 6, 36443 (2016).
[2] A. Fan, P. Somasundaran and N. J. Turro, Langmuir, vol. 13, pp. 506-510 (1997).
[3] R. Zhang and P. Somasundaran, Advances in Colloid and Interface Science, vol. 123-126, pp. 213-229 (2006).
[4] S. Alila, S. Boufi, M. Belgacem and D. Beneventi, Langmuir, vol. 21, pp. 8106-8113 (2005).
[5] S. Santer, Journal of Physics D: Applied Physics, 51, pp. 013002 (2017).

Combined fluorescence/phase-contrast imaging reveals novel chemotaxis strategies of bacteria with multi-mode motility

P5

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Active navigation in chemical concentration gradients is key for bacteria to find sources of food or to flee from poisons. The soil bacterium *Pseudomonas putida* self-propels its motion with a polar bundle of rotating, helical flagella. It senses changes in its environment via a chemosensory system and responds to it by adapting the flagellar rotation. Our earlier research demonstrated that the motion pattern of *P. putida* is characterized by persistent runs which are interrupted by sharp reversals [1]. Recently, we showed that the flagella of *P. putida* may operate in three different modes during swimming: the bundle can push, pull, or wrap around the cell body, corresponding to certain swimming modes [2]; changes in the direction of motion are induced by transitions of the flagellar configuration. Based on a novel experimental setup, we are now able to acquire a large number of trajectories together with information on the bundle configuration for each run. We used this data to study the statistics of transitions between the different swimming modes and to elucidate *P. putidas*' swimming strategy when navigating in the direction of a nutrition gradient. Our results reveal that the wrapped mode plays the most prominent role for directional navigation: the run time in the wrapped mode depends on the swimming direction with respect to the gradient orientation. We interpret and discuss these experimental findings in the light of efficiency and robustness of bacterial chemotaxis strategies within a coarse-grained theoretical model.

[1] M. Theves, J. Taktikos, V. Zaburdaev, H. Stark and C. Beta, Biophys. J., 105, 1915 (2013).
[2] M. Hintsche, V. Waljor, R. Großmann, M. J. Kühn, K. M. Thormann, F. Peruani and C. Beta , Sci. Rep., 7, 16771 (2017).

Division of multinucleated *Dictyostelium discoideum* cells | P6

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The precise interplay between shape, size and mechanics during cell division is not yet fully understood. Defects in cell growth and division can lead to multinucleated cells which compared to mononucleated cells has different division processes. We have investigated the division of multinucleated *Dictyostelium discoideum* cells which were generated by electric pulse induced cell fusion. Our investigations have shown that there are two different processes of division. First, attached to a surface the cells divide several times. These cells separate by traction forces until the connection between them disrupts resulting in two daughter cells. These daughter cells vary over a large scale in size indicating that they are not mononuclear. Further depending on the cell size these daughter cells divide adhesion dependent themselves. Second, cells divide by rounding up, detaching from the surface and then divide simultaneously yielding many daughter cells which do not divide again. The size of the daughter cells are all in the same range indicating that they are mononuclear. Analysis of microtubules and centrosomes demonstrate that the simultaneous division process is associated with mitosis.

Partial synchronisation in yeast cell populations P7

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The transition between synchronized and an asynchronous behaviour of intact, immobilized yeast cells of the strain Saccharomyces carlsbergensis is investigated. In populations of intermediate cell densities the individual cells remain oscillatory, whereas on the level of the cell population, both a partially synchronized and an asynchronous state are accessible for experimental studies. In the partially synchronized state, the mean oscillatory frequency is larger than that of the cells in the asynchronous state. This suggests that synchronization occurs due to entrainment from the cells that oscillate more rapidly. This is typical for synchronization due to phase advancement. Furthermore, the synchronisation of the frequency of the glycolytic oscillations precedes the synchronisation of their phases. However, the cells do not synchronize completely, as the distribution of the oscillatory frequencies only narrows but does not collapse to a unique frequency. Furthermore, no spatial clusters were found, where all cells oscillated at exactly the same phases. Chimera states, i.e., the coexistence of a synchronized and an asynchronous part of the population, could not be observed.

How actin wave dynamics governs the evolution of cell shape

P8

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Motile cells like macrophages, stem cells, or cancer cells show complex spatiotemporal pattern formation in the actin cytoskeleton. These patterns can be influenced by external cues like chemoattractants, which lead to directed movement. But they can also occur spontaneously, for example, as self-sustained actin oscillations or waves. Recently it has been shown that one of the main genetic determinants for actin waves in *Dictyostelium discoideum* is a homologue of the RasGAP NF1. While *D. discoideum* wild type cells with an intact NF1 gene do not display any self-sustained cortical wave patterns, a strain with a single knockout of the NF1 gene exhibits fully developed traveling waves. Here, we study actin wave dynamics in giant cells produced by electric pulse induced fusion of NF1 knockout cells. In contrast to actin waves in common lab strains, waves in these cells appear more stable. They travel in a highly persistent fashion and induce distinct deformations of the cell membrane. We use this setting to study in detail how wave formation impacts shape dynamics and motility. For example, waves may induce transitions between different distinct cell shapes, or they can form broad actin fronts that push the cell boundary in a way that is reminiscent of a lamellipodium. We compare our experimental observations to numerical solutions of a model that combines a noisy excitable reaction-diffusion system with a dynamic phase field for the cell shape and identify key factors that are required for wave-driven cell motility.

Inferring the dynamics underlying protrusion-driven cell motility

P9

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Amoeboid cell motility is essential for a wide range of biological processes including wound healing, embryonic morphogenesis, and cancer metastasis. It is based on localized deformations of the cell membrane called pseudopodia. Pseudopodia are formed by coordinated actions of the actin cytoskeleton, a complex biopolymer network at the inner side of the plasma membrane. Its dynamics is controlled by a signalling network that integrates intra- cellular information as well as external receptor cues. Current models of eukaryotic motility typically fall into one of the following two categories: models based on an effective intracellular mechanism that drives cell locomotion (mechanistic models); or models that phenomenologically reproduce the statistics of cell protrusion or position dynamics based on experimental data (empirical models). The long-term aim of our project is to develop a model of protrusion-driven cell motility based on a space-time stochastic process that over- comes this division. We started with the detection of cell membrane protrusions by analyzing images of the model organism *Dictyostelium discoideum*. Therefore, we developed mathematical tools to track the flow of the cell outline over time. With these tools at hand we are now developing an automated protrusion detection to assimilate data from experimental recordings, while we simultaneously start developing the mathematical model for protrusion formation based on a point process. Our project is part of the CRC 1294 Data Assimilation (sfb1294.math.uni-potsdam.de).

"Rewarding" cargo-carrier interactions: a story on cell-mediated particle transport

P10

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As society paves its way towards devices miniaturization and precision medicine, micro-scale actuation and guided transport become increasingly prominent research fields, with high potential impact in both technological and clinical contexts. To date, a promising strategy is to exploit living cells as smart, steerable and biochemically powered carriers, developing the so-called bio-hybrid systems. Still, in applications like targeted drug delivery, a guided transport through complex environments as living tissues remains challenging.

Inspired by leukocytes, efficiently moving through our body to reach target sites, we propose to exploit the amoeboid motion of eukaryotic crawling cells for transport of drug-loaded microparticles.

Our experiments point out the ability of amoeboid cells to displace cargos in a directed fashion, by means of chemotaxis, both across 2D substrates and through 3D matrices. Remarkably, the random walk of cell-cargo systems shows faster spreading than the one of lone cells, suggesting cell-particle interaction as stimulus promoting cell motility. Further, by comparing experiments with different particle sizes, a non-monotonic behavior emerges for the cargo diffusivity-size relation.

To get insights into the cell-cargo dynamics, the maximum pulling force a cell can exert on a cargo is being quantified with the aid of microfluidic devices. Using a microfluidic channel of known geometry and hydrodynamics, cells experience a negligible shear stress under laminar flow conditions. Therefore, the drag force acting on the particle, before its rapture from the cell body, can be determined from the particle size and flow profile.

By analysing cell-particle relative dynamics, we find reproducible features of the underlying interaction, such as recurrent bistable dynamics and effective interaction potential shapes. On the basis of such evidences, we developed a physical model of our bio-hybrid system, which we then embed into stochastic simulations to generate in-silico trajectories.

Our model successfully compares to experimental data, reproducing realistic values of diffusivity that scale non-monotonically with cargo size. Remarkably, a good quantitative agreement between experiments and simulations was achieved by adopting empirical values for all the simulation parameters, with no fitting procedure.

Although simplistic, our model seems to grasp the main motility aspects of such peculiar system, while giving new understandings on eukaryotic cell motion in general.

Controllable switching between stable modes in network of four pulse-coupled chemical oscillators

P11

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Computationally and experimentally, we analyze switching between stable oscillatory modes in a network of four Belousov–Zhabotinsky oscillators coupled on a ring via unidirectional inhibitory pulses with a time delay [1]. There are five stable modes in this network: in phase, anti-phase, walk, walk reverse, and three-cluster modes. Switching between the modes can be carried out by external pulses applied to one or several oscillators and can be classified into three types: (i) 'forced' switching, where the phases of oscillators of an initial mode are reset in such a way that they correspond to the phases of the desired mode; internal pulses of the network play no role in this resetting; (ii) 'specific'' switching, when the phase of only one oscillator is changed by an external perturbation which induces a chain of phase changes in other oscillators due to internal coupling between oscillators; and (iii) multistep switching through the intermediate modes, which can be either stable or unstable attractors. All of these types of switching have been found in simulations and verified in laboratory experiments with macro- reactors. Also, we implement the "all-to-all" type of coupling by means of pulses of light using micro-reactors.

[1] Pavel S. Smelov, Ivan S. Proskurkin and Vladimir K. Vanag, Phys. Chem. Chem. Phys. (2019), v.21, pp.3033 – 3043.

Useful phone numbers

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