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PART I

WHO WE ARE
WHO WE ARE

Dynamics and self-organization are omnipresent in nature; in living systems self-organization plays a vital role, which is however still enigmatic. Generally, one finds similar physical principles at work on multiple scales from the very large - as in the formation of galaxies, to the intermediate - as in the formation of clouds, turbulence, and swarming phenomena, to the small - as in the cooperative activity of neurons and heart cells, and to the very small - as in the nanoscale machinery inside living cells. All dynamical self-organization occurs in nonlinear complex systems that are far from equilibrium. These systems often are highly nonlinear, are composed of large numbers of interacting units, have multiple levels of organization, and are spatially extended or form interconnected networks. Current understanding of these systems is quite limited. It is the objective of the Max Planck Institute for Dynamics and Self-Organization to uncover the fundamental principles and functions of complex matter in nature.

Our Institute was founded in 2003 as a research institution dedicated to the physics of dynamics and self-organization. It is the successor of the Max Planck Institute for Flow Research. Now ten years young, with three departments, an independent research group and six centrally funded Max Planck Research Groups it has established itself at the forefront of this rapidly advancing research field. On the national and international level it has taken leadership roles in the federally funded German Heart Centers and Bernstein Centers initiatives, it is a node in the Max Planck Synthetic Biology Initiative, it leads the Göttingen Exploration of Microscale Oil Reservoir Physics (GeoMorph), which is part of the Exploratory Research Initiative of BP International Inc., and it is coordinating the European High-Performance Infrastructures in Turbulence Research (EuHIT) funded by the European Community. It houses the Göttingen Focus on Complex Fluid Dynamics, which is scheduled to move into a new building at the end of 2014.

The institute is an integral part of the Göttingen Research Campus and is tightly collaborating with departments of the neighboring Max Planck Institutes for Experimental Medicine and Biophysical Chemistry, the German Primate Center, the Georg August University and its Medical Center. It is participating in five Collaborative Research Centers (SFBs) funded by the German Science Foundation. Together with the neighboring Max Planck Institute for Biophysical Chemistry and the GWDG, a competence center for IT services, it forms the Max Planck Campus Göttingen with more than 1200 employees; it is one of the largest research establishments focusing on fundamental science in Lower Saxony.
Fred Wolf, Eleni Katifori, Jean-Christophe Baret, Marc Timme (front row, from left to right), Eberhard Bodenschatz, Tobias Schneider, Stephan Herminghaus, Stefan Luther, Theo Geisel (standing, from left to right).
Göttingen, October 2013
DEPARTMENTS

The core of the Max Planck Institute for Dynamics and Self-Organization (MPIDS) consists of three departments: Nonlinear Dynamics; Dynamics of Complex Fluids; Fluid Dynamics, Pattern Formation, and Biocomplexity. While the Department of Nonlinear Dynamics was established in 1996, the Department of Dynamics of Complex Fluids and the Department of Fluid Dynamics, Pattern Formation, and Biocomplexity are both seven years younger. The MPIDS is led by the three directors Eberhard Bodenschatz, Theo Geisel and Stephan Herminghaus, each a Scientific Member of the Max Planck Society and heading one of the three departments.

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Nature confronts us with numerous dynamical phenomena, many of which are easy to dissect for a human observer, while others have challenged theoreticians for decades. Simple mathematical models that give rise to chaotic behaviour have long been studied as paradigms for complex systems and have provided us with new tools, but mostly have had little direct application to physical reality. Twenty five years ago my group underwent a paradigm shift of a second kind, i.e., shifting away from paradigms to real applications. We then began to focus on chaos and quantum chaos in mesoscopic systems such as semiconductor nanostructures and the dynamics of biological neural networks. Today looking at our contributions in this volume, it is amazing to see how far this approach can reach, e.g., in uncovering brain function.

In neuroscience, in particular, many important problems and questions are related to dynamics and self-organization. How do the neurons in our brain cooperate when we perceive an object or perform a task? What is the role of different dynamical states, e.g., critical avalanches, for brain function? How do cortical networks quickly switch between different states, e.g. for context-dependent information routing? While computer simulations of even very large neuronal networks are becoming fashionable, they are of only limited use for answering such questions in depth.

On the other hand rigorous mathematical analyses of the dynamics of neural networks cannot rely on mainstream recipes but pose formidable mathematical challenges. Neural systems exhibit several features that elude standard mathematical treatment: the units of the network communicate or interact only at discrete times and not continuously as in many-body theory in physics; there are significant interaction delays that make the systems formally infinite-dimensional; and complex connectivities give rise to novel multioperator problems - enough "raisons d’être" for a group of theoreticians. Meeting such challenges has often been facilitated by cross-fertilization within the wide scope of problems addressed in our department, from diverse stochastic processes in complex environments to wave phenomena in random and complex media such as the random focussing of rogue waves and tsunamis or the localization of Bose-Einstein condensates in optical lattices. Our recent research achievements demonstrate that abstraction and mathematical rigor do not impede but in fact deepen our understanding of complex systems.

The Department of Nonlinear Dynamics was created by the Max Planck Society in 1996 to start a scientific reorientation of the former MPI for Flow Research towards modern nonlinear dynamics. The department has initiated and hosts the federally (BMBF) funded Bernstein Center for Computational Neuroscience Göttingen, in which it cooperates with experimental neuroscience labs. Our group is closely linked to the Faculty of Physics, where Theo Geisel teaches as a full professor. It is financed to a large extent by the Max Planck Society and to a smaller extent by the University of Göttingen through its Institute for Nonlinear Dynamics and plays a bridging role between the Faculty of Physics and the MPIDS.
Dr. Demian Battaglia studied physics at the University of Turin and received his PhD in 2005 at the International School for Advanced Studies (SISSA, Trieste), doing research at the interface between statistical mechanics and theoretical computer science. From 2006 to 2008 he was postdoctoral researcher at the Laboratory of Neurophysics and Physiology (University Paris Descartes). In 2009 he joined the group of Theo Geisel as a Postdoc at the MPI for Dynamics and Self-organization. Since May 2010, he has been principal investigator of the Bernstein Center for Computational Neuroscience Göttingen and has been appointed as Bernstein Fellow in 2013.

Dr. Stephan Eule studied physics at the Westfälische-Wilhelms University in Muenster where he received his PhD in 2008. In 2009 he joined the Department of Nonlinear Dynamics at the Max Planck Institute for Dynamics and Self-Organization. He works on problems related to stochastic population dynamics and fluctuating physical and biological systems with a focus on the description of anomalous diffusion processes.

Dr. Ragnar Fleischmann studied physics at the Johann-Wolfgang-Goethe University in Frankfurt am Main and received his PhD in 1997. The thesis was awarded the Otto-Hahn-Medal of the Max-Planck-Society. From 1997 to 1999 he was postdoctoral researcher in the group of Theo Geisel at the Max-Planck-Institut für Strömungsforschung and from 1999 to 2000 in the group of Eric Heller at Harvard University. Since 2000 he has worked as a scientific staff member in the Department for Nonlinear Dynamics. His research focuses on the theory of mesoscopic systems and wave propagation in complex and random media.

Dr. Denny Fliegner studied physics at the University of Heidelberg and received his doctoral degree in theoretical particle physics in 1997. From 1997 to 2000 he was postdoctoral researcher at Karlsruhe University working on parallel computer algebra and symbolic manipulation in high energy physics. He joined the group of Theo Geisel at the Max Planck Institute for Dynamics and Self-Organization as an IT coordinator in 2000. Since 2007 he has been the leading IT manager for high performance computing at the MPIDS.

Dr. Anna Levina studied mathematics at the St. Petersburg State University (Russia) and received her doctorate in mathematics from the University of Göttingen in 2008. Her thesis was carried out in the group of Theo Geisel at the Max Planck Institute for Dynamics and Self-Organization and was awarded the Otto-Hahn-Medal of the Max Planck Society. In 2011 she started working part-time again on self-organized criticality in neuronal networks as a postdoctoral fellow at the MPIDS and the Bernstein Center for Computational Neuroscience Göttingen.
Dr. Jakob Metzger studied physics at Imperial College in London and the University of Freiburg. He received his doctorate from the University of Göttingen in 2010, working in the group of Theo Geisel at the Max Planck Institute for Dynamics and Self-Organization. He was awarded the Otto-Hahn-Medal for his work on particle and wave flows in random media. He also applies methods from nonlinear dynamics and stochastic processes to the study of population genetics.

Dr. Jan Nagler studied physics at the Christian-Albrechts-University Kiel and received his doctorate in theoretical physics from Bremen University in 2003. He worked as a postdoctoral researcher at Bremen University and Boston University (USA). He joined the Department of Nonlinear Dynamics of the MPIDS as a senior postdoctoral researcher in the SPICE group in 2008. His research comprises nonlinear dynamics, statistical physics and stochastic processes with applications in biology, ecology, epidemiology and social sciences.

Dr. Viola Priesemann studied physics at the Technical University Darmstadt and the Universidade Nova de Lisboa (Portugal). She started her PhD as a joint project between the Ecole Normale Supérieure (France) and Caltech (USA), and subsequently moved with her supervisor to the Max Planck Institute for Brain Research in Frankfurt. She worked experimentally on the turtle visual system and theoretically on subsampling effects in self-organized critical systems. In September 2013 she started working as a postdoctoral fellow on self-organized criticality and subsampling at the Max Planck Institute for Dynamics and Self-Organization and the Bernstein Center for Computational Neuroscience Göttingen.

Dr. Olav Stetter studied physics at the Ludwig Maximilian University of Munich and wrote his diploma thesis at the Max Planck Institute for Biochemistry in Martinsried on extracellular stimulation of neurons. In 2009 he joined the Max Planck Institute for Dynamics and Self-Organization to work on his PhD on the relationship between structure and dynamics in neuronal networks in vitro. Since December 2012 he has been a postdoctoral researcher at the Bernstein Center for Computational Neuroscience Göttingen.

Dr. Annette Witt studied mathematics at the Humboldt-University Berlin and received her doctorate in theoretical physics from the University of Potsdam in 1996. Her thesis was awarded the Otto-Hahn-Medal of the Max Planck Society. Annette worked as postdoctoral researcher at several physical and geoscientific institutes in Potsdam, Florence (Italy) and London (U.K.). In 2007, she joined the Department of Nonlinear Dynamics at the MPIDS where she develops tools for characterizing recordings of complex systems and applies them to neuro-scientific problems. Since 2010 she has been a principal investigator of the Bernstein Center for Computational Neuroscience Göttingen.
Yorck-Fabian Beensen studied physics at the Georg-August-University Göttingen and the University of Aarhus (Denmark). In 1997 he received his diploma from the faculty of geophysics for a work in the field of seismological data analysis which earned him the Berliner-Ungewitter-Prize. He joined the department of Nonlinear Dynamics in 2000 as an IT administrator. In 2001 he was elected as a member of the institute’s staff council and has been the head of the council for the last three terms.

Barbara Guichemer has been working as an IT assistant of the Department of Nonlinear Dynamics and the HPC group since February 2007. She assists the administration of the HPC cluster and HPC infrastructure, the procurement of hard- and software as well as in the organization of tender procedures. Within the central IT service she is responsible for the management, procurement, distribution and support of scientific software licenses throughout the institute.

Viktoryia Novak has been working as a foreign language assistant of the department since March 2011. Beyond office management tasks she is responsible for the organization of conferences and visits of international guests as well as for supporting Prof. Fred Wolf in administrative issues and the management of external funds. Ayse Bolik is a European Business Assistant certified in English and French and has been administrative assistant to Prof. Theo Geisel and the Bernstein Center for Computational Neuroscience since 2010. Regina Wunderlich is a General Business Administrator and has been administrative assistant to Prof. Theo Geisel at the Institute of Nonlinear Dynamics of the Georg-August-University Göttingen since June 2001 and previously at the Bernstein Center for Computational Neuroscience since 2005.
1.2 DEPARTMENT OF DYNAMICS OF COMPLEX FLUIDS

Our research focuses on mechanisms of self-organization and self-assembly. A wide scope of methods is employed for their investigation, including analytical statistical theory, advanced simulation tools and cutting edge experimental techniques. The most challenging question is: are there general common ‘principles’ behind the various instances of structure formation and emergence in open systems?

On the fundamental side, wet granular materials have proved to be versatile model systems for studying collective behavior in systems violating detailed balance on the microscopic level. Their particular charm is in being placed right at the border of complex interfaces, soft matter and systems far from thermal equilibrium. Thereby granular systems connect fields of expertise of different subgroups of the department. On the complex side, biological matter and bio-systems are the most intricate systems we are studying, but we try to concentrate on those which are still simple enough to be described by physical and physicochemical principles.

Our strength in investigating the dynamics of soft matter interfaces has won us a grant from BP Exploration Operation Company Ltd. since 2009. It has enabled us to significantly augment our research on liquid interfaces in complex environment to make it applicable for basic research related to the pore scale physics in oil reservoirs. The grant provides a total of eleven full time equivalents plus consumables for five years, and we are currently preparing the extension of the project for another five years (2014-2019).

Other projects are spanning the range from complex soft interfaces to the generation of artificial micro- and nano-devices, which play important roles as building blocks of soft functional systems. These projects involve the development of unconventional concepts in microfluidic systems. They are strongly fertilized by the insight we gain in non-equilibrium systems and pushed by the need for soft manipulation techniques for our bio-related projects.

During the last three years there have been substantial fluctuations in our personnel. Thomas Pfohl left our group for a professorship at the University of Basel (Switzerland) and Manfred Faubel has retired. Marco Mazza and Oliver Bäumchen have joined our department as new group leaders in 2012 and 2013, additionally Lucas Goehring (joined in 2011) has extended his group. With the new group leaders we have widened our scope towards the theoretical modeling of liquid crystals, the investigation of interface dynamics and the pattern formation in geo-systems, respectively.
Dr. Oliver Bäumchen studied physics and mathematics at Saarland University (Saarbrücken, Germany) between 2000 and 2006 where he received his Diploma in Physics in 2006. He concluded his studies with a thesis in experimental physics on the wetting properties of nanostructured materials. In 2010 he received his PhD from Saarland University for his work on the fluidics of thin polymer films in the group of Prof. Karin Jacobs. He taught experimental physics as a lecturer at the University of Applied Sciences (Saarbrücken, Germany) from 2007 to 2008. In 2011 he was awarded a DFG research fellowship and joined the group of Prof. Kari Dalnoki-Veress at McMaster University (Hamilton, Canada). During his postdoctoral stay he explored the structure and dynamics of soft matter at interfaces. Aside from instabilities of complex liquids, he became interested also in biological systems. Since August 2013 he has been a group leader at the Max Planck Institute for Dynamics and Self-Organization.

Dr. Christian Bahr studied chemistry at the Technical University Berlin and received his PhD in 1988. Research stays and postdoctoral work took place at the Raman Research Institute (Bangalore, India) and the Laboratoire de Physique des Solides of the Université Paris-Sud (Orsay, France). After his habilitation for physical chemistry at the Technical University Berlin in 1992, he moved to the Physical Chemistry Institute of the University Marburg as a holder of a Heisenberg-Fellowship in 1996. From 2001 to 2004 he worked as a software developer in industrial projects. In 2004 he joined the group of Stephan Herminghaus at the MPI for Dynamics and Self-Organization. Research topics comprise experimental studies of soft matter (mainly thermotropic liquid crystals): Structures and dynamics in thin smectic films, surfactant-laden liquid crystal interfaces, active liquid crystal/surfactant/aqueous systems, and microfluidics of nematic liquid crystals.

Dr. Lucas Goehring studied physics at the University of British Columbia (B.Sc. 2002) and the University of Toronto (M.Sc. 2003, Ph.D. 2008). He received his doctorate in the group of Prof. S. Morris for his studies on the scaling and ordering of columnar joints in starch and lava. He has since continued to study geophysical pattern formation, for example in fossil biofilms or permafrost soils, through experimentally accessible analogues. Between 2008 and 2011 he was elected a research fellow of Wolfson College at the University of Cambridge, where he investigated the cracking behavior of colloidal materials with Prof. W. Clegg and Dr. A. Routh. He joined the MPI for Dynamics and Self-Organization in 2011 and is currently studying pattern formation in geophysical systems, the solidification of colloidal systems, and the ordering of crack networks.

Dr. Kristian Hantke studied physics at the University of Manchester Institute of Science and Technology (Bachelor of Science 2000) and at the Philipps-University Marburg (Diploma 2002). In 2005 he received his PhD from the University of Marburg working on the optical properties of dilute III-V nitrides in the experimental semiconductor-physics group of Prof. W. Rühle. After studying the optical injection of spin currents during a post-doctoral stay at the University of Marburg he joined the group of Prof. S. Herminghaus at the Max Planck Institute for Dynamics and Self-Organization as a scientific staff member in 2007. Being the lab coordinator for the laser and microscopy setups, his work centers around the application of new experimental techniques based on nonlinear vibrational imaging and multi-photon laser scanning microscopy.
Dr. Marco G. Mazza received his Master’s degree in physics in 2001 from the University of Catania (Italy) with the thesis “Proper time formulation of Wilson renormalization group” under supervision of Paolo Castorina, followed by a research grant. In 2005 he joined the Boston University as a teaching and research assistant. In 2009 he received his PhD with the thesis “Thermodynamics and dynamics of supercooled water” under supervision of H. Eugene Stanley. Between 2009 and 2012 he worked as a postdoc and lecturer at TU Berlin in the group of Martin Schoen. Since 2012 he has been working as a group leader at the MPI for Dynamics and Self-Organization in the Department of Dynamics of Complex Fluids.

Dr. Matthias Schröter studied philosophy and physics at the Universities of Frankfurt and Kassel. He obtained his PhD in 2003 from the University of Magdeburg while working in the group of Ingo Rehberg on pattern formation in electrodeposition. During his postdoctoral stay with Harry Swinney at the Center for Nonlinear Dynamics at the University of Austin he studied the statistics and dynamics of granular media. Since May 2008 he has been a senior research fellow in the Department of Dynamics of Complex Fluids. Main research topics are the statistical mechanics of static granular media and x-ray tomography of complex materials.

apl. Prof. Dr. Jürgen Vollmer studied physics in Bielefeld and Utrecht. In 1994 he received his doctorate in Prof. Harry Thomas’ group at the University Basel (Switzerland), where he worked on dynamical systems theory and became interested in the theory of phase transitions. After pursuing postdoctoral studies in Essen, Brussels and Mainz, he joined the working group Complex Systems at the Philipps University Marburg, and since April 2007 he has been a group leader in the Department of Dynamics of Complex Fluids. He holds an appointment as an Associate ("außerplanmäßiger") Professor at the Faculty of Physics of the Georg-August-Universität Göttingen, and he is a faculty member of the Göttingen Graduate School for Neurosciences, Biophysics, and Molecular Biosciences. He has organized the Dynamics Days in 2002 and 2009 and was the secretary of the Dynamics Days Advisory Committee from 2008 to 2011. In 2013 he became an Associate Editor of Frontiers in Interdisciplinary Physics.

Associated Scientists

Dr. Martin Brinkmann studied physics and mathematics at the Free University of Berlin between 1990 and 1998 where he received his Diploma in Physics. After an internship at the Dornier Labs (Immenstaad, Lake Constance) in 1999 he joined the theory group of Prof. Reinhard Lipowsky at the MPI of Colloids and Interfaces (Potsdam, Germany) to work on wetting of chemically patterned substrates. In 2003 he received his doctorate from the University of Potsdam. During a postdoctoral stay in the Biological Nanosystems Group at the Interdisciplinary Research Institute in Lille (France) he explored wetting of topographic substrates as a possible way to manipulate small liquid droplets. Since the beginning of 2005 he has been investigating wetting of regular and random geometries in the Department of Dynamics of Complex Fluids at the MPIDS. Since 2012 he holds a senior scientist position at Saarland University in the Group of Prof. Seemann. He is still associated with the DCF department by the GeoMorph project funded by BP, the DFG SPP 1486 “Partikel im Kontakt (PiKo)” and the SFB 937.
apl. Prof. Dr. Folkert Müller-Hoissen received his doctorate in theoretical physics from the University of Göttingen in 1983. After postdoc positions at the MPI for Physics in Munich and the Yale University in New Haven (USA) he returned to the University of Göttingen as an assistant professor (Hochschulassistent), obtained his habilitation in 1993 and became a Privatdozent. Since 1996 he is carrying on his research in mathematical physics at the MPI for Flow Research, which meanwhile evolved into the MPIDS. Since 2000 he is adjunct professor at the University of Göttingen. His present research focus is the theory of integrable partial differential and difference equations, applications in theoretical physics and related mathematical structures.

Prof. Dr. Ralf Seemann studied physics at the University of Konstanz where he received his Diploma in 1997. The diploma work was carried out at the MPI of Colloids and Interfaces in Berlin-Adlershof. He received his doctorate in 2001 from the University of Ulm where he experimentally studied wetting and rheological properties of complex fluids. In 2003 he received the Science Award of Ulm. During his stay as postdoctoral researcher at the University of California in Santa Barbara, he explored techniques to structure polymeric materials on the micro- and nano-scale. Since 2003 he was a group leader at the MPIDS, Göttingen. Ralf Seemann was appointed as professor at the Saarland University in 2007. Among other topics he is concerned with wetting of topographic substrates, wet granular media, and discrete microfluidics. He is still associated with the DCF department in the framework of the GeoMorph project funded by BP.

Barbara Kutz, Dr. Guido Schriever and Monika Teuteberg, support the head of the department. Monika Teuteberg and Barbara Kutz run the offices as secretaries and take care of administration issues at Faßberg and at Bunsenstraße, respectively. Guido Schriever’s tasks as the scientific assistant imply among other things scientific reporting and organization of visits and events.

Sibylle Nägle and Thomas Eggers take care of the information technology. Sibylle Nägle focuses on the webpage of the department as well as image creation and processing, while Thomas Eggers supports the desktop computers of the scientists, the computer clusters, the DCF network and the email accounts.

Christian Jacob, Wolf Keiderling and Markus Benderoth belong to the service group of the department. Wolf Keiderling operates the mechanical work shop, Markus Benderoth is responsible for our chemical and biological laboratories and Christian Jacob works in the electronics work shop.
1.3 DEPARTMENT OF FLUID DYNAMICS, PATTERN FORMATION, AND BIOCOMPLEXITY

Dynamics and self-organization occurs in many-body systems that are out of energetic equilibrium. If we want to understand the world around us, we must rely on simplifying descriptions that capture the fundamental physical principles. Thus we need to identify "complex systems" that include all necessary parameters, boundary conditions and initial conditions. These together with a rigorous mathematical description, must allow for a quantitative understanding. The analyses of complex systems pose a major challenge both to physics and mathematics, since the equations are usually coupled, nonlinear and nonlocal. Nevertheless, though very different in detail, the fundamentals of complex systems can be described by unifying concepts. Our aim is the search for and the understanding of those concepts in the physics of fluid- and biomechanics. In our approach we rely on methods from non-equilibrium statistical mechanics and pattern formation. Currently we are investigating spatiotemporal chaos and turbulence in thermal convection; fundamentals of turbulence; inertial and tracer particle transport in fully developed turbulence with implications for fundamental theories, but also for practical issues like turbulent mixing, particle aggregation and cloud micro-physics; the spatio-temporal dynamics of the electric signals in the heart; and the intra-cellular and self-organizing processes leading to eukaryotic cell motility, chemotaxis and tissue development.

The laboratory provides a microscopy facility, a cell biology laboratory, and shares with the other groups a class 1000 clean room for micro-fabrication. It established the Göttingen Turbulence Facility, which consists of a set of experimental systems and a compressed gas facility to achieve ultra-high turbulence levels. The latter is part of the European Infrastructure Network EuHIT, which is coordinated by the department. For investigations of cloud micro-physics we have an outpost at the Environmental Research Station Schneefernerhaus on the Zugspitze, Germany's highest mountain, where we are also part of the Virtual Alpine Observatory. In 2012, with Stefan Herminghaus we have created the Focus on Complex Fluid Dynamics to be opened soon in direct vicinity of the MPIDS.

Our research has been and will continue to be truly interdisciplinary from engineering, material science, physics, geophysics, and applied mathematics, to chemistry, biology, and medicine. We connect seamlessly to the other departments and research groups and are a member of the International Collaboration for Turbulence Research and the German Centre for Cardiovascular Research. We collaborate with groups at the MPI for Biophysical Chemistry, the Physics Department, and the Medical Center at the University of Göttingen. In addition, we are embedded in a network of national and international collaborations.
**Prof. Dr. Guenter Ahlers** received his Ph.D. from UC Berkeley in 1963 and carried out research on critical phenomena and chaos at AT&T Bell Laboratories from 1963 to 1979. Then he joined UC Santa Barbara as Professor of Physics and studied pattern formation and turbulence in nonlinear fluid-mechanical systems. Since 2007 he is involved in studies of turbulence in a very large convection system at the MPIDS. He is a fellow of the APS, AAAS and the American Academy of Arts and Sciences. He is a member of the US National Academy of Sciences. He received the Fritz London Award of IUPAP and the APS Fluid Dynamics Prize.

**Prof. Dr. Carsten Beta** studied chemistry in Tübingen, Karlsruhe and Paris. In 2001, he joined the Department of Gerhard Ertl at the Fritz Haber Institute (MPG) and received his PhD from the Free University Berlin in 2004. After working as a postdoctoral fellow at Cornell and UCSD, he became a group leader at the MPIDS in Göttingen in 2005. In 2007, he was appointed Professor of Biological Physics at the University of Potsdam, where he is acting as head of the Institute of Physics and Astronomy since 2012. His research concentrates on biophysics, in particular, on cell motility and chemotaxis as well as pattern formation in reaction-diffusion systems.

**Dr. Gregory Bewley** received his bachelor’s degree from the mechanical engineering department at Cornell University in 2000. He was awarded a PhD from Yale University in 2006 for discovering how to observe quantized vortex dynamics experimentally. He continued this work at the University of Maryland before joining the MPIDS in 2007. His work now focuses on turbulence, both its intrinsic properties and its role in various environmental settings.

**Dr. Azam Gholami** studied physics at the Sharif University in Tehran and graduated in 2001 from the Institute for advanced studies in Basic Sciences (IASBS), in Zanjan (Iran). In 2003, she joined the group of Prof. E. Frey to start her PhD studying semiflexible polymers and cell motility. She received her PhD in 2007 from the Ludwig-Maximilian-University of München. In January 2008, she joined the MPIDS as a postdoctoral researcher in the group of Prof. Bodenschatz to work on *in-vitro* actin-based motility as well as pattern formation in *Dictyostelium discoideum* in the presence of an external flow.

**Dr. Dennis P. M. van Gils** received his PhD in Applied Physics from the University of Twente (The Netherlands) in 2011. There he helped construct a Taylor-Couette setup able to probe the ultimate turbulent regime, with which he later published experimental work on torque scaling and drag reduction. In 2012 he joined the MPIDS as postdoctoral researcher where he experimentally studies turbulent heat convection at the High Pressure Convection Facility. His research topics involve convection in/near the ultimate state and the influence of global rotation on this system.
Dr. Isabella Guido studied electrical engineering at the University of Bologna (Italy). In 2006 she joined the Lab-on-Chip Technology group at Fraunhofer (IBMT). In 2010 she received her PhD in engineering from the TU Berlin. She moved to China as a postdoc at the Cell Mechanics Lab of the Peking University and in 2012 to the UK as visiting scientist in the Dept. of Biomedical Engineering of the University of Glasgow. Her studies focused on the development of microsystems for cell manipulation and the characterization of cellular mechanical properties. In June 2013 she joined the MPIDS as a postdoctoral researcher working on chemo- and electrotaxis.

Dr. Xiaozhou He received his PhD in physics from the Hong Kong University of Science and Technology (HKUST) in 2009. His PhD research was on the experimental study of the thermal dissipation rate and temperature statistics in turbulent thermal convection. From January to October in 2010, he was a postdoctoral fellow at the HKUST. In November 2010, he joined the group of Prof. Bodenschatz at the MPIDS as a postdoctoral fellow. In 2011, he won the Young Scientist Prize at the 13th European Turbulence Conference. His current research projects focus on the turbulent Rayleigh-Benard convection at very high Rayleigh numbers.

Dr. Dimitry Ivanov received his M.D. (1999) in physics from the Belorussian State University. In 2001, he started his graduate work in physical chemistry at the MLU Halle-Wittenberg, where he investigated diffusion processes for multicomponent mixtures. In 2006-2007 he was a postdoc at the TU Eindhoven. In 2008 he continued to study fluid mixtures by dynamic light scattering at the University of Maryland. From 2010 to 2011 he was a postdoc at the Reykjavik University and developed experimental techniques. In 2011 he joined the MPIDS as a postdoc. His research interest is the experimental study of the interaction between turbulence and inertial particles.

Dr. habil. Alexei Krekhov received his PhD in theoretical physics from the Perm State University (Russia) in 1990 studying defects in liquid crystals. During his Humboldt Research Fellowship at the University of Bayreuth from 1994 to 1996 his studies focused on pattern forming instabilities in liquid crystals. In 1999 he joined the University of Bayreuth as a researcher. His research topics involve nonlinear dynamics, pattern formation in complex fluids and soft matter theory. In 2010 he received the habilitation in theoretical physics from the University of Bayreuth. Since October 2013 he is a researcher at the MPIDS and works on convection in binary mixtures.

Prof. Dr. Valentin Krinski studied physics at the Institute of Physics and Technology (Moscow, Russia), where he received his PhD in 1964. After 12 years at the Institute of Biological Physics in Puschino, he was appointed Head of the Autowave Laboratory in 1976 and Prof. of Biological Physics at the Institute of Physics and Technology in 1980. He was Directeur de Recherche, CNRS, INLN, (Nice, France) as of 1993. His research interests include vortices in biological excitable tissues and novel approaches for the termination of life-threatening chaos in the heart. In 2007 he joined the MPIDS to work with Prof. Luther and Prof. Bodenschatz on cardiac dynamics.
Dr. Jan Moláček studied mathematics at the University of Cambridge (UK), where he received his BA and MA degrees. He received his PhD in applied mathematics from the Massachusetts Institute of Technology (Cambridge, USA) in 2013 for his experimental and theoretical investigation of droplets bouncing and walking on a vibrating liquid bath. He joined the MPIDS in September 2013 as a postdoctoral researcher working on the in-situ investigation of drop-turbulence interaction in warm clouds.

Dr. habil. Holger Nobach received his doctorate in electrical engineering from the University of Rostock in 1997. During his postdoctoral research at Dantec Dynamics in Copenhagen (Denmark) and at the Technical University of Darmstadt, he developed measurement techniques for flow investigations. Since 2005 he has been a senior scientist at the MPIDS with a research visit at Cornell University (NY, USA). In 2007, he received the habilitation in mechanical engineering from the Technical University of Darmstadt. He works on the experimental investigation of turbulent flows and thermal convection and is editor for ISRN Signal Processing.

Dr. Ganapati Sahoo studied physics at Utkal University (Bhubaneswar, India) where he received his BSc and MSc degrees. He received his doctorate in theoretical physics from the Indian Institute of Science (Bangalore, India) in 2010. During his PhD he carried out various direct numerical simulations of magnetohydrodynamic (MHD) turbulence. He then joined IIT University (India) as an assistant professor. Since March 2011, he has been a member of Prof. Bodenschatz’s group at the MPIDS and works on tracking particles in a turbulent jet flow. His research interests also include direct numerical simulations of fluid flows and MHD turbulence.

Dr. Marco Tarantola received his diploma in biology at the University of Würzburg in 2005 and his PhD at physical chemistry, University of Mainz, in 2010, studying dynamics of epithelial monolayers by acoustic and impedimetric biosensors. In 2010, he became coordinator of the CRC proposal SFB 937. He then joined the MPIDS as a postdoctoral scientist until 2012, before leaving for a second postdoctoral stay at the UC San Diego until 2013. Since 2013, he is a senior scientist at the MPIDS and, besides continuing his work on Dictyostelium, he also studies beating patterns of fibrotic cardiac cocultures.

Dr. Huixuan Wu studied at the Johns Hopkins University (Baltimore, USA) starting 2005. He received his PhD in 2011 from the Mechanical Engineering Department for his work on measurements of the complex vortical flow within the rotor tip region of turbomachinery. In November 2011, he joined the MPIDS as a postdoctoral fellow. He received an Alexander von Humboldt Scholarship in early 2013. His current project is simultaneous velocity and vorticity measurement in complex flow fields. Dr. Wu is also interested in thermodynamics and heat transfer, applied optics, and turbomachinery flows.
Dr. Haitao Xu received his PhD from Cornell University in 2003. From 2003 to 2006, he was a post-doctoral researcher at the Laboratory of Atomic and Solid State Physics, Cornell University, where he, together with other colleagues, developed the Lagrangian particle tracking technique for high Reynolds number turbulence measurements. In August 2006, he joined the MPIDS, where he is now a senior scientist. His main research interest is the Lagrangian properties of fluid turbulence and the interactions between turbulence and additives, such as particles or flexible long-chain polymers.

Dr. Vladimir S. Zykov studied physics at the Institute of Physics and Technology (Moscow, Russia). He graduated in 1973, received his PhD in 1979, was habilitated in 1990 and occupied the position of leading scientific researcher at the Institute of Control Sciences (Moscow, Russia). In 1992 he joined the group of Prof. Mueller first at the MPI of Molecular Physiology and since 1996 at the Magdeburg University. From 2001 he was a research scientist at the TU Berlin and joined the MPIDS in 2010. His research interests include pattern formation processes in nonlinear reaction-diffusion media and control methods of self-organization.

Sabrina Volkmar is responsible for travel expenses and supports the EuHIT project. She has worked at the MPIDS since December 2011.

Angela Meister is a foreign language correspondent certified in English and French. She has been the Administrative Assistant to the Director Prof. Eberhard Bodenschatz since May 2005.

Andreas Renner has been a technician for the Bodenschatz Group since January 2007.

Marcel Meyer completed his education in the MPIDS machine shop in 2012 and has worked as a mechanic since October 2012. He supports the scientists in technical matters and services the experimental hall and laboratories.

Dr. Artur Kubitzek supports scientists in preparing their experimental setups. He is involved in the design, construction and development of scientific facilities and manages the service team.

Andreas Kopp has been a technician for the Göttingen Turbulence Facility since 2009 and supports the scientists in their practical work.
Ortwin Kurre is an electronics technician. He is responsible for education in electronics at the MPIDS and supports the team in electronical matters. Lukas Ackermann is a trainee in electronics. Gerhard Nolte has been responsible for the IT infrastructure and user support of the department since 2005. He joined the institute in 1993.

Katharina Schneider has worked at the institute since April 2005. She is a laboratory assistant for the chemotaxis group and takes care of the Dictyostelium discoideum cells and maintenance of the biological laboratories. She is currently on maternity leave. Marion Kunze has been a biological technical assistant for Prof. Luther’s Biomedical Physics Group since 2009. She is responsible for the primary cells and biological perfusion systems, and she takes care of the maintenance of the biomedical laboratories. Tina Althaus has been a biological lab assistant at the MPIDS since April 2013. Her main task is the cultivation of Dictyostelium discoideum and assisting the scientists in the biological lab. Maren Stella Müller has been a biological technical assistant at the MPIDS since April 2013. She is responsible for genotyping cell lines of Dictyostelium discoideum.
Nine research groups complement the institute’s three departments as pillars of its research structure. While some of these groups add to the institute’s scientific endeavors temporarily, others are permanent. Six temporary groups are Max Planck Research Groups – having a distinguished status in the Max Planck Society. They are led by principal investigators who work independently within the framework offered by the institute and have the opportunity to establish themselves in their respective fields. In addition, Annette Zippelius, Chair of Theoretical Physics at the University of Göttingen, has been appointed Max Planck Fellow, offering a strong link for collaborations with the University. Two permanent Research Groups are headed by Stefan Luther (Biomedical Physics) and Fred Wolf (Theoretical Neurophysics in the Department for Nonlinear Dynamics).

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2.1 MAX PLANCK RESEARCH GROUP: DROPLETS, MEMBRANES, AND INTERFACES

Soft interfaces are ubiquitous in our daily lives, widely represented in natural and technological systems. Membranes are, for example, an essential feature of living systems while soap films, foams and emulsions are man-made systems, based on soft interfaces, of practical interest as advanced materials. The group focuses on soft interfaces in a multidisciplinary approach mixing soft-matter physics, physical-chemistry and biotechnology. Self-assembly processes in soft matter provide basic means to construct soft interfaces. We control and study these processes using microfluidics. We visualize the transient processes occurring at short time-scales and measure dynamic properties of system out of equilibrium, for example surfactant monolayers or polymer shells upon polymerization. The same microfluidic tools are also of practical interest for biological applications, through the controlled manipulation of biomaterials at the appropriate lengthscale. Single cells are, for example, easily encapsulated in surfactant stabilized droplets and quantitatively assayed in microcompartment of typical sizes of approx. 20 μm.

A wide range of operation is now also envisioned based on cell-free systems to circumvent the cellular complexity in applications such as protein engineering. Elaborating on this idea, the control of self-assembly processes in microfluidics provides new methods to prepare tailored compartments made of soft-matter with controlled properties mimicking minimal cells. Combining microfluidics, soft interfaces and biotechnology will provide new tools and methods to prepare biomimetic systems based on controlled micro-compartments, capable to sustain out-of-equilibrium conditions similar to those found in living systems. We believe that these systems are perfectly well suited to study the emergence of life from prebiotic compounds or to create artificial biomimetic functional cells from soft matter.

Dr. Renaud Dufour received a Master’s degree in 2009 from the University of Lille with a focus on micro and nanotechnologies. For his PhD he worked on the development and characterization of polymeric super-omniphobic surfaces at the Institute of Electronic, Microelectronic and Nanotechnologies (IEMN, France). Since 2013 he has been a postdoctoral researcher in the research group Droplets, Membranes and Interfaces in a joined project with the Department Dynamics of Complex Fluids. He develops experimental tools to measure wettability on complex structures and investigating the wetting of rough surfaces in the frame of the Geomorph project financed by BP.
Dr. Erfan Kadivar received his Master’s degree in theoretical physics in 2002 from University of Isfahan (Iran), with a focus on nematic liquid crystal flow. For his PhD he worked at University of Isfahan in the field of simulation of defect in nematic liquid crystal and finished the PhD in 2007. In a first postdoctoral position he worked on the simulation of two-phase flow in microfluidic channel. In 2013, he joined the research group Droplets, Membranes and Interfaces to work on numerical simulations of droplets in channels and surfactant adsorption.

Dr. Jiseok Lim received his Master’s degree in mechanical engineering in 2006 from Yonsei University (Korea) in the field of nano-fabrication technology. For his PhD he worked at the Nanofabrication and microoptics National Research Laboratory at the Yonsei University to develop imaging system with microoptics. In 2011 he joined the Enzyme Biochemistry Research Group of Dr. Manfred Konrad at the MPI for biophysical chemistry as a postdoctoral researcher. He joined the research group of Dr. Jean-Christophe Baret from 2012, working on a project for directed evolution of therapeutic enzymes and developing novel microfluidic devices.

Dr. Florine Maes received her Master’s degree in engineering in 2008 from the Polytech Lille Engineer School in Lille (France) in material sciences. In 2011, she received her PhD diploma from the Mines ParisTech School in Paris (France). During her PhD, she worked on the self-healing properties of supramolecular rubber in collaboration with the Soft Matter and Chemistry lab of ESPCI (Paris, France). Since 2012, she is a postdoctoral researcher in the research group Droplets, Membranes and Interfaces at the MPIDS where she works on active and reactive interfaces in droplet-based microfluidics.

Dr. Deniz Pekin received her Diploma in molecular biology in 2009 from the University of Strasbourg (France). She received her PhD in 2013 from the University of Strasbourg for a project on droplet-based microfluids techniques for the detection of cancer biomarker. The project was a collaboration between the Institut de Science et d’Ingénierie Supramoléculaires (Strasbourg) and the Université Paris-Descartes. Since August 2013 she is a postdoctoral researcher in the research group Droplets, Membranes and Interfaces to construct biomimetic systems made of soft matter using biochemical reactions.

Dr. Ingmar Polenz received his Diploma in organic chemistry (with Prof. Dr. K. Banert) in 2009 and his PhD in polymer chemistry (with Prof. Dr. Stefan Spange) in 2012, both from the Chemnitz University of Technology. He worked on the novel imine base isocyanate mediated radical polymerization and its applications. From 2012 to 2013, he was a research fellow of the BASF Advanced Research Initiative at Harvard University in the group of Prof. David A. Weitz working on reactive encapsulation techniques in microfluidic devices. In May 2013 he joined the research group Droplets, Membranes and Interfaces to study of the dynamics of shell formation at reactive interfaces and the properties of the resulting materials.
2.2 MAX PLANCK RESEARCH GROUP: BIOLOGICAL PHYSICS AND EVOLUTIONARY DYNAMICS

Biological evolution is driven by at least partially random events, such as birth, death and mutations. As a result, randomness has left a marked footprint in the biological world we see today. Numerous emergent phenomena in biology, such as the complex patterns of genetic and phenotypic diversity within populations or the peculiarities of genomic architectures and developmental pathways, are difficult to explain without invoking the effects of stochasticity in evolution. In recent years, our research has focused on rationalizing the inherently stochastic trajectory of evolutionary dynamics in theoretical models and experimental model systems, using methods of statistical physics. This focus is part of our general research goal to reveal essential structures of emergent phenomena in complex biological systems, which is a truly interdisciplinary endeavor that combines quantitative biology, non-linear dynamics, and statistical physics.

Our projects extend from fundamental studies on stochastic reaction diffusion systems to explicit models of adaptive evolution. We are driven by basic evolutionary puzzles such as “How fast is evolution?”, or “Under which circumstances is evolution driven by survival of the luckiest rather than the fittest?”. In order to test our models in the lab, we use microbes grown in liquid media, on agar plates and in micro-fluidic devices. Amongst others, combination theory and experiment has revealed novel patterns of chance and adaptation, that have also been found in natural populations of multicellular species. Our evolutionary experiments also fuel biophysical research questions, such as “What forces can be generated by microbial populations when they grow in confined geometries?”

More generally, we want to understand how organized microbial colonies as a result of proliferation interacting with hydrodynamics and viscoelasticity of the surrounding matrix. Ultimately, this interdisciplinary approach might help to control the formation and adaptation of biofilms, which are microbial communities involved in numerous infectious disease and responsible for significant industrial costs.

Dr. Jean-François Flot studied biochemistry at the Ecole Normale Supérieure de Cachan in France, at the University Paris Diderot and at the University of Stockholm before moving to Okinawa (Japan) for a master in marine science at the University of the Ryukyus. He received his PhD in molecular systematics at the Paris Museum of Natural History in 2007, then did research in evolutionary genetics at the University of Göttingen in Germany, at the University of Namur in Belgium and at Genoscope (French National Genome Center) in France. In 2012 he joined the research group Biological Physics and Evolutionary Dynamics at the MPIDS where he is currently investigating the effect of spatial structure on mutation accumulation and adaptation in bacteria and yeast.
The dynamics encountered in nonlinear systems are often extremely complex and chaotic. One of the most familiar and at the same time most relevant example is the turbulent motion of fluids. Turbulent flows are ubiquitous in nature and occur on many different scales ranging from astrophysical examples like the formation of stars and planets to flows in the atmosphere, rivers and blood vessels. The classical way to approach turbulence is to consider the asymptotic Reynolds number limit and to assume flows to be homogeneous and isotropic. This idealized case however is hardly ever realized in practice and many of the fundamentally most important questions have been left unanswered. We take a different approach and instead of the large Reynolds number limit we investigate turbulence when it first arises. Here the dynamics are less complex and may allow us to obtain a conceptual understanding of the origins and nature of turbulence. As our recent studies show, in this regime tools from nonlinear dynamics and critical phenomena are applicable and substantial progress can be made. We focus on flows where turbulence arises despite the stability of the laminar flow such as pipe, channel and plane as well as circular Couette flows. These flows play a central role in fluid dynamics and are of great practical importance. Unlike in situations where transition follows a linear instability, here a physical understanding of the onset of turbulence has been lacking. By combining detailed experiments with highly resolved simulations and the simultaneous study of different flows we could for the first time describe the transition process and uncover a phase transition at which turbulence becomes sustained.

These insights now provide a unique opportunity to determine universal features of turbulence close to onset (e.g. scale invariance and critical exponents) and to extend concepts to the increasing complexity encountered at higher Reynolds numbers. At the same time we exploit our knowledge of the sustaining mechanisms to control turbulent flows. In initial experiments we have demonstrated that it is even possible to fully relaminarize turbulent structures in the transitional regime. We have meanwhile developed new methods that also allow us to relaminarize pipe flows in experiments at higher Reynolds numbers where the entire domain is turbulent. More detailed studies are presently being carried out.

Recently we have extended our interests to situations where complexity arises through the interaction of shear flows with other self organizing processes. These projects presently take up more than one third of the group’s activities and include the influence of polymers on phase transitions in shear flows, the formation of biofilms and the swimming of plankton larvae.

The group was started by Björn Hof in March 2008 who was appointed full professor at the Institute of Science and Technology Austria in June 2013. Part of his group (2 PhD students, 2 postdocs and 1 technician) will remain at MPIDS until the end of May 2014. An
important aspect of our group is the multidisciplinary background of the group members, comprising physicists, mathematicians and engineers. Currently we are collaborating with Prof. B. Eckhardt, University of Marburg (theoretical physics), Prof. D. Barkley, University of Warwick (applied mathematics), Dr. G. Jekely, MPI for developmental biology Tuebingen (biology), Prof. P. Cvitanovic, Georgia Tech (theoretical physics), Dr. Fernando Mellibovsky, UPC Barcelona (aerospace engineering), Dr. Ashley Willis, University of Sheffield (applied mathematics) and Professor Marc Avila, University of Erlangen (mathematics).

Dr. Jose Manuel Gallardo Ruiz studied engineering at University of Malaga (Spain) finishing 2005. During the last year of his studies he joined a research group at Istituto Motori from the National Research Council of Italy (CNR) in Naples (Italy), where he experimentally investigated flame propagation inside internal combustion engines through optical and pressure measurements methods. After working in different companies as a project manager, he started his PhD in 2008 focusing on the discharge of a swirling light gas into a heavier ambient, with coflow with application to combustion using experimental and numerical methods. During his PhD he spent five months as a researcher visitor in the Istituto Motori in Naples (Italy) and four months in the group of Dr. Hof at the Max Planck Institute for Dynamics and Self-Organization in Göttingen. He received his PhD in engineering from the University of Malaga in 2013. The title of the thesis was "On the influence of the density ratio and the co-flow on the 3D structures of swirling jets, and their relevance in combustion processesing". In 2013 he joined the MPIDS in Dr. Hof group at Göttingen as a postdoctoral researcher.

Dr. Duo Xu studied engineering at Beijing University of Aeronautics & Astronautics and aerodynamics at the Institute of Mechanics, Chinese Academy of Sciences. His PhD focused on experimental investigations of turbulent stratified flows. He received his PhD in 2012 from the Mechanical Engineering Department of Purdue University. Then he joined the research group of Dr. Hof at the MPIDS as a postdoctoral researcher. Here he carries out experimental studies of transition to turbulence in plane Couette flow.
The complex shapes and intricate structures that are found in living organisms arise partially as adaptive advantages and partially as the inevitable results of physical constraints during growth. The spiral arrangement of the seeds in a sunflower is determined by simple physical principles acting without a direct evolutionary cause, whereas the architecture of the branching structures in the lung is designed for high efficiency in gas exchange. The group Physics of Biological Organization is interested in deciphering the role of physics in biological form. Motivated and inspired by the complexity of living organisms, we look at questions regarding morphogenesis and function. Our work is theoretical and computational but the questions we address either bear directly on current biological questions or are motivated by experiments. To achieve this, we have multiple close collaborations with several experimental groups in Europe and the Americas.

Our primary focus is on biological transport networks, such as those found in leaf vasculature. It includes a variety of projects aimed at understanding the architecture of distribution networks that can be as simple as the single vein of a pine needle (Ch. 8.1) or as complex as the vasculature of the human body. We want to know how auxin canalization, diffusion of morphogens and mechanics work together to dictate the initiation of the main vein in the young leaf (Ch. 7.9), and how the curvature imposed by confinement affects the higher order reticulate vascular patterns (Ch. 7.8). Inspired by the foraging protoplasmic veins of physarum we investigate how a network reorganizes under local adaptive rules (Ch. 8.2). Leaf veins and other transport networks present many complex phenotypes. We are developing algorithmic tools to accurately digitize the networks and mathematical tools to quantify their metric topology (Ch. 8.3).

Our secondary focus on thin shell elasticity is inspired by the thin curved structures that are very common in biology, such as the walls of pollen grains and seed pods. Their geometry can dictate how they deform under load, and the pathway of the transformation is important for their function (Ch. 7.5).

The group was established in May 2012, it is currently composed of six members (including MSc and Bachelor students) and there are plans for expansion to a total size of eight in the near future. The group also maintains a number of collaborations with scientists both from within the MPIDS (L. Goehring and M. Timme) and outside institutions (Freiburg, Harvard, Copenhagen, Lyon, Rockefeller, Santiago de Chile).
In transitional shear flows local perturbations of the quiescent flow generate patches of turbulence that invade the surrounding laminar flow like a bush fire. Likewise, crystal growth from a solution can create intricate, coral-like solids. How can viscous momentum transport in shear flows, diffusion and chemical reactions in crystal growth as well as similarly simple physical mechanisms in other systems give rise to complex shapes and complex spatio-temporal patterns? These are typical questions our group studies using several aspects of continuum mechanics and transport theory entwined with dynamical systems methods and pattern-formation theory.

One dominating theme are spatial laminar-turbulent patterns in the flow of a viscous liquid between parallel plates moving in opposite directions. Here we recently detected a set of exact solutions, all unstable, fully 3D and fully nonlinear equilibria. They are spatially localized and organized in a bifurcation structure previously found in simpler differential equations serving as pattern forming model systems, see Ch. 7.2. Those solutions together with their entangled stable and unstable manifolds form the dynamical network supporting chaotic turbulent dynamics. Due to their spatial localization the solutions allow us to capture the full spatio-temporal evolution of laminar turbulent patterns and thus are a key step towards truly establishing dynamical systems as a new paradigm to study turbulence, see Ch. 7.2 and Ch. 5.3.

We recently started to extend our studies to convectively driven systems as well as boundary layers. While the former allows for additional theoretical approaches and will be studied in close collaboration with the Department Fluid Dynamics, Pattern Formation and Biocomplexity headed by Prof. Eberhard Bodenschatz, the latter is highly relevant for engineering applications and connects to studies of flows characterized by high Reynolds numbers conducted at MPIDS.

Throughout our research we combine analytical methods with large-scale computer simulations. Thereby we solve the multi-dimensional non-linear partial differential equations describing continuum mechanical systems and perform continuation and bifurcation studies in millions of coupled degrees of freedom. Taking advantage of our state-of-the-art computer infrastructure including the group’s parallel HPC clusters we develop custom-tailored software in-house [Ch. 7.3]. Moreover we combine our continuation methods with pre-existing numerical packages. Together both approaches provide an adequate simulation infrastructure for a broader range of projects.

The new projects beyond shear flows to which we apply our computational and theoretical tools include: patterns in actively forced Navier-Stokes which models biological systems; the role of elasticity in micro-swimmers [Ch. 3.6]; reaching beyond mechanical systems – reaction-diffusion dynamics underlying the formation of biomorphs [Ch. 7.10]. Additionally we are setting up the infrastructure to study
free-surface flows in microfluidic applications as well as complement experimental studies on fully developed turbulence by numerical simulations.

The group was established in March 2013. It currently consists of five scientists and postdoctoral researchers as well as visiting students. Two more students will join the group in fall 2013. We represent various backgrounds including chemical and mechanical engineering, physics, and applied mathematics. We are involved in multiple local, national, and international collaborations.

Dr. Arvind Gopinath studied chemical engineering in Bombay (India) after which he decided to sample the cold weather at Cornell university in New York. Graduating with a doctorate specializing in fluid mechanics and applied mathematics, he then moved to Cambridge, USA working first with Prof. Robert Armstrong at MIT and then with Prof. L. Mahadevan at Harvard university. Prior to coming to Göttingen he was a faculty fellow at JNCASR (Bangalore, India) and has held research scientist positions at A*STAR (Singapore), at MIT and at Brandeis University.

Dr. Johannes Schönke received his Diploma in physics in 2005 from Jena University with a thesis about planet formation in the field of theoretical astrophysics. After working in the nonlinear dynamics group in the Department of Theoretical Physics at Bremen University, he joined the Institute for Theoretical Astrophysics at Heidelberg University. There he obtained his PhD in 2010 with a thesis on theoretical aspects of star formation. As a PostDoc he worked on the numerical implementation of FEM methods and the theory of nonlinear PDE at the Interdisciplinary Center for Scientific Computing at Heidelberg University in the Bernstein Center for Computational Neuroscience. In 2013 he joined the research group of Dr. Tobias Schneider and develops numerical algorithms for surface growth problems and turbulent fluid flow.

Dr. Hecke Schrobsdorff received his Diploma in theoretical physics in 2005 from Göttingen University in the field of theoretical neuroscience. In 2006 he received a diploma in mathematics also from Göttingen University with a focus on algorithms in quantum computing. For his PhD he worked at the BCCN Göttingen in a joint project with the Institute for Pedagogical Psychology and finished the PhD in 2009. In a first postdoctoral position he developed efficient algorithms for holographic photostimulation of optogenetic neurons. In 2012 he joined the Max Planck Research Group of Dr. Tobias Schneider and develops parallel applications for high performance computers for flow simulations and microfluidics.

Dr. Priya Subramanian completed her Bachelor’s degree in aeronautical engineering in 2004 from Madras University. She then completed her doctorate at the Department of Aerospace Engineering, IIT Madras in 2012. Her PhD focused on the interaction between acoustics and premixed flames which can lead to thermoacoustic instabilities in rockets, aero-engines and gas turbines. Since her doctorate, she has been a postdoctoral researcher in the Max Planck Research Group of Dr. Tobias Schneider and works in the areas of pattern formation in transitional flows, emergent dynamics in elastic swimmers along with continuing her investigation into the nonlinear dynamics of thermoacoustic systems.
2.6 MAX PLANCK RESEARCH GROUP: NETWORK DYNAMICS

Networks are everywhere. And most of them are dynamic. From biochemical reactions in the cells of our bodies to the neuronal circuits in our brains that make us behave; from social ties forming networks of our friendships to the power grids that provide huge amounts of electric energy; all of these systems form networks of units that interact to yield complex, emergent forms of functions – and all are crucial to our everyday life.

Scientific research on the dynamics of networks thus is an intrinsically transdisciplinary endeavor and as such not represented by traditional subjects focused on by institutes and departments at most universities and research institutions. A researcher starting to work on what is on its way to become “Network Science” in the future thus needs to read text books and articles on graph theory and stochastics, nonlinear dynamics, statistical physics, computation, and algorithms, as well as the specific subject she is aiming to investigate, e.g. in biology, physics or engineering.

In the Network Dynamics team, we are working towards a unifying understanding of the fundamentals underlying the dynamics of large, nonlinear interconnected systems. We theoretically study topical questions arising from a broad range of phenomena in physics, in neurobiology, in evolution, and in the engineering of self-organizing “intelligent” systems. Moreover, a substantial part of our work is investigating emergent mathematical objects and developing mathematical and computational tools necessary to understand the novel phenomena arising in network dynamical systems.

These seemingly disjoint research topics are strongly overlapping as they are joined by two types of links: The first set of links is methodological, resulting from developing mathematical and computational tools of nonlinear dynamics and statistical physics of networked systems. The second set of links exists on a systems level; most of our work focuses on the theory of collective dynamics of excitable and oscillatory networks (and their constituents). For instance, much of our progress, highlighted below, results from theoretical studies on the collective dynamics of such networks; on the emergence of neural synchrony and spike patterns (Ch. 8.9); on collective stochastic oscillations in evolutionary dynamics (Ch. 8.8); on intelligent, self-organizing solutions to communication in ad-hoc networks and new forms of natural computational principles (Ch. 6.2); and on oscillatory networks modeling modern electric power grids (Ch. 8.11).
Dr. Hinrich Arnold studied physics at the Universities of Göttingen and Padua (Italy). In 2007 he joined the Network Dynamics Group to work on his Diploma thesis “Precise spike timing in neural systems with static and dynamic synapses”. After receiving his Diploma from the University of Göttingen in 2009 he remained in the group to analyze the impact of horizontal gene transfer on stochastic evolutionary dynamics. He obtained his PhD in 2013 and is now working on the analysis of spiking neuronal dynamics and on questions in evolution theory raised in his thesis.

Dr. Sarah Hallerberg did her PhD project on time series analysis and predictability of extreme events in stochastic processes under the supervision of Prof. Dr. H. Kantz at the MPIPKS in Dresden. In 2007 she was also a visiting scientist at the Centre for the Analysis of Time Series at the London School of Economics, working on the predictability of forecast errors in meteorological ensemble forecasts. In 2008 she received her PhD in theoretical physics and started to work as a temporary lecturer at the Department for Applied Mathematics at the University of Cantabria. There she also became interested in scaling properties of perturbations in spatio-temporal chaotic systems. In 2011 she joined the MPIDS to work on the analysis of whale vocalizations, perturbations in high dimensional chaotic systems and several other data analysis projects.

Dr. Fabio Schittler Neves studied physics at the Federal University of Rio Grande do Sul (Brazil), where he obtained his Bachelor’s degree in 2003 and his Master’s degree in theoretical physics in 2006 with a thesis on the effects of non-monotonicity. He received his doctorate from the University of Göttingen in 2010 with a thesis on the computational properties of neural networks exhibiting heteroclinic cycles. He continues studying this novel paradigm of computing by heteroclinic switching and its real-world applications in autonomous agent control and general-purpose computation.

Dr. Dirk Witthaut studied physics at Technical University Kaiserslautern and received his PhD in 2007 for his work on the nonlinear dynamics of Bose-Einstein condensates in optical lattices. After working as a guest lecturer at the Kigali Institute for Science and Technology in Rwanda for one semester, he stayed at the Niels Bohr Institute in Copenhagen funded by a DFG research fellowship. Since 2009 he has been leading a research project on the self-organized nonlinear dynamics of modern power grids in the group of Prof. Timme. Recently, he has been offered a research position (tenure track) to head a Helmholtz Young Investigators Group at Forschungszentrum Jülich.
2.7 RESEARCH GROUP: BIOMEDICAL PHYSICS

Self-organized complex spatial-temporal dynamics underlie dynamic physiological and pathological states in excitable biological systems including heart and brain, one example being life-threatening cardiac arrhythmias, a major cause for morbidity and mortality worldwide. The term dynamical disease was coined for arrhythmias, suggesting that they can be best understood from the dynamical system’s perspective. We are driven by the vision that the systematic integration and evaluation of dynamics on all levels from sub-cellular, cellular, tissue and organ to the in vivo organism is key to the understanding of complex biological systems and will open, from a long-term perspective, new paths for translating fundamental scientific discoveries into practical applications that may improve human health.

The theory of dynamical systems plays a central role in integrating biological experiments with mathematical modeling. Our group focuses on the following objectives: physiological modeling of cardiac dynamics and electro-mechanical instabilities; multivariate analysis; classification and prediction of biosignals; control of arrhythmias by novel approaches. These aims will be achieved by a data driven, integrative strategy that combines high-resolution imaging techniques with state of the art numerical modeling through innovative state and parameter estimation and model evaluation methods. Based on this approach, we have successfully developed a novel method for low-energy termination of electrical turbulence in the heart. In collaboration with our research partners, we demonstrated a sustained in vivo energy reduction of 80-90% compared to standard defibrillation, opening the path towards painless and non-damaging termination of life-threatening arrhythmias. For this achievement, we received the award Gründungssoffensive Biotechnologie 2012 from the German Federal Ministry of Education and Research (BMBF). Following our successful evaluation in 2012, the Max Planck Research Group Biomedical Physics has been granted tenure by the President of the Max Planck Society. Enjoying a scientifically independent status at the MPI DS, our Research Group continues to strive for excellence in research and training of young scientists. We contribute to the curriculum “Biophysics and Physics of Complex Systems” of the Faculty of Physics at the Georg-August-Universität Göttingen. The Biomedical Physics Group participates in several large-scale cross-disciplinary collaborative initiatives including EUTrigTreat, DZHK e.V., and SFB 1002.

Honorarprofessor Dr. Stefan Luther studied physics at the Georg-August-Universität Göttingen, where he received his doctoral degree in 2000. This was followed by postdoctoral research on non-ideal turbulence (University of Twente, 2001-2004) and cardiac dynamics (Cornell University, 2004-2007). Since 2007 he has been head of the Max Planck Research Group / Research Group Biomedical Physics (tenured 2012) at MPI DS and Honorarprofessor at the Georg-August-Universität Göttingen (since 2008). He received the Medical Technology Innovation Award 2008 and the GO-Bio Award 2012. He is faculty member at the Institute for Nonlinear Dynamics, GAUSS, and a founding member of the Heart Research Center Göttingen.

Dr. Philip Bittihn studied physics at the Georg-August-Universität Göttingen as a scholar of the Studienstiftung des deutschen Volkes (German National Academic Foundation). In 2009, he obtained his diploma with honors from the university, before joining the MPRG Biomedical Physics at the MPI DS. He received his PhD in June 2013 for theoretical and experimental work on the complex structure and dynamics of the heart and is currently continuing his research as a postdoctoral fellow. His interests include the nonlinear dynamics and emergent phenomena of biological systems, numerical simulations, partial differential equations and experimental data analysis.
**Prof. Dr. Valentin Krinski** studied physics at the Institute of Physics and Technology (Moscow, Russia) where he received his PhD in 1964. After 12 years at the Institute of Biological Physics in Puschino, he was appointed Head of the Autowave Laboratory in 1976, Prof. of Biological Physics at the Institute of Physics and Technology (Moscow, Russia) in 1980. He was Directeur de Recherche, CNRS, INLN (Nice, France) as of 1993. His research interests include vortices in biological excitable tissues and novel approaches for the termination of life-threatening chaos in the heart. In 2007 he joined the MPIDS to work with Prof. Luther and Prof. Bodenschatz on cardiac dynamics.

**Gisa Luther** studied physics at the Universität Hannover and the Carl von Ossietzky Universität Oldenburg, graduating in 1996. From 1997 to 2001, she worked for Bull GmbH (Langen) as an assistant project manager in software engineering and system integration. In 2002, she joined WestLB Systems GmbH (Münster) as project manager in software engineering. From 2004 to 2007 she was a visiting scientist at LASSP, Cornell University (Ithaca NY). Since 2004 she has been a senior researcher at the MPIDS. Her research interests include numerical modeling of complex hydrodynamic and biological systems.

**apl. Prof. Dr. Ulrich Parlitz** studied physics at the Georg-August-Universität Göttingen, where he received his PhD in 1987. After five years at the Institute for Applied Physics of the TU Darmstadt he returned to Göttingen in 1994 where he was habilitated in 1997 and appointed apl. Prof. of Physics in 2001. He was a visiting scientist at the Santa Fe Institute (1992), the UC Berkeley (1992), and the UC San Diego (2002, 2003). His research interests include nonlinear dynamics, data analysis, complex systems, and cardiac dynamics. In September 2010 he joined the Max Planck Research Group Biomedical Physics. He is faculty member at the Institute for Nonlinear Dynamics, GAUSS, and principal investigator at the BCCN.

**Dr. Claudia Richter** studied biology at the University of Rostock, with focus on animal physiology and forensic biology (2000-2005). After graduation she worked as research associate at the Department of Forensic Genetics at the Institute of Legal Medicine in Rostock. She received her PhD in February 2011 and since March 2011 has been working as a postdoctoral associate in the Max Planck Research Group Biomedical Physics at the MPIDS. Her research interests include cardiac dynamics, biophysical and molecular research, biomaterials and tissue engineering.

**Dr. T K Shajahan** studied physics at the Indian Institute of Technology (Madras) where he received his MSc. He received his PhD from the Department of Condensed Matter Theory at Indian Institute of Science (Bangalore) in 2008. During his PhD he studied the formation of spiral waves and their interactions with heterogeneities in mathematical models of cardiac tissue. After spending a year teaching at the Indian Institute of Science Education and Research in Trivandrum, he accepted a postdoctoral position at the Department of Physiology, McGill University (Canada). His research interests include pattern formation in excitable media and initiation and control of cardiac arrhythmias. In April 2013 he joined the Max Planck Research Group Biomedical Physics as a postdoctoral fellow.
The brains of humans and animals arguably are among the most complex systems in nature. Understanding their operation crucially depends on the ability to analyze the cooperative dynamics of spatially distributed multi-component systems: Even the most elementary sensory stimulus engages large ensembles of interacting nerve cells distributed throughout the brain. The processing power of biological neuronal circuits exactly results from their collective dynamics. In addition, complex nervous systems utilize processes of dynamical self-organization to generate and maintain their processing architecture. The amount of information in a mammalian genome is by far insufficient to specify the wiring of biological neuronal networks in microscopic detail. Functionally useful processing architectures are thus dynamically generated by self-organization on the level of neuronal circuits. Ultimately, even an individual nerve cell is a complex dynamical system. Virtually all single neuron computations critically depend on the dynamical interaction of a multitude of subcellular components such as ion channels and other interacting biological nano-structures. It is due to this ubiquity of collective behaviors that neuroscience provides a rich source of attractive research questions for the theoretical physics of complex systems.

The Research Group Theoretical Neurophysics examines neurobiological and biophysical phenomena which require mathematical and theoretical treatment and can be approached in precise quantitative experiments. Our work extends from the formulation of novel mathematical approaches for addressing dynamical phenomena in neuronal systems, over analysis methods for turning biological experimental observations into theoretically informative quantitative data, to the development of experimental paradigms designed to provide insight into cooperative and dynamical aspects of neuronal function. To achieve a seamless interaction of theory and experiment, many projects are pursued in collaboration with experimental biological research groups around the world. Three problems are at the core of our research agenda: (1) The self-organization of neuronal circuits in the visual cortex. In this system our analyses revealed that the architecture of biological neural networks precisely follows invariant quantitative laws. Our mathematical theories of neuronal self-organization demonstrate that these laws are exactly predicted by a novel universality class of pattern forming dynamical systems. (2) The dynamics of large networks of pulse-coupled neurons and its impact on the representation of sensory information. Here the ergodic theory of network dynamical systems promises to provide a natural language that links details of the network dynamics to information preservation, decay and flux. (3) The biophysical nature and dynamics of high-bandwidth action potential encoding. Here we are integrating concepts from non-equilibrium statistical physics with the biophysics of membranes and ion channels. The identification of dynamically realistic models of single neuron operations is essential for understanding collective computations in the brain.
Dr. Andreas Neef received his Diploma in physics in 2000 from the University of Jena, Germany. He joined the MRC Laboratory of Molecular Biology, Cambridge (UK) as a visiting scientist to work on retinal neurons and then worked on his PhD at the Research Centre Jülich, Germany, where he received his doctorate from Cologne University in 2004. After being a postdoctoral researcher at the Institute for Biological Information Processing I in Jülich (2004) and at the Bernstein Center for Computational Neuroscience, Göttingen he became a Bernstein Fellow associated with the Department of Fluid Dynamics, Pattern Formation, and Nanobiocomplexity in 2006. Since 2013 he heads the research group Biophysics of Neuronal Computation at the Bernstein Center for Computational Neuroscience.

Dr. Guillaume Lajoie studied mathematics at the University of Ottawa (Canada) and applied mathematics at the University of Washington (USA) where he received a PhD in Applied Mathematics in 2013. In 2010 he worked as a visiting scholar at the Instituto de Mathematica Pura e Aplicada in Rio de Janeiro (Brazil). His research focuses on the development and application of dynamical systems techniques to understand information processing in networks of spiking neurons. He recently joined the MPI-DS and the Bernstein Center for Computational Neuroscience Göttingen as a Bernstein Fellow.

Dr. Achmed ElHady studied pharmaceutical sciences at Cairo University (Egypt) and attended the International Max Planck Research School for neuroscience master courses. He obtained his PhD in 2012 at the Max Planck Institute for Dynamics and Self Organization studying neuronal network dynamics using optogenetics. Since then, he is a postdoctoral fellow at the Max Planck Institute for Dynamics and Self Organization where he uses a combination of multielectrode arrays recording and optogenetics in order to experimentally test theoretical models of neuronal encoding and its underlying biophysical mechanisms and to study network-level plasticity.

Dr. Lars Reichl studied physics at the University of Heidelberg. He received his diploma in 2003 about cosmological models in extra dimensions. In 2004 he joined the the group of Theo Geisel at the MPI for Dynamics and Self-Organization. He received his PhD degree in physics in 2010 about his studies on visual cortical development. Since 2012 he works a postdoctoral researcher on optimization models for visual cortical processing architectures and on the quantitative description of pattern formation processes during morphogenesis in drosophila.

Dr. Yvonne Reimann studied biology at the University of Göttingen and finished her PhD at the Max Planck Institute for Biophysical Chemistry in Göttingen in 2008 for work on cell fate determination during cortical development. From 2008 to 2009 she was a Postdoc in the Department Molecular Cell Biology at the Max Planck Institute for Biophysical Chemistry. She did postgraduate studies in science management at the German University of Administrative Sciences Speyer from 2009 to 2010. From 2010 to 2012 she worked as scientific coordinator at the Leibniz Research Laboratories for Biotechnology and Artificial Organs at Hannover Medical School before changing to the Research Department of University of Göttingen. Since December 2012, she is the administrative coordinator of the Bernstein Center for Computational Neuroscience Göttingen and Bernstein Focus Neurotechnology Göttingen.
Our research is devoted to the further development and application of magnetic resonance imaging (MRI) and localized magnetic resonance spectroscopy for noninvasive studies of animals and humans. Current projects range from advanced methods that monitor the dynamics of myocardial functions and blood flow in real time to neurofeedback training in humans by functional brain mapping. The use of genetically modified animals allows us to link molecular and genetic information to MRI-accessible functions at the system level.

Our recent breakthrough towards real-time MRI is based on the use of non-Cartesian spatial encoding, pronounced data undersampling, and image reconstruction by regularized nonlinear inversion. Pertinent techniques bear the potential to alter the future of (clinical) MRI. They allow for movie recordings of speech production, turbulent flow or the beating heart – without synchronization to the ECG and during free breathing. The computational demand is met by a parallelized algorithm and multiple graphical processing units which could be fully integrated into the software framework of a commercial MRI system.

A second area of research focuses on studies of the functional organization of the human brain and its axonal connectivity. Diffusion MRI provides information about the orientational dependence of the anisotropic water mobility in brain tissue and may be exploited for three-dimensional reconstructions of nerve fiber tracts. In order to overcome limitations of the standard echo-planar imaging technique we developed a single-shot stimulated-echo MRI sequence which is now further extended by radial undersampling and nonlinear inverse reconstruction. Functional brain mapping deals with the neural encoding of sensorimotor functions. Our results for fine-scale finger somatotopy in humans indicate consistent intra-digit topographic maps for the little but not the index finger within the primary somatosensory cortex. Neurofeedback training of brain activity is a potential treatment option for psychiatric diseases offering access to arbitrary structures. Our aim is to investigate the role of fMRI-based neurofeedback in the anterior mid-cingulate cortex which relates to higher-order cognitive processes.

Animal MRI research addresses the pathophysiologic mechanisms underlying human brain disorders. The development of MRI techniques for transgenic mice allows for structural, metabolic, and functional assessments of the mouse brain at high spatial resolution. An observation of utmost importance is the high but reversible elevation of brain lactate in response to volatile anesthetics. The metabolite responses to various neuromodulators indicate a stimulation of adrenergic pathways as well as an inhibition of the respiratory chain. Corresponding findings in conditional Cox10 mutant mice, in which oligodendrocytes suffer from impaired oxidative energy metabolism, suggest the use of lactate as brain energy source, so that oligodendrocytes survive by enhanced nonoxidative glucose consumption which in turn secures the maintainance of myelin as well as long-term axonal integrity.
2.10 MAX PLANCK FELLOW GROUP: POLYMERS, COMPLEX FLUIDS, AND DISORDERED SYSTEMS

In our research group we try to understand how macroscopic complexity appears in the collective behavior of strongly interacting many particle systems.

Very complex behavior of physical systems can originate from very simple ingredients. Polymers, for instance, can be idealized as hard spheres (monomers) linked together randomly in a network. Even though this is an extremely idealized point of view, many macroscopic properties of polymer melts, solutions or gels can be understood from this model, for example the random localization of particles in the gel as well as rheological properties. In recent years our research has focused on biopolymers, such as actin-filaments and microtubules, which determine the elastic properties of biological cells. We use simple models of statistical mechanics for analytical calculations and large scale simulations to study the elastic properties of cross-linked biopolymers.

The behavior of a simple system can become very complex as soon as it is pushed out of equilibrium. A biological cell is inherently out of equilibrium: the cytoskeleton is an active, dissipative polymer structure which uses motor proteins to drive dynamic processes, such as cell motility or growth. As a first step to understand an active polymer structure we simulate a combined model of polymers and motors.

A granular fluid is another prototype of a system which is relatively simple in equilibrium and extremely complex as soon as dissipation is switched on, showing for instance clustering instabilities, correlations between translation and rotation or highly non-Gaussian energy distributions. At sufficiently high densities granular fluids can undergo a jamming transition into an amorphous solid state. The emergent solid turns out to be highly fragile and susceptible to even minute changes in the external control parameters. It is this interplay and coexistence of flowing and solid states that poses challenging new questions, like for example the origins of flow localization or shear thickening. Complexity can also be induced by disorder. Disorder is present in most, if not all, systems encountered in reality and its influence is often such that it cannot be neglected, on the contrary, even infinitesimal disorder can lead to effects which are absent in an idealized ordered state. A particular challenge is disorder in low dimensions, a typical example being the spin glass. Here, the nature of the low temperature phase is far from being understood. Recent development of new methods and tools has made significant progress possible in this area. Our research group consists of the head of the group, one postdoctoral researcher and two PhD students in physics. Additionally, visiting scientists and Master students contribute to the research program. Given that soft and biological matter is a research focus of both, the Georg-August University and the MPIDS, we were able to establish a new collaborative research center (SFB 937) in 2011. Four scientists from the MPIDS are involved in the research program “Collective Behavior of Soft and

Prof. Dr. Annette Zippelius studied physics at the Technical University of Munich and at the University of Colorado in Boulder. She received a Master’s degree in 1973 in Boulder, her PhD in 1977 in Munich and the habilitation in 1983 in Munich. She was a postdoc in Harvard and Cornell universities. In 1983 she became a scientific staff member at the Forschungszentrum Jülich. Since 1988 she has been a full professor in the Faculty of Physics at the University of Göttingen. She was awarded the Leibniz-Prize of the DFG in 1998, was a member of the Wissenschaftsrat from 2005 to 2011 and became a Max Planck Research Fellow in 2006. She is speaker of the SFB 937, established in 2011.
Biological Matter”, further strengthening the cooperation between the MPIDS and the university.

Dr. Karina E. Avila completed her Master’s degree in physics in 2010 from Ohio University. She then started her doctorate research at the Department of Physics and Astronomy at Ohio University in 2010. Her PhD research focuses on studying the origin of spatial-temporal fluctuation, called dynamical heterogeneity, in structural glasses. In 2010 she joined the group of Prof. Annette Zippelius, in the Max-Planck Fellow Group, in a collaboration with the Department of Physics and Astronomy at Ohio University. In this collaboration she is investigating dynamical heterogeneity in a simulated granular system by observing and extracting the extent of these fluctuations.

Dr. Andrea Fiege studied physics and mathematics in Göttingen, Helsinki and Halifax. She received her Diploma in theoretical physics in 2007 from Göttingen University with a thesis on diffusion in driven granular matter. For her PhD she joined the MPI Fellow Group of Annette Zippelius. She completed her PhD in 2013 in Göttingen. She has been working on driven granular matter close to the granular glass transition, active particles and fluidized beds of granular particles.

Matthias Grob completed his Bachelor’s degree in physics in 2010 at Göttingen University. After he spent half a year at Groningen University (Netherlands) in 2011, he received his Master’s degree in physics also from Göttingen University in 2012 with a focus on molecular dynamics simulation on graphics processing units and rheology of dense frictional particulate systems. His PhD is ongoing work and continues the work on rheology.

Dr. Till Kranz studied physics at the Universities of Augsburg and Göttingen where he received his PhD in 2011. From 2007 to 2012 he worked in the group of Annette Zippelius in the MPIDS. In 2012 he joined the Department of Theoretical Physics of the University Göttingen as a postdoctoral researcher continuing his work on the glass transition in nonequilibrium fluids.
2.11 MAX PLANCK EMERITUS GROUP: MOLECULAR INTERACTIONS

Together with the late Hans Pauly (1928–2004) we came to Göttingen in 1969 from the University of Bonn to establish the new research direction of molecular beam investigations of chemical elementary collision processes. In the following years the Institute became one of the leading international centers for experimental and theoretical research in determining with unprecedented precision the van der Waals forces between atoms and molecules. These forces are of fundamental importance for understanding both the static and dynamic properties of gases, liquids and solids as well as their phase transitions. Our research led to the development of a new model for the van der Waals interaction, the Tang-Toennies potential, which is widely used for accurate simulations in place of the well-known Lennard-Jones potential.

In the course of these studies our group observed in the late 1970’s that helium free jet gas expansions behaved in a remarkable way. Instead of the usual velocity distributions with \( \Delta v / v \approx 10\% \), the helium atom beams had very sharp velocity distributions and were nearly monoenergetic with \( \Delta v / v \leq 1\% \). This unexpected observation was found to be related to the extremely weak interatomic forces between He atoms, with the consequence that their collision cross section, at the ultra-low ambient temperatures \( (\approx 10–3\text{ K in the expanding gas}) \) rises to 259,000 Å, more than 4 orders of magnitude larger than the cross section at room temperature. These nearly monoenergetic helium atom beams have found widespread applications. In expansions with small concentrations of molecules the excess of helium atoms serves to cool the molecules down to temperatures of several degrees K. This became a great boon for molecular spectroscopy since at these temperatures the hot bands that otherwise obscure the molecular spectra are eliminated.

Our group exploited the helium atom beams for exploring the structures and vibrations at the surfaces of solid crystals. In complete analogy to neutrons which are routinely used to study the structures and phonon dispersion curves inside solids, helium atoms are the ideal scattering probe method for investigating the structures and dispersion curves of phonons at solid surfaces, which are not accessible with neutrons. The study of over 200 different surfaces by helium atom scattering (HAS) and the complimentary method of inelastic electron scattering (EELS) have lead to a much more profound knowledge of interatomic forces at surfaces and how atoms and molecules interact with metal surfaces, which is of basic importance for understanding catalysis. In the following years we became even more fascinated by this unusual element helium, which is the only substance which exhibits superfluidity, a collective quantum phenomena similar to superconductivity. In its superfluid state below 2.2 K liquid helium flows without friction, just as the electrons in a superconductor flows without resistance. Thus it was natural to ask if small clusters and droplets of helium might also exhibit superfluidity. Our finding that atoms and molecules were trapped in the droplet’s interior opened up the possibility of employ-
ing their spectroscopy to interrogate the physical properties of helium droplets. Surprisingly the sharp spectral features of the embedded molecules indicated that the molecules rotate freely as if they were in a vacuum and not at all strongly hindered as expected for an ordinary liquid. Subsequent experiments revealed that this remarkable behavior was related to the superfluidity of these droplets and has since been accepted by the science community as a new microscopic manifestation of superfluidity.

Helium nanodroplets are now being used in more than 25 laboratories worldwide as a uniquely cold (0.15–0.37 K) and gentle matrix for high resolution molecular spectroscopic investigations of atoms, molecules, and “tailor made” clusters, their chemical reactions, and their response to photoexcitation. Our group used this technique to provide the first evidence that para-hydrogen molecules which, like He atoms are spinless bosons, can also exhibit microscopic superfluidity. Our most recent experiments were directed at exploring the nature of small pure clusters ($N \leq 100$) of helium and hydrogen molecules. To this end we developed an apparatus to study the matter-wave diffraction of cluster beams from nanostructured transmission gratings. These experiments led to the first evidence for the existence of the dimer and the precise measurement of its size and of the van der Waals interactions of a number of atoms and molecules with solid surfaces. Unexpected magic numbers were found in larger clusters ($N \leq 50$), which have led to the first insight into the elementary excitations of these nano-sized superfluids.

At present we are collaborating with several groups in three main areas of research: (1) With a theory group at the University of Milan we are preparing a comprehensive review article on “The Interaction of Atoms with Surfaces and Surface Phonons” for a new Landolt Boernstein volume LB III/45A-B, titled "Physics of Solid Surfaces" edited by Prof. G.Chiarotti and Prof. P. Chiaradia. This review will provide an update of results from helium atom scattering experiments and the related theory for the interaction of atoms with surfaces; (2) We have recently completed the analysis of experimental data relating to the flow of solid helium through a 100 micron capillary. The analysis indicates that the flow is non-classical in that it does not follow the Hagen-Poiseuille law. Rather it exhibits an unexpected large velocity which is independent of the pressure gradient. This phenomenon is attributed to a type of Bose-Einstein Condensation of a solid with a high concentration of vacancies. (3) In collaboration with a group at the University of Innsbruck we are currently investigating the creation of short lived helium anions and related kinetic processes occurring in large superfluid helium droplets subjected to electron bombardment. The results have important implications for understanding the mobility of negative charge carriers in superfluid helium. Other investigations are devoted to preparing publications on experimental research carried out in our group while we were still active. Today, new insight coming from developments in the theory make the results of topical interest.
PART II

RESEARCH
FRONTIERS FAR FROM EQUILIBRIUM – STATISTICAL PHYSICS OF STRONGLY DRIVEN SYSTEMS

Many systems of practical interest are driven to states far from thermal equilibrium. Driving can be external, as in turbulent flows or agitated granular matters, or internal, as in bacterial colonies, where each particle (i.e., cell) provides its own active drive. As a consequence, the formalisms of equilibrium physics do not apply. Despite significant recent theoretical advances for non-equilibrium physics, provided, e.g., by fluctuation theorems and large-deviation functionals, a general framework for modeling systems far from equilibrium is still lacking. At the MPIDS, we are studying paradigmatic non-equilibrium systems to identify overarching commonalities and modeling concepts.

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Three-dimensional turbulent flows gain the energy for their motion from forcing at large length scales and dissipate the kinetic energy to heat through molecular interaction, which occurs at small length scales. A defining feature of turbulence is that the energy transfer from the large, energy-containing scales to the small, dissipative scales through successive agitation of smaller and smaller scales, a process called the energy cascade. Kolmogorov’s classical 1941 theory (K41) [1] distills the cascade picture into an elegant and concise mathematical description. In particular, it shows that when the energy injection scale and the dissipative scale are widely separated, energy is transferred by non-linear interactions through the intermediate scales without loss. This intermediate range is termed the “inertial range”. For homogeneous turbulence, K41 further establishes a quantitative relation between two-point velocity correlations (or velocity structure functions) and the mean energy flux through scales, a central quantity for describing turbulence.

Despite this breakthrough, exactly how the energy cascade proceeds, or what the dynamics in the inertial range are, remains at the heart of the turbulence problem. The self-similarity hypothesis of K41 was proven wrong. Many attempts were proposed with limited success [2]. At the MPIDS, we carried out a series of experiments to study the energy cascade at all the scales involved: the energy-containing range, the inertial range, and the dissipative range.

The new Variable Density Turbulence Tunnel (VDTT, see Fig. 3.1, top) produces a wide inertial range, or a wide separation between the energy-containing scales $L$ and the dissipative scales $\eta$. It achieves this by circulating gases (e.g. air or sulfur hexafluoride, SF$_6$) pressurized up to 15 bar [3]. With a classical grid of crossed bars in the VDTT, we produced Taylor-microscale based Reynolds numbers, $R_\lambda$, up to about 1800. Here, $u$ is the fluctuating velocity, $\lambda$ the Taylor microscale, and $\nu$ the kinematic viscosity. Such high Reynolds numbers are associated with very wide scale separation (see Fig. 3.1, bottom) and make the VDTT an ideal test bed to revisit long-standing questions whose answers are usually obscured by small inertial ranges.

One such question concerns the rate at which the total kinetic energy in a turbulent flow dissipates when it is left freely to decay. Even in the simplest case of homogeneous and isotropic turbulence, competing theories have been proposed and different experiments have given different answers [4]. Because the experiments were confined to low Reynolds numbers, the question remained unsettled. In the VDTT, we reached $R_\lambda$ higher by an order of magnitude than in any previous, systematic study. We found no Reynolds number dependence,
as shown in Fig. 3.2, which challenges some arguments that different decay laws would appear at high Reynolds numbers.

The turbulence in the VDTT is nearly isotropic, but what if it were anisotropic, as are most flows in nature? To answer this question, we let turbulence decay from various prescribed anisotropic states in a “soccer ball” apparatus [5], and found that the anisotropy decayed much more slowly than the energy.

The cascade of energy from large to small scales can produce power-law scaling in the statistics of the velocity differences, which implies similarity in the dynamics at different scales and is supported by an exact theoretical prediction for the third moment of velocity differences [1]. It is generally believed that scaling occurs for all moments at sufficiently high Reynolds numbers. Surprisingly, we did not observe scaling from measurements of velocity differences in the VDTT, even at the highest Reynolds numbers. Instead, the data show that power-law scaling was approached only algebraically with increasing $R_\lambda$, and that it arises only locally, not over a broad range of scales. It was possible, however, to observe relative scaling between the moments of velocity-differences of different orders, a phenomenon called “Extended Self-Similarity (ESS)” [6]. The unique capabilities of the VDTT allowed us to measure with great precision the scaling of several even-order moments relative to the third, which is the only moment with known exact scaling. As evident from Figure 3.3, the relative scaling exponents were constant over a wide range of $R_\lambda$, showcasing their universality and reproducibility.

Compared to turbulence under constant forcing, much more of the energy cascade can be studied by purposely varying the external forcing and observing the response of the turbulence. In one experiment, we abruptly change the energy injection by suddenly increasing or decreasing the rotation speed of the propellers that stir the water flow in an icosahedron-shaped container (the Lagrangian Exploration Module, see Figure 3.4). Some preliminary results of the response of turbulence to this Heaviside-function-like perturbation are shown in Figure 3.5, from which we see an overshoot of the turbulence kinetic energy, followed by a slow decay to the corresponding steady state. The transient process lasts for many large-eddy turnover times, in contrast to the estimate of a few turnover times from the usual scaling argument. Moreover, our measurements show that turbulence at different length scales responded differently to the change of large-scale forcing. As
Figure 3.5: Left: Response of turbulence kinetic energy (symbols) to external forcing (dashed line). Right: Response of the turbulence at different scales, measured by the instantaneous second moments of the velocity differences as a function of scale \( r \), normalized by that at the initial state \( (t < 0) \).

we are collecting more statistics from experiments, the scatter of the data will reduce to reveal the details of the scale-dependent response, precisely the information needed to understand the energy cascade.

In another experiment we use a new “active grid” with many movable flaps in an open-circuit air tunnel to slowly modulate the intensity of the turbulence by changing the amplitude of the flap agitation. We find that the inertial-range scaling coefficients for the structure functions of various orders are determined by the amplitude of the modulation, which explains the non-universality of the scaling coefficients and will help to build more accurate turbulence models.

From the Lagrangian point of view, the cascade of energy to smaller scales leads to the short-time decrease of the relative velocity between two tracer particles in turbulence, which in turn causes asymmetry between the forward and backward relative dispersions of two tracer particles. This is reported in detail in Section 3.2 of this report, where we also discuss our recent attempts to understand the physical implications of energy dissipation for single-particle statistics.

The energy cascade changes when long-chain polymers are added into the flow. Through stretching and coil-back, polymers can extract turbulence fluctuation energy from certain scales and distribute it back to the flow at other scales. The seminal work by Tabor and de Gennes [7] proposes that the effect of polymers is captured by a length-scale at which the elastic energy stored in polymers balances the turbulence kinetic energy. This “energy-balance” theory explains some experimental observations such as the concentration dependence, but quantitative tests with experiments have not been reported. In our recent work [8], we suggest that it is not the balance of the energy itself, but the energy flux, that determines the scale below which polymer effects are dominant. Predictions from this “energy-flux balance” theory agree well with experimental data (see Figure 3.6). Further implications of the theory, such as the critical concentration, are under investigation.

3.2 LAGRANGIAN PERSPECTIVE OF TURBULENCE

E. Bodenschatz, J. Mutschall, S. Schütz, H. Wu, H. Xu
G. Falkovich (WIS, Israel), N. T. Ouellette (Yale, USA),
A. Pumir (ENS-Lyon, France), M. Wilczek (Johns Hopkins U., USA)
L. Biferale (U. Roma “Tor Vergata”, IT), G. Boffetta (U. Turino, IT),
A. S. Lanotte (ISAC, IT), F. Nicolas, M. Shats, H. Xia (ANU, AUS),
W. Pesch (U. Bayreuth, DE), F. Toschi (TU Einhoven, NE)

When studying a fluid flow, we, the observer, often stand aside and
examine the flow as it passes by. This Eulerian view is the prevailing
method in fluid mechanics due to the well-developed tools for analyz-
ing continuum fields. It is sometimes, however, desirable to plunge into
the fluid and observe the flow while moving with it. This Lagrangian
view has been proposed since the beginning of fluid dynamics and was
shown almost a century ago to be the natural choice for the study of
turbulent dispersion and mixing. It is however only very recently that
the breakthrough in theoretical understanding [1, 2] and the advance
in experimental technique [3] drew broad attention to the Lagrangian
approach for turbulence research. At the MPIDS, we study turbulence
from the Lagrangian perspective by following tracer particles moving
and spinning in turbulent flows.

The Lagrangian aspects of turbulence have been probed mostly
through the statistics of the temporal velocity increments of a fluid par-
ticle, $\delta V = V(t + \tau) - V(t)$. The probability density functions (PDFs)
of $\delta V$ were found to be not self-similar when the time-lag $\tau$ was in
the intermediate interval between the small, Kolmogorov time, $\tau_K$, and
the large, correlation time, $T_E$. In particular, the PDFs, $P(\delta V)$, at
small $\tau$ deviate strongly from the nearly Gaussian PDFs of $\delta V$ at large
time-lags. Previous studies, mainly phenomenology-based, connected
this “Lagrangian intermittency” with the interaction between small
and large scales. Using the fine-grained-PDF approach, we derived a
Liouville equation for $P(\delta V)$, which showed that the evolution of
$P(\delta V)$ is controlled by an “intermittency generating function” whose
key ingredient is the mean conditional acceleration at given values of
the velocity increments [4]. This finding thus clearly revealed how a
small-scale quantity (acceleration) interacted with a larger-scale quan-
tity (velocity increments) to produce intermittency. Interestingly, data
from experiments and direct numerical simulations (DNS) showed
that while the PDFs of $\delta V$ were not self-similar for different $\tau$, the
underlying driving forces for the change of the PDFs, the intermittency
generating functions, were approximately self-similar (Figure 3.7).

At present, most work on the statistics of $\delta V$ has used the analogy
with the spatial velocity difference in the Eulerian frame. Based on
K41-type universality hypotheses, the statistics of $\delta V$ were expected
to depend only upon the time-lag, $\tau$, and the energy dissipation rate, $\epsilon$, when
there is a wide separation between the largest and the smallest
time scales, i.e., when $T_E/\tau_K \gg 1$. With the postulation that the mo-
ments of $\delta V$ possess power-law scaling with $\tau$ in this intermediate
time-lag range, dimensional arguments led to predictions of the scaling

![Figure 3.7: (a) The PDFs of normalized Lagrangian velocity increments, $v = \delta V/\sigma$, for dif-
cerent time-lags $\tau$ are not self-
similar, where $\sigma = \langle \delta V^2 \rangle^{1/2}$. For clarity, the PDFs are shifted
vertically. The time-lags shown
are, from top to bottom, in-
creasing from 0 to $T_E/2$. The
dashed lines are correspond-
ing model predictions [4].
(b) The non-dimensionalized,
intermittency-generating func-
tions collapse for time-lags
between $2\tau_K$ and $T_E/2$.]

![Figure 3.8: The kinetic energy $E(t)$ following a tracer particle
in a turbulent water flow. Dur-
ing the event with large change
of $E(t)$ (blow-up plot), the par-
ticle lost kinetic energy faster
than it gained energy.]

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exponents. In particular, it was believed that the second-order moment \( \langle \delta^2 V \rangle \) scales as \( \epsilon \tau \), which is special because linear dependence on \( \epsilon \) means that intermittency would not affect the scaling and hence \( \langle \delta^2 V \rangle \) could be used as a reference to determine the scaling of other moments. Experimental and numerical data available to date (up to \( R_1 \geq 10^3 \)), however, do not support such a linear scaling. Our recent examination raised doubts about this dimensional argument [5]. A notable limitation of the expected scaling \( \langle \delta^2 V \rangle \sim \epsilon \tau \) is that \( \langle \delta^2 V \rangle \) remains the same when the “arrow of time” is flipped, while \( \epsilon \) must change sign under such transformation as the energy dissipation signifies the irreversibility of the flow.

Surprisingly, we found that, unlike the velocity increments, the large changes of kinetic energy following a particle trajectory typically have the feature of “slow gain but fast loss” (see Figure 3.8 for an example), a phenomenon resembling driving in dense traffic. The temporal increments of kinetic energy, \( W(\tau) = E(t + \tau) - E(t) \), are therefore sensitive to the flipping of the arrow of time. More specifically, we found that for all of the turbulent flows analyzed, including a wide variety of experiments and DNS, the third moments of \( W(\tau) \) were negative for \( 0 < \tau < T_e \) (Figure 3.9(a)), which suggested that even single-time statistics, (the rate of change of the kinetic energy, or the instantaneous power \( p = \frac{dE}{dt} = \frac{dW}{dt} \)), could also detect the arrow of time. As shown in Figure 3.9(b), the PDFs of \( p \) were negatively skewed. For large magnitudes of \( p \), the probabilities for negative \( p \) (energy loss) were higher than for positive \( p \) (energy gaining). The non-dimensionalized third moment of power, \( \langle p^3 \rangle / \epsilon^3 \), could therefore be used as a measure of irreversibility [6].

A fundamental question to ask regarding single-particle Lagrangian statistics is how are single-particle statistics connected with the energy dissipation rate (energy flux through spatial scales)? The casual dimensional argument is most-likely not justified. Is there another deep relation, similar to the 4/5th-law for Eulerian quantities? Perhaps involving energy increments? This is a challenging but very important question and is currently under active research.

In contrast, there exists an exact relation between Lagrangian statistics involving multiple particles and the energy dissipation rate: The rate of change of the relative velocity between two fluid particles is given by \( \frac{d}{dt} \langle (V_1(t) - V_2(t))^2 \rangle = -4\epsilon \), when the distance between the two particles, 1 and 2, is in the inertial range [2, 7, 8]. This is because two particles already provide access to energy flux through scales. This flux law dictates that in three-dimensional turbulence, on average, two fluid particles will initially lose their energy for separation, in sharp contradiction to Richardson’s postulation on relative dispersion, which requires particles to gain separation energy. This partially explains why it is so difficult to observe Richardson dispersion, even in flows with very large Reynolds numbers. Another interesting implication is that the relative dispersion is faster if viewed backwards in time than forwards in time, which was confirmed by our experimental data.

Unexpectedly, we observed Richardson’s \( t^3 \) law when Brownian particles with small diffusivity were added into a simulated large-
aspect-ratio Rayleigh-Bénard convective flow that was driven slightly above the onset of instability [9] (see Figure 3.10). This $r^3$ law was found in both spiral-defect-chaos and in straight-roll-convections, and independent of the diffusivity of the particles. This somewhat surprising finding points out that Richardson’s conjecture assumes that two particles in turbulence experience δ-correlated relative acceleration in the inertial range, which in reality violates a simple kinematic constraint due to stationarity.

While two-particle statistics provided access to energy flux, following a group of particles allowed us to examine shape deformation in the Lagrangian frame, which is inherently tied to the inertial range dynamics. For example, from the evolution of an initially isotropic tetrahedron formed by four tracers, we could identify the “vortex stretching” mechanism, the growth of the vorticity vector and its aligning with the largest stretching direction (Figure 3.11). Vortex stretching has long been considered the most important mechanism by which energy cascades down to smaller scales. Eulerian measurements showed, however, that at any instant time, vorticity aligned preferentially with the weakly stretching direction. The Lagrangian perspective helped resolve this puzzle by showing that vorticity was indeed enhanced by stretching and turned to align with the largest stretching direction. However, during this process, the largest stretching direction turned away so that the vorticity always lagged behind. Therefore, at any instant in time, vorticity was not aligned with the largest stretching [10, 11]. This is a clear example of where the Lagrangian perspective provides a better understanding than the Eulerian one.

All Lagrangian studies to date have concerned only the velocities following fluid tracers. By measuring how tracer particles spin, we are able to follow vorticity along tracer trajectories. This direct vorticity measurement technique uses the “Vorticity Optical Probe (VOP)” principle [12] as shown in Figure 3.12. An incident laser beam is reflected by a micron-sized mirror embedded in a tracer particle that spins in turbulence. The reflected beam then rotates and leaves a trajectory on the image plane of a camera, which can be used to calculate the direction and the speed of the rotation of the mirror and hence the vorticity. Our initial test in a Taylor-Couette flow demonstrated its feasibility. We are now extending the technique to simultaneously measure vorticity and velocity along the same particle trajectory, which would provide unprecedented information for the study of Lagrangian statistics.

3.3 TURBULENT THERMAL CONVECTION

G. Ahlers, E. Bodenschatz, H. Nobach, D. Funfschilling (CNRS, France), D.P.M. van Gils
X. He, F. Winkel, S. Grossmann (University of Marburg), S. Horn (DLR IAS), D. Lohse (University of Twente, Netherlands), O. Shishkina (DLR IAS), A. Tilgner (University of Göttingen), C. Wagner (DLR IAS)

Turbulent convection in a fluid heated from below and cooled from above (Rayleigh–Bénard convection, RBC) has been at the center of scientific inquiry for a long time [1]. RBC serves as a model system for buoyancy-driven convection as found in numerous astrophysical, geophysical, atmospheric, and industrial processes. One important question is the dependence of the heat transport, the Nusselt number $Nu$, on the dimensionless temperature difference, the Rayleigh number $Ra$.

Well past the onset of turbulence and up to $Ra \approx 10^{11}$, basically all experiments and numerical simulations reveal a similar $Nu(Ra)$ scaling amongst one another. In this regime, the bulk has transitioned into turbulence but the viscous and thermal boundary layers (BLs) are still of a laminar, Prandtl-Blasius type [2]. Here, the heat transport is limited by the thermal and viscous diffusivities of the BLs. This is regarded as the ‘classical’ state.

As originally predicted by Kraichnan [3], a transition should happen at large $Ra$ where the BLs will also have transitioned into turbulence due to the increasing amount of shear induced by either the large-scale circulation or the turbulent fluctuations inside of the bulk [2]. This state is regarded as the ‘ultimate’ or ‘Kraichnan’ state: The heat transport is no longer dominated by the BLs but by the convection occurring inside of the bulk. The $Nu(Ra)$ scaling in the ultimate regime is predicted to reach an asymptotic dependence, $Nu \propto Ra^{1/2}$, times logarithmic corrections due to viscous sublayers [2, 3].

Understanding the ultimate state is relevant in order to validate the extrapolation of laboratory measurements to geo-/astrophysically relevant ranges. Interestingly, in the regime $Ra > 10^{11}$, many experiments reveal very different $Nu(Ra)$ scalings and different $Ra$ numbers where a transition takes place [2]. To elucidate this we performed experiments in the high pressure convection facility at the MPIEDS.

The facility comprises of a general-purpose pressure vessel, known as the "U-Boot" of Göttingen, which can be filled with sulfur hexafluoride ($SF_6$) at pressures up to 19 bars with a nearly constant Prandtl number of 0.8 (see figure 3.13). The vessel can house two different RBC cells alongside each other. They have aspect ratios $\Gamma = D/L = 1.00$ and $\Gamma = 0.50$, both with a diameter $D = 1.12$ m and with a length of, respectively, $L = 1.12$ and $L = 2.24$ m. The maximum Rayleigh numbers that were achieved with these cells at near Oberbeck-Boussinesq conditions [9] are, respectively, $Ra \approx 2 \times 10^{14}$ and $Ra \approx 10^{15}$.

The experimental results obtained from both RBC cells are summarized here. We first focus on the global $Nu(Ra)$ scaling and define a local effective exponent, $Nu \propto Ra^{\gamma_{\text{eff}}}$. For $\Gamma = 0.50$, we reported...
\( \gamma_{\text{eff}} = 0.312 \pm 0.002 \) in the classical range at \( Ra \leq Ra^*_1 \simeq 1.5 \times 10^{13} \) (see figure 3.14 and [4, 5]). Likewise for \( \Gamma = 1.00 \) in the classical range we found \( \gamma_{\text{eff}} = 0.321 \pm 0.002 \) [6]. These scaling exponents are close to one another, are slightly dependent upon the aspect ratio and are in good agreement with other experiments, direct numerical simulations and the Grossmann and Lohse model [2]. Remarkably, a transition sets in for both cells above a nearly identical value \( Ra \gtrsim Ra^*_1 \), viz. \( \gamma_{\text{eff}} \) starts to increase. For \( \Gamma = 0.50 \) we were able to increase \( Ra \) well enough to recover a new, well-defined local scaling exponent, \( \gamma_{\text{eff}} \simeq 0.38 \) at \( Ra \gtrsim Ra^*_2 \simeq 5 \times 10^{14} \). This effective exponent is not only predicted as the ultimate-state scaling for the investigated control parameters, but the \( Ra \) number at which the ultimate-state transition should occur also matches [2, 3]. This convinces us that we have successfully entered the ultimate state of RBC in the lab. The range \( Ra^*_1 < Ra < Ra^*_2 \) appears to be a transitional range from the classical state towards the ultimate state. The transitions found by us are, within the resolution of the data, independent of \( \Gamma \). We believe that a \( \Gamma \)-independent \( Ra^*_1 \) suggests that the BL shear-transition is induced by fluctuations on a scale less than the sample dimensions rather than by a global \( \Gamma \)-dependent flow mode. Above \( Ra^*_1 \), any difference between the heat transport for the two \( \Gamma \) values is too small to be resolved, suggesting a universal aspect of the ultimate-state transition and properties [6].

In [4] we additionally determined the effective Reynolds number, \( Re_{\text{eff}} \), of the \( \Gamma = 0.50 \) cell based on local temperature time series measurements. By assuming that temperature is a passive scalar and by using the elliptical approximation [7] we were able to determine \( V_{\text{eff}} = \sqrt{U^2 + V^2} \) and the corresponding \( Re_{\text{eff}} = V_{\text{eff}}L/\nu \). Here, \( U \) is the time-averaged vertical velocity component, \( V \) is the root-mean-square of the velocity fluctuations and \( \nu \) is the kinematic viscosity. Our data showed that \( Re_{\text{eff}} \) is dominated by the contribution in \( V \). Furthermore, we examined the local effective scaling, \( Re_{\text{eff}} \propto Ra^5 \) (see figure 3.15). For \( Ra \leq Ra^*_1 \), the \( Re_{\text{eff}} \) results are consistent with expectations for classical RBC [1, 2]. For \( Ra \geq Ra^*_2 \), the data matches well with a pure power law with an exponent of 1/2 and no logarithmic corrections as predicted by Grossmann and Lohse [2]. For the range \( Ra^*_1 < Ra < Ra^*_2 \), complex behavior associated with the transition from the classical to the ultimate state was observed for \( Re_{\text{eff}} \), analogously to \( Nu \). In this range the \( Re_{\text{eff}} \) values correspond to estimated shear Reynolds numbers ranging from about 200 to 400. These values are consistent with the expected transition to turbulent BLs in shear flows. Thus, the \( Re_{\text{eff}} \) results also support our view that we have found and characterized the transition to the ultimate (asymptotic) state of RBC.

For both the classical and the ultimate state, we found by experiment [8] that beyond a thin BL or thermal sublayer the temperature \( T(z) \) and its root-mean-square fluctuation vary logarithmically as a function of the distance \( z \) from the bottom plate. Specifically, the temperature \( T(z) \) can be fitted well by the function \( \Theta(z) = A \times \ln(z/L) + B \), as is shown in figure 3.16. Here, \( \Theta \) is the deviation of the local temperature from the sample mean temperature, scaled by the applied temperature difference. For the classical state at \( Ra \leq 2 \times 10^{12} \), these results were confirmed.
and extended by direct numerical simulation. To our knowledge there is no theory at present that predicts a logarithmic temperature profile in the bulk for $Ra < Ra_c$. For the ultimate state at $Ra > Ra_c$ these findings agree with the logarithmic dependence predicted by [2] as a result of the BLs having transitioned into turbulence and extending vertically throughout the entire sample. Thus, there is no ‘bulk’ in the same sense as there is for the classical state. Global and local measurements on a $\Gamma = 0.33$ cell at up to $Ra = 4 \times 10^{15}$ are underway, which should allow us to probe deeper into the ultimate regime.

Global rotation is common for geo- and astrophysical situations and we will approach this in the lab by rapidly rotating the RBC cells about their vertical axes. Depending on the $Ra$ number and the overall rotation strength, different regimes can be entered, each with unique overall heat transport and complex flow dynamics. Ultimately, we wish to probe the geostrophic turbulent regime, important in geo- and astrophysical contexts. This regime is poorly understood especially at large Rayleigh numbers. The construction of a rotating table (see Figure 3.17) onto which the RBC cells will be put is finished and the rotating RBC facility is currently being tested. In order to house the rotating table with the 2-meter-high RBC sample inside the U-Boot it was necessary to extend the height of the dome by $1.8 \text{ m}$ (see Figure 3.18).

Recently, we also performed moist turbulent RBC experiments in a two-phase binary gas mixture composed of SF$_6$ and He at $Ra$ numbers of up to $10^8$ in a small, $\Gamma = 3.0$ cell slightly below the critical point, at a pressure of $54 \text{ bar}$. The liquid phase of SF$_6$ fills about half of the convection cell and the gas space is He rich. After a temperature difference of 0.5 K is applied, we observe clouds of nucleating SF$_6$ droplets in a thin layer above the liquid phase of SF$_6$ (see figure 3.19). The SF$_6$ clouds are driven by the turbulent flow in the gaseous phase of the binary mixture. In addition, we observe a wetting instability at the cold top plate, where the SF$_6$ vapor condenses in a hexagonal array of dimples and drops. We are currently exploring the origin of the clouds and the nature of the droplet instability.

Although turbulence is relevant to a multitude of processes throughout nature, our conceptual understanding of this phenomenon is very limited. The equations describing fluid motion, the Navier Stokes equations, have been known for a long time. However, for the vast majority of situations we are unable to solve these equations analytically. The problem stems from the nonlinear nature of these partial differential equations and as common for nonlinear systems, at large amplitudes the dynamics are extremely complex and chaotic. Most studies of turbulence attempt a statistical description of the dynamics at very large Reynolds numbers (Re). Our approach is different: we attempt to obtain a more fundamental understanding of the structures underlying turbulence in parameter regimes where turbulence first occurs. Our expectation is that the dynamics here are less complex and possibly sufficiently low-dimensional to be able to identify the structures (unstable solutions) underpinning the turbulent dynamics. The main focus here is on elucidating the temporal complexity of turbulence in pipe flow at low Re.
at fairly low Reynolds numbers. Due to their instability, individual solutions can not persist in practical flows and if at all can only be expected to show up transiently. In analogy to other chaotic systems, such unstable states can form a complex entity [1] (i.e., a turbulent repeller) through further bifurcations and entanglement, which gives rise to chaotic motion. Indeed, such unstable solutions have been found numerically for a variety of flows including that of a fluid down a straight pipe [1] (see Figure 7.1, bottom row). Our earlier experiments [7] (Figure 7.1, top row) have given a first indication that these unstable states can be observed transiently in a turbulent flow and therefore that they are indeed relevant to fluid turbulence. The formation of a chaotic repeller is also supported by our observation that the decay of spots of turbulence is a memoryless process [2, 3, 5]. Such behavior is well known from lower-dimensional systems where chaotic dynamics are observed for very long times until the system suddenly escapes to a local attractor in a different part of the phase space (here, the laminar flow).

Figure 3.21: Axial vorticity isosurfaces. (a) The experimental measurement and (b) the traveling wave converged as a result of seeding the experimental snapshot to the Newton iteration. A second experimental snapshot is shown in (c), together with the traveling wave converged from it in (d) (from [3]).

**Edge states in decaying turbulence**

In this project we focus on decaying turbulence, testing whether clearer visits to unstable solutions occur in fading turbulence. The investigation is limited to low Reynolds numbers (here, Re=1900). Indeed, we observe that approximately 20 diameters downstream from where the decay sets in, flow fields frequently show a simple, one-fold symmetry with two high-speed streaks close to the wall, separated by one low-speed region.
and corresponding streamwise vortices in between. This structure is reminiscent to a particular state that has been identified recently in numerical simulations of pipe flow, the so-called ‘edge state’ [5]. The important feature of this state is that it separates initial conditions that become turbulent from those which go directly to the laminar state. The edge state itself is chaotic and it has been shown that imbedded in it are several unstable travelling wave solutions of similar symmetry. As it marks the border between the laminar and turbulent flows, it is plausible that it may play an important role during the transition to and from turbulence. Using experimentally measured velocity fields we have been able to directly converge the flow fields (Figure 7.2) from the experiment to invariant travelling wave solutions [3] which are known to be embedded in the laminar turbulent edge. This is the first direct link obtained between turbulent flow fields in laboratory experiments and invariant numerical solutions of the Navier-Stokes equations.

![Figure 3.22: First observation of localized invariant periodic orbits for pipe flow. (a) Streak isosurfaces of a turbulent puff. (b) Lower branch localized periodic orbit. (c) Upper branch solution (from [8]).](image)

**Localized periodic orbits and the onset of chaotic motion**

While all numerical solutions observed so far are periodic in the streamwise direction, in experiments and DNS with large domains, turbulence in the transitional regime is spatially localized. It is hence plausible to assume that those invariant solutions, acting as building blocks of turbulent puffs, must also be streamwise localized. We carried out direct numerical simulations in a symmetric subspace (2-fold and mirror symmetric) for pipe flow [8] to try to find some such streamwise localized solutions. When identifying the edge between turbulent and laminar motion we indeed observed that the edge is not only localised but also corresponds to a periodic orbit (Figure 7.3) [8]. By following this solution to smaller Reynolds numbers we could identify the saddle node bifurcation (Figure 3.23) where this solutions first arises and identify the upper-branch solution, which is stable in the subspace (the lower branch edge state has a single unstable direction). With increasing Re, the upper branch was found to undergo a secondary Hopf bifurcation and a further instability to chaos. At slightly higher
Re, the chaotic attractor underwent a boundary crisis to transient chaos (see Figure 3.23), giving rise to turbulent puffs of finite lifetime. We could hence identify how the turbulent repeller is first formed for this subspace of pipe flow. While turbulence is likely to arise from other solutions for full space, it is likely that a qualitatively similar sequence of events also prevails there.

Figure 3.23: A saddle-node bifurcation gives rise to localized RPOs at $Re = 1430$: UB is stable up to $Re = 1530$, where it undergoes a supercritical Neimark-Sacker bifurcation, leading to a relative 2 torus. Subsequently, the torus breaks up to chaos at $Re = 1540$ and the chaos becomes transient at $Re = 1545$. The bars show the variation of energy over a period (Newton-converged LB and UB) and over long runs (torus and chaos). LB has a single unstable direction and is the edge state (from [8]).

To understand turbulence in a fundamental sense and to make predictions useful in real-world applications, one needs not only to observe turbulence at high Reynolds numbers, but also to control the turbulence. As in any experiment, control means not only the ability to fix the conditions of the experiment, so that precise measurements are possible, but also the ability to adjust the conditions in various ways, so that dependencies can be uncovered. The facilities at the MPIDS make it possible not only to generate turbulence with the highest Reynolds numbers yet possible under laboratory conditions, but to do so with unprecedented control. Matching our achievements in the control of turbulent flows is our advancement of measurement technologies. We have even adapted some of these to record in field experiments the full richness of natural flows. In this section, we describe our various experimental facilities and their unique capabilities.

The Variable Density Turbulence Tunnel (VDTT), see Fig. 3.24 and Ch. 3.1, is a recirculating pressurized wind tunnel that consists of two measurement sections with cross-sectional areas of 1.9 m$^2$ and lengths of 9 m and 7 m. The chief merits of the VDTT are that it produces high Reynolds number flows and stable operating conditions. Furthermore, the Reynolds number is finely adjustable by changing the pressure of the gas in the tunnel, usually sulfur hexafluoride ($\text{SF}_6$). In its current configuration, a grid of crossed bars generates Reynolds numbers ($\text{Re}_\lambda$) up to 1700, much higher than in any comparable facility.

Yet higher Reynolds numbers and increased control will be possible in the VDTT once we install a novel “active grid” with position-controlled flaps that agitate the flow. Uniquely, our active grid has a large number of degrees of freedom (129). Among other attributes, the homogeneity, isotropy, and intensity of the turbulent fluctuations can be set by programming the motions of the flaps appropriately. Once in the VDTT, we predict that we will reach Reynolds numbers up to 8000. This grid is presently operating in the Prandtl tunnel, an open-circuit wind tunnel dating to the 1930’s.

The High Pressure Convection Facility (HPCF) utilizes a general-purpose pressure vessel called the “U-Boot”, see Fig. 3.25, which is 5.3 m long and has a diameter of 2.5 m. We precisely control both the temperature and the pressure in the vessel. Within the vessel are two cylindrical Rayleigh–Bénard (RB) experiments (diameter 1.1 m, heights 2.2 m and 1.1 m) that reach Rayleigh numbers as high as $10^{15}$, as discussed in Ch. 3.3. Uniquely, a large range of Rayleigh numbers can be accessed in the facility while holding the Prandtl number fixed. Recently, we constructed a rotating table for the RB cells, which allows for the study of turbulent heat convection under the influence of rotation.
The “Cigar” is a general-purpose pressure vessel with a length of 4 m and an inner diameter of 1.5 m, see Fig. 3.26. It contains a free jet powered by a 2 kW ducted fan, which we anticipate will produce Reynolds numbers of several thousand, as high as any free jet yet built.

Two von Kármán mixers generate high Reynolds number turbulent water flows between two counter-rotating baffled disks. One is shown in Fig. 3.27. Because the average displacement of fluid particles near the middle of the mixers is close to zero, their motions can be followed for a long time. The mixers are about a half-meter in diameter, and $R_\lambda$ can be as high as 1200. Large glass windows provide optical access for imaging techniques.

Theoretical knowledge is most developed for turbulence that is stationary and isotropic. But real flows are neither. Two novel “soccer ball” apparatuses, see Fig. 3.28, make it possible for the first time to control the degree to which a turbulent flow is anisotropic. The soccer balls are about one meter in diameter. In one of them, we produce cloud-like conditions, as discussed in Ch. 4.14. A second apparatus called the LEM, see Ch. 3.1, has a similar geometry. We use it to study the dynamic response of turbulence to changes in forcing conditions.

The facilities make use of state-of-the-art three-dimensional Lagrangian particle tracking (LPT) technologies that we have developed in-house. The technology relies on multiple movie cameras viewing the same particles from different angles, with megapixel resolution and kilohertz frame rates. We also employ a Dantec hot-wire system in conjunction with nano-fabricated hot-wires from Princeton University, a LaVision tomographic particle image velocimetry system, and a TSI laser Doppler velocimetry and particle sizing system. All of this equipment is compatible with pressures up to 15 bar. Some of these techniques require substantial light, which we typically produce with Nd:YAG or argon-ion lasers. The systems all produce data at rates that necessitate high-performance computing and storage clusters, which we maintain in-house.

Another large-scale turbulence facility is being installed on top of the Zugspitze, Germany’s highest mountain, in order to investigate the dynamics of water droplets in warm clouds in natura. The particle-turbulence interactions in clouds play an important role in their evolution, and is one of the uncertainties that most limit our ability to predict climate change. In addition to standard fluid dynamical and meteorological measurements (wind velocity, droplet size and velocity, temperature, water vapor content, etc.), the unique apparatus of this facility is the “see-saw”, a platform that moves high-speed cameras at the mean wind speed to track the full three-dimensional motion of cloud droplets. The linear motors in the seesaw can drive a payload of 350 kg up to 7.5 m/s. The seesaw is currently under testing at the MPIDS (Fig. 3.29) and is planned to be installed on the roof of the Umweltsforschungsstation Schneefernerhaus on top of the Zugspitze at an altitude of 2700 m (Fig. 3.30). A similar such moving platform is also under development for installation inside the test sections of the VDTT (see above).
3.6 LOCALIZED STRUCTURES AND EMERGENT DYNAMICS IN ACTIVE SYSTEMS

A. Gopinath, P. Subramanian, T. M. Schneider

Generalized hydrodynamic theory can be employed to describe the dynamics of complex fluids such as polymers and gels. This approach can also be extended to describe systems with non-vanishing energy flux due to internal sources. Such active fluids are intrinsically out of equilibrium. A subclass among them are active polar fluids, which consist microscopically of elongated, self-propelled particles. A wide class of physical systems, ranging from the cytoskeleton of a living cell to herds of animals and flocks of birds, fall under this generic paradigm [1, 2, 3].

We investigate pattern formation in such polar active systems using a phenomenological mean-field model based on symmetry principles. In this reduced-dimensional approximation, the state of the system is described in terms of a vector order parameter, the polarity field, such that behaviors like swarming/flocking or macroscopic flow are identified through spontaneous symmetry breaking. Furthermore, dissipation is accounted for by treating the fluid as a momentum sink. In this modeling approach, the hydrodynamic equations for the polarization and the density (a conserved scalar quantity) serve to track the dynamics of the active fluid. We find that three physical parameters dominate the dynamics of the system, the mean propulsion speed, \( w_0 \), of the particles, the mean density, \( \rho_0 \), which measures their response to fluctuations, and the active elasticity, \( \lambda \), which quantifies interactions between individual particles. Using linear and weakly nonlinear analysis [4], we have demonstrated the existence of two primary persistent stable structures: convective solitary waves and localized asters.

The solitary wave structures arise from a convective instability dominated by the interplay between the density and polarity even in the absence of non-linear elastic interactions. In these waves, the polarity and density are in phase and the waves consist of ordered, high-density regions moving through a disordered low-density medium. This is reminiscent of the entry of a liquid phase into an isotropic gas phase. The aster is a localized stationary non-linear structure that does not exist unless active elasticity (the \( \lambda \) term) is present. As shown in Figure 3.6(a), this structure consists of a renormalized core defect with the polarity field pointing radially inward (the polarity exhibits a clear separation of length scales). The density is however maximum at the center of the core and decays radially. The inward flow due to polarity is balanced by the flow outward due to diffusion and maintains the structure. When self propulsion becomes large enough, the aster becomes unstable and yields to the solitary wave as seen in Figure 3.6(b).

The example discussed above represents a limit where the activity and elasticity come from the polar particles and their interaction. The suspension is itself comprised of multiple, monopolar particles. In

![Image](image-url)

Figure 3.31: (a) The structure of a localized aster in an active polar fluid. Asters occur when active elasticity dominates propulsion speed. Radial density (color map) and polarity (arrows) profiles are shown. Inset: The polarity field is symmetric about the center of the aster and exhibits a clear inner core (b). Symmetry breaking from asters to waves in an active polar fluid, visualized in terms of maximum density (solid circles) and maximum polarity (crosses). As self-propulsion speed increases, the peak density and peak polarity of the aster increases. The subsequent sharp decrease is the signature of an aster to wave transition.
the other limit, one may ask what happens if a number of these polar particles are attached via elastic constraints so as to force them to move together. As the next step, we consider such a composite filament comprised of connected polar particles constrained at one end. The geometric constraint coupled with the polarity results in an active compressive deforming force density, \( f_p \), that tends to buckle the filament. Motivated by the experimental actin assays, we study the emergent dynamics of this animated filament constrained to move in a plane.

We begin by considering the dynamics when the composite filament of length \( \ell \) with bending stiffness \( \kappa \) is anchored at one end - the head. We consider a generalized boundary with the head constrained by a torsional spring of stiffness \( C \). Thus the limit \( C \to \infty \) yields a clamped head, while \( C = 0 \) corresponds to a frictionless pivot. Linear stability analysis of the equations for the deformation of this forced filament indicates two interesting instabilities (Figure 3.32). Positive values for the real part of eigenvalue \( Re_d \) indicate the linear instability in Figure 3.32(a) for increasing dimensionless force \( \beta \equiv f_p \ell^3 / \kappa \). For small forcing the filament remains straight. As \( f_p \) increases, a clamped filament becomes unstable to an oscillatory instability beyond a critical value of \( f_p \), with well-defined frequencies at onset. A pivoted filament, however, exhibits a divergent instability, the divergence being cut off by nonlinear terms to eventually yield coiled, steadily rotating shapes. We have studied the nature of these critical points. Specifically, for finite \( C > 0 \), we observe the existence of a flutter boundary. For follower loads below the limiting threshold, oscillatory instabilities are supported similarly to a clamped end. When the follower forces exceed this limit, the end behaves as a purely pivoted end condition with a strictly divergent instability with no oscillations [5].

Modifying the end constraint and instead affixing the composite filament to a larger bead (generating thus a larger viscous drag) allows us to build an active swimmer. We have simulated the motion of such an over-damped swimmer in a viscous fluid and find that tuning the properties, geometric as well as material of the swimmer allows us to achieve not only sustained propulsion but also various swimming gaits (Figure 3.32b). While the most efficient form of the propulsion arises from a balance between isotropic viscous dissipation due to the head and the buckling activity of the tail, anisotropic friction on the tail dominates for large tail lengths [5].

Our preliminary work thus sets the stage for a more detailed exploration of the complex interplay between intrinsic activity, elasticity, and response to extrinsic fields in low-Reynolds number swimmers. We aim to ultimately identify efficient gaits as observed in biological organisms.

3.7 ANOMALOUS VELOCITY DISTRIBUTIONS IN ACTIVE BROWNIAN SUSPENSIONS

A. Fiege, A. Zippelius
B. Vollmayr-Lee (Bucknell)

In recent years, there has been growing interest in so-called active matter, referring to the ability of the constituents to move actively by either extracting energy from the environment or depleting an internal energy depot. Examples are motor proteins, bacterial swimmers or motile cells [1]. Whereas the mechanism that drives the individual active particle has been studied for many years [2, 3, 4], the collective behavior of a large number of individuals has been addressed only recently. Very rich behavior has been observed, ranging from pattern formation and nonequilibrium phase transitions to turbulence [5, 6]. Active particles on mesoscopic to macroscopic scales have also been realized in the form of self-propelled colloids (Janus particles) and vibrated polar granular rods [7]. More generally, granular particles that are driven by random kicks may be considered to be active matter, though with their direction of motion being random.

We have studied a simple model of active particles [8]: hard spheres placed in a fluid with a viscous drag \( \gamma \), that are accelerated at discrete times and undergo elastic collisions. The equation of motion for particle \( i \) reads as

\[
\partial_t \mathbf{v}_i = -\gamma \mathbf{v}_i + \frac{\Delta \mathbf{v}_i}{\Delta t_{\text{coll}}} + \frac{\Delta \mathbf{v}_i}{\Delta f_{\text{Dr}}}.
\]

The driving force is modeled as discrete kicks with amplitude \( \Delta \mathbf{p} = m \Delta \mathbf{v} \) and frequency \( f_{\text{Dr}} \). The components of the kick velocity, e.g. \( \Delta v_x \), are drawn from a Gaussian distribution, \( P(\Delta v_x) \), with zero mean and variance \( \sigma^2 \).

![Figure 3.33: Velocity distributions for volume fraction \( \eta = 0.35, f_{\text{Dr}} = 7.11 \), and several values of \( \beta = \gamma / f_{\text{Dr}} \) = 0.1, 1, 3, 5, 10, taken from [8]. The dashed-dotted line shows the Maxwell-Boltzmann distribution. The coloured solid lines show the first iterative solutions of the single-particle model (see text below) for \( \beta = 3, 5, 10 \).](image)

We have simulated a 3-dimensional system of 2,122,416 monodisperse spheres with volume fractions \( \eta = 0.05 \) and 0.35, using event-driven simulations of hard spheres, generalized to include viscous drag. We have determined that the velocity distribution, \( f(v) \), is dependent upon 3 parameters in the stationary state: \( \gamma, f_{\text{Dr}}, \) and \( \eta \). In Fig. 3.42, we show \( f(v) \) for \( \eta = 0.35 \) and \( f_{\text{Dr}} = \omega_{\text{coll}} \) and various values of the damping constant, \( \gamma \). The curves are labeled by the ratio \( \beta := \gamma / f_{\text{Dr}} \).
Whereas for very small $\beta$ the distribution is approximately Gaussian, we observe increasingly strong deviations for larger $\beta$. Small velocities are highly overpopulated with an indication of a singularity in the limit of large $\beta$. High velocities are overpopulated as well, as compared to the equilibrium Maxwell-Boltzmann distribution. These deviations can be understood intuitively as follows: particles which have not been recently kicked are damped to nearly zero velocity, whereas the recently kicked particles populate the tail.

The main results of our simulations are the following:

- The distribution is independent of volume fraction for the investigated range of $\eta$.
- It is also independent of the ratio of the driving frequency, $f_{Dr}$, to the collision frequency, $\omega_{coll}$; we obtain the same distribution regardless of whether a particle is kicked once or 100 times between collisions.
- Consequently, the distribution is almost exclusively determined by the ratio $\beta = \gamma / f_{Dr}$, even though the model contains the three independent timescales, $\gamma, f_{Dr}$ and $\omega_{coll}$.
- The single-particle velocity distribution is Gaussian only in the limit $\beta \to 0$. The distribution shows increasingly stronger deviations at small and large velocities for increasing $\beta$.
- The distribution seems to develop a singularity at small argument as $\beta \to \infty$.

These observations, in particular the insensitivity to collision rate, have led us to derive an approximate analytical theory for the velocity distribution based on a single-particle model that neglects collisions. The idea of the calculation is the following: we use the single-particle distribution at the beginning of a small time interval, $\Delta t$, as input and compute the resulting single-particle distribution at the end of the interval, taking into account changes of the velocity due to damping and due to random kicks. We then require the two distributions to be the same in the stationary state.

The probability distribution within this single-particle model, $f(v)$, is a function of $\beta = \gamma / f_{Dr}$ only, in agreement with the multi-particle simulation data. In the limit $\beta \to 0$, the stationary distribution of the single-particle model goes to the Maxwell-Boltzmann distribution, as expected for thermal equilibrium. In the limit of large $\beta$, we can identify three regions for $f(v)$:

$$f(v) \approx \begin{cases} 
\frac{e^\beta - 1}{2\sqrt{\pi \beta^3}} & |v| \ll \sigma e^{-\beta} \\
\frac{1}{2\beta |v|} & \sigma e^{-\beta} \ll |v| \ll \sigma \\
\frac{1}{\sqrt{\pi \beta}} \frac{1}{v^2} e^{-v^2/4\beta} & |v| \gg \sigma
\end{cases} \quad (3.2)$$
In Fig. 3.43 we plot the velocity distribution data for $\beta = 10$ and $\beta = 5$ and compare to the analytic expressions (dashed lines) from Eq. (3.2) and their ranges (dotted lines). The three regions are clearly distinguishable and match the simulation data well. Note that the $1/|v|$ region shrinks as $\beta$ decreases.

For intermediate values of $\beta$ we solved the equation for the stationary distribution numerically by iteration, starting from a Maxwell-Boltzmann distribution. The convergence of the iteration process is very fast; there is almost no difference visible between the first three iterations. The iterative solution is compared to the data from simulations for several values of $\beta$ in Fig. 3.42. No deviations can be detected within the scatter of the data. We find similar good agreement for all values of $\beta$.

To conclude, we have shown that Brownian suspensions of interacting particles, subjected to random accelerations, exhibit strongly anomalous velocity distributions. These distributions are largely universal and are well described by the analytical solution of a single particle model. Our approach can be generalised in several ways. Both the simulations as well as the analytical theory can be generalised to other distributions for the kick amplitudes and times. It also of interest to include dissipation in the collisions in order to make closer contact with experiments on granular media. Furthermore we plan to study directed motion, polar particles and rotational degrees of freedom, modeling other swimmers.

3.8 JAMMING OF FRICTIONAL PARTICLES

M. Schröter, M. Neudecker
S. Herminghaus, C. Heussinger (Uni Göttingen),
G. Schröder-Turk (Uni Erlangen)

The shape of the individual particles (spheres, ellipsoids, cubes ...) inside a granular packing influences both the number of inter-particle contacts and their type (such as point contacts or face-to-face contacts). Because contacts are the backbone of the load-bearing force chains, they are fundamental to the mechanical properties of the packing. The contact number is also of prime importance in the jamming paradigm [1] where mechanical properties are expected to scale with the distance to isostaticity (the state where each degree of freedom is exactly blocked once). However, the jamming paradigm has mostly evolved around frictionless spheres. While jamming in frictional systems is controversial on its own, no work at all has been done for particles which allow different types of contacts. Face-to-face, edge-to-face or point contacts will each fix a different amount of constraints, adding another layer of complexity.

In the last three years we tested experimentally the jamming paradigm for tetrahedra (figure 3.37 a and b). We find that even the loosest packings have twice the number of constraints required for isostaticity (Figure 3.37 c). Together with the fact that the contact number depends on the packing protocol, these results pose a serious challenge to the jamming paradigm in its present form [2].

Ongoing work includes packings of cylinders (Figure 3.35, in collaboration with Claus Heussinger) and ellipsoids (Figure 3.36, with Gerd Schröder-Turk). Preliminary results show that in the latter systems the contact number is controlled by the distribution of Voronoi volumes.

Figure 3.35: Tomography of a cylinder packing.

Figure 3.36: Voronoi tessellation of an ellipsoid packing.

Figure 3.37: Packing tetrahedra. a) Polypropylene tetrahedra with a side length of 7mm, made by injection molding. b) Raytracing of the same packing after determining particle positions and orientations from a X-ray tomography. c) Number of mechanical constraints imposed on each tetrahedra by its contacts with neighboring particles. An isostatic packing, where each degree of freedom of a particle is blocked exactly once, would require only 6 constraints. Symbols refer to different packing protocols, data are extracted from 5000 particles. b) and c) are from [2].

3.9 PHASE SEPARATION IN AGITATED GRANULAR MATTER

M. G. Mazza, S. Herminghaus
J. Clewett, K. Roeller, M. R. Swift (Nottingham, UK)

A challenge of modern statistical physics is to create a general framework for the collective behavior of far-from-equilibrium systems. Granular systems provide an excellent model for study such phenomena. We have started to unravel the physics of granular systems confined between two walls oscillating with a sinusoidal time dependence. At filling fractions between 0.05 and 0.15, and when the amplitude of oscillation is of the order of a few particle diameters, the system exhibits a striking separation between a high-density, liquid-like phase and a low-density, gas-like phase [1, 2]. This non-equilibrium phase separation carries some surprising similarities to liquid-gas phase separations in molecular fluids. For example, a spinodal and a binodal line can be identified, spinodal decomposition obeys the predictions of Model B (in the classification of Hohenberg and Halperin), and the system exhibits a surface tension even though there is no microscopic attraction [2].

The liquid-gas phase separation stops above a certain shaking amplitude. We have now focused our attention on the details of this region of the phase diagram. In a molecular fluid, identifying the amplitude with the “thermal field”, the liquid-gas critical point is the terminus of the transition line. From ongoing work based on molecular dynamics simulations, we find evidence that there might be a critical point in a system of dry, vibrated granular matter. We calculate the Binder cumulant of the density $U_B \equiv \langle \rho^4 \rangle / \langle \rho^2 \rangle^2$ and find an intersection of curves calculated with different cell sizes. Additionally, the system displays critical slowing down in this region. We have also started experiments to verify our theoretical predictions.

Figure 3.38: Dependence of the Binder cumulant $U_B$ on the amplitude (normalized to the particle diameter $d$) in a system of dry, vibrated granular matter under confinement. Different curves correspond to different cell sizes in a finite-size scaling analysis. The red circle indicates the approximate location of the putative liquid-gas critical point.

3.10 DYNAMICS OF DRIVEN SUSPENSIONS

A. Fiege, W. Pätzold, M. Schröter, A. Zippelius

In fluidized beds an initially stationary column of solid particles is transformed into a fluid-like state by an upward stream of gas or liquid, when the pressure drop across the column of particles exceeds the buoyant weight of the particles, normalized by the bed area. In the chemical processing industry fluidized beds are used in cooling, heating, drying, coating, granulation, and heterogeneous catalytic and non-catalytic reactions.

From a more basic research perspective, fluidized beds are a unique tool to study driven granular fluids in a steady state with controlled volume fraction \( \phi \). This can be understood from a simple force balance argument: granular particles of mass \( m \), density \( \rho_s \) and radius \( R \) are immersed into a fluid of density \( \rho_f \) and viscosity \( \eta \), flowing upwards with velocity \( v = v_{fl} \hat{z} \). Each particle is subject to viscous drag by the surrounding fluid, which can be modeled by a volume fraction dependent term \( \gamma(\phi) \) times \( v \). In its stationary, expanded state this viscous drag will in average be balanced by the sum of the gravitational force, \(-mg\hat{z}\), and the buoyancy force, \( F_b \hat{z} \):

\[
0 = -\gamma(\phi)v_{fl} - mg + F_b
\]  

where \( v_{fl} \) is directly proportional to the liquid flow rate \( Q \), therefore \( Q \) will control the value of \( \phi \) at which the fluidized bed reaches its stationary state. This is demonstrated in the left panel of Figure 3.39 using experimental data from a water-fluidized bed [1]. The right panel of Figure 3.39 demonstrates for a wide range of particle diameters that \( \gamma(\phi) \) is well approximated by the empirical Richardson-Zaki relation [2]:

\[
m\gamma(\phi) = 6\pi\eta R (1-\phi)^{-n}
\]

Figure 3.39: Water-fluidized bed. Left: Initial expansion of a sample of 25 µm large glass spheres at different flow rates \( Q \). After 400 s the fluidized bed reaches a steady state. Right: Flow velocity needed to prepare a fluidized bed at a given volume fraction. The different symbols correspond to glass beads of different diameters, the orange line is a fit of equation 3.4 (the free parameter is \( n \)). Data taken from [1]
The dynamics in the fluidized bed are described by the equation of motion for the \( z \)-component of the velocity \( \dot{v}_i^z \) of particle \( i \) \[3\]:

\[
\dot{v}_i^z = -\gamma (v_i^z - v_f^z) - g + \frac{F_b}{m} + \left( \frac{\dot{v}_i^z}{\varepsilon} \right)_{\text{coll}} \]  

(3.5)

The last term in the above equation accounts for inelastic collisions, parameterized by the coefficient of restitution, \( \varepsilon \).

The equations of motion, linearized around the stationary state, have been simulated with an event driven algorithm, generalized to include viscous drag. We have studied fluidization and sedimentation, monitoring relaxation into the stationary state as well as the density profile in the stationary state. An example is shown in Fig. 3.42. In the left panel we show the time evolution of the profile into the stationary state; in the right panel the profiles in the stationary state are shown for various volume fractions.

![Figure 3.40: left: Interface formation of a fluidized bed of packing fraction \( \phi = 0.3 \); time step in between two subsequent density profiles: 20, 50, 100, 200, 400 collisions per particle. right: Density profiles in fluidized states for different flow rates. The packing fractions of the corresponding homogeneous state are \( \phi = 0.3, 0.35, 0.4 \) and 0.45. The symbols represent the data; the lines show fits according to Eq. 3.7. Data taken from[3].]

The probability to find particle \( i \) at position \( z \) in the homogeneous state is given by

\[
p_{\text{hom}}(z) = \begin{cases} 
\frac{1}{h}, & 0 \leq z \leq h \\
0, & \text{else.} 
\end{cases} \]  

(3.6)

At the interface, several processes disturb the particle position. We assume them to enter Gaussian distributed, \( p_c = \frac{1}{\sqrt{2\pi}\sigma} e^{-z^2/(2\sigma^2)} \). Hence the probability to find the particle at position \( z \) is given by a convolution

\[
p(z) = (p_{\text{hom}} \ast p_c)(z) \]. \]  

(3.7)

Using the width of the Gaussian, \( \sigma \), as a fit parameter, the profiles are well reproduced by the above simple model.

3.11 GRANULAR MATTER: MOTION FAR FROM EQUILIBRIUM

J. Blaschke, K. Roeller, S. Herminghaus, J. Vollmer
S. H. Ebrahimnazhad Rahbari (Tabriz)

Most real-world systems with a large number of degrees of freedom are not in equilibrium. As an intriguing model system we study the arrest of granular flow and the motion of a variation of the granular Brownian motor [1], where the gas is non-Maxwellian. This motor is a triangular wedge (the Brownian motor), confined to move along the x-axis only. The motor is immersed in a granular gas with inelastic collisions between the motor and the particles (see Figure 3.41). The dissipation due to the coefficient of restitution in itself causes the system to be out of equilibrium, even if the gas is in equilibrium. This is sufficient for the motor to acquire a finite steady-state drift [1].

Gases with dissipative gas particle-particle interactions which are kept in a steady-state by shaking from the walls have a squeezed-Gaussian particle velocity distribution [2] with an anisotropy \( a^2 = \langle \theta^2 \rangle / \langle \theta^2 \rangle \). Our asymptotic theory for large motor gas-particle mass ratio, \( \mathcal{M} \), yields a dimensionless parameter, \( \beta = 4\mathcal{M}(a - 1)/(1 - r) \), characterizing the relevance of anisotropy [3]. For \( \beta \ll 1 \) the drift of the motor is independent of anisotropy. For \( \beta \gg 1 \) the drift is independent of the restitution coefficient \( r \) (see Fig. 3.41 b).

Commonly, mechanical work is considered a consequence of heat flow. As this is clearly not the case for motors coupled to non-Maxwellian gasses, a deeper exploration of the stochastic dynamics is currently under investigation.

Besides the origin of non-trivial motion in granular systems, we are also interested in their spontaneous arrest. We have shown that the minimal force required to induce sustained flow can be analytically calculated based on the balance of the injected power and the power dissipated in creeping flow. This not only holds for a shear flow in a two-dimensional system driven by a body force [4], but also for a shallow gravity-confined layer of particles [5], and our argument can even be adapted to calculate the residual stress in a system where the flow rate is controlled and gradually decreased [6].


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3.12 THE GRANULAR GLASS TRANSITION

Till Kranz, Annette Zippelius
Matthias Sperl (DLR Köln)

The non-equilibrium stationary state of a fluidized quasi-2d assembly of steel balls has been investigated recently by Abate & Durian [1]. In particular, they measured the mean square displacement (MSD), \( \delta r^2(t) = \langle (\vec{r}(t) - \vec{r}(0))^2 \rangle \), as a function of time. For low packing fractions \( \varphi \), they found the well known crossover from ballistic motion on short times to diffusive motion on longer time scales. At the highest packing fraction they observed the formation of a plateau in the MSD for intermediate times. For colloidal fluids, such a plateau has been interpreted as a signature of the glass transition [2]. A similar plateau can also be found in the coherent scattering function \( \phi_q(t) \). The Debye-Waller factor \( f_q(t \to \infty) \) serves as a order parameter for the fluid-to-glass transition. While \( f_q = 0 \) in the (ergodic) fluid phase, the glass is characterized by \( f_q > 0 \), signaling an arrested state. Mode-Coupling Theory (MCT) [3] derives a nonlinear equation of motion for the coherent scattering function \( \phi_q(t) \) that captures this behavior.

We succeeded in generalizing MCT to the non-equilibrium stationary state of randomly driven inelastic hard spheres and disks [4, 5, 6]. Here, the dissipative collisions are characterized by a constant coefficient of normal restitution \( \varepsilon \). In particular, we find the equation of motion

\[
\ddot{\phi}_q(t) + q^2 C_q^2 \phi_q(t) + \int_0^t d\tau M_q(t - \tau)\dot{\phi}(\tau) = 0 \quad (3.8)
\]

where \( C_q \) is the speed of sound and the memory kernel is given in the mode-coupling approximation

\[
M_q(t) \approx \sum_{k+p} V_{\vec{k},\vec{p}} W_{\vec{k},\vec{p}} \phi_{k}(t) \phi_{p}(t). \quad (3.9)
\]

The coupling constants \( W_{\vec{k},\vec{p}} = \frac{1+\varepsilon^2}{2} V_{\vec{k},\vec{p}} \) have been calculated explicitly. That they are unequal reflects the loss of detailed balance in the dissipative collisions.

The Debye-Waller factor is the solution of the nonlinear equation

\[
\frac{f_q}{1 - f_q} = M_q[f] / q^2 C_q^2 \quad (3.10)
\]

which shows a bifurcation from \( f_q = 0 \) to \( f_q > 0 \) at a critical packing fraction \( \varphi_c(\varepsilon) \). The resulting phase diagram is shown in Fig. 3.42. Note that the critical packing fraction increases substantially with increasing dissipation but that there is a fluid-glass transition for all degrees of dissipation.

The full dynamics is shown in Fig. 3.43 for several packing fractions close to the glass transition. The approach to the plateau (\( \beta \)-relaxation) and the departure from the plateau (\( \alpha \)-relaxation) can be described...
Figure 3.43: Coherent scattering functions $\phi_q(t)$ as a function of time in 3D for wave number $q_d = 4.2$. At the transition point at packing fraction $\phi_c(\varepsilon = 0.5) = 0.548$ with a critical glass form factor of $f_q = 0.4$, and at higher ($1.1\phi_c$, $1.01\phi_c$, $1.001\phi_c$) and lower ($0.9\phi_c$, $0.99\phi_c$, $0.999\phi_c$) packing fractions.

in terms of critical exponents, $a(\varepsilon), b(\varepsilon)$, that depend weakly on the coefficient of restitution

$$\phi_q(t) - f_q \simeq t^{-a}, \quad t < t^*$$  \hspace{1cm} (3.11a)

$$\phi_q(t) - f_q \simeq -t^b, \quad t > t^*$$  \hspace{1cm} (3.11b)

where $t^* \propto (\phi - \phi_c)^{-1/2}$ diverges at the critical density. The second relation is also known as the von Schweidler law.

Similar mode-coupling arguments lead to an equation of motion for the MSD

$$D_0 \delta \dot{r}^2(t) + \delta r^2(t) + \int_0^t d\tau m_0(t - \tau) \delta r^2(\tau) = 6D_0 t$$  \hspace{1cm} (3.12)

describes the coupling between the coherent- [$\phi_k(t)$] and incoherent [$\phi_s(t)$] dynamics [5]. The resulting MSD as a function of time is shown in Fig. 3.44. Close to the critical packing fraction it shows a plateau like the experimentally measured MSD [1]. This was also confirmed by simulations [8].

With event driven simulations the randomly driven inelastic hard sphere fluid has been analyzed further in terms of its macro- [9] and micro-rheology [10]. Work on the integration through transients formalism [11] for a sheared granular fluid is in progress.

3.13 QUANTIFYING THE RANDOM FIXATION OF DELETERIOUS MUTATIONS IN ASEXUAL POPULATIONS

S. Eule, J.J. Metzger

In populations of finite size, deleterious mutations may occur due to an unfavorable stochastic fluctuation, a phenomenon that can be described by Muller’s ratchet, a paradigmatic model of population genetics [1]. Obtaining quantitative predictions of the ratchet rate, i.e. the frequency with which a deleterious mutation fixes, is expected to be important for understanding a broad range of effects ranging from the degeneration of the Y-chromosome to the evolution of sex as a means of avoiding the accumulation of deleterious mutations.

Two quantities are of central interest for the understanding of the dynamics of the ratchet: the rate at which deleterious mutations occur and the distribution of the frequency of the fittest individuals, which may be experimentally more accessible than the rate, particularly when the ratchet rate is very large.

To obtain a better understanding of how Muller’s ratchet operates, we have considered a Moran model with overlapping generations. Since this model can be represented in terms of a master equation, it allows for the application of methods tailored for the analysis of rare stochastic fluctuations which drive the ratchet [2]. More specifically, we have performed a two-class approximation of the ratchet, combining all individuals that carry one or several mutations into one class, which then interacts with the class of individuals that carry no mutation. Using a WKB-approximation originally derived in the context of semiclassical quantum mechanics, we can perturbatively treat the master equation obtained from the two-class model to obtain concise and accurate analytical results for the rate of Muller’s ratchet, which are confirmed by extensive numerical simulations. Additionally, we are able to predict the hitherto elusive full distribution of the frequency of the fittest individuals. Our expression for the ratchet rate complies with recent results that were obtained by a semi-analytical investigation of the full ratchet with path integral methods [3].

Our study allows insight into an important fundamental mechanism of population genetics and also offers several opportunities for analyzing Muller’s ratchet in a more general context, like, for example, in spatially extended systems.

3.14 DYNAMICS OF CELL MOVEMENTS IN DROSOPHILA MORPHOGENESIS

F. Wolf, L. Reichl
J. Großhans (University of Göttingen)

In gastrulating embryos, cells perform a complex choreography of large-scale tissue rearrangements. Germband extension during gastrulation of Drosophila embryos is based on directional cell intercalation. Cells exchange with their neighbors by a characteristic series of junction constriction and expansion, which can be described as a topological T1 process. Previous studies have revealed the molecular mechanism of the constriction of vertical junctions, especially how the anisotropic distribution of RhoGEF2/Dia signaling and E-Cadherin endocytosis controls directed myosin flow. In contrast, the mechanisms for the resolution of 4x vertices and the expansion of new horizontal junctions have not yet been studied. Also, whether and how the force generation and movement of individual cells are actively coordinated during morphogenetic transformations is largely unknown. To shed light on this question we study cell shape fluctuations during one of the major morphogenetic tissue transformations in the Drosophila embryo, axis elongation. We found that cell shape fluctuations are in fact actively coordinated. Furthermore, coordinated shape fluctuations are essential for axis elongation in Drosophila development.

Figure 3.46: Dynamic cell shape changes during morphogenesis in a Drosophila embryo. The graphs show the dynamics of cell areas of old (blue) and new (purple) neighbors in comparison to AP junction length (black). Red arrows indicate the time when the images shown above were recorded. Analyzing hundreds of such intercalation events, we find that area fluctuations are strongly anti-correlated. This type of intercellular coordination is lost when the cell-adhesion molecule E-cadherin is genetically depleted. Notably, cell area fluctuations persist under genetic depletion, demonstrating that anti-correlations do not directly result from the geometry of shared cell borders.

Cells surrounding emerging anterior-posterior cell junctions perform anti-correlated contractions of cross-sectional area. When E-Cadherin was depleted by RNAi or in the novel mutant xit, individual cell contractions persisted but became uncoordinated. 4x vertices were arrested in persistent, undirected fluctuations. Microsurgical cuts in the tissue disrupted coordinated cell contractions and impaired the formation of new junctions in a similar manner, indicating that E-Cadherin is not per se able to drive extension and that tissue integrity is a prerequisite for coordination of cells. We conclude that E-Cadherin promotes axis elongation in Drosophila by coordinating contractions amongst cells surrounding nascent cell junctions.

[1] Zhang, Reichl, Kong, Vogt, Wolf, and Großhans (under review)

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Most information transfer in neuronal systems occurs through action potentials. The first quantitative description of action potential generation was published over 60 years ago [1]. Considering the huge importance of AP generation for the functioning of the nervous system, it came as a large surprise when we realized that the community is to this day far from a quantitative understanding of the AP generation in mammalian neurons. Biophysically motivated multi-compartment models of neurons fail to reproduce the shape of individual action potentials and fail to reproduce the ability of central neurons to encode frequencies as high as 200 or 300 Hz. We identified two core problems in the field: 1. Sodium channels activate so rapidly that the 1 to 2 kHz resolution typically used in previous studies significantly distorts the measurements. 2. The surface density of sodium channels at the soma, often used as a reference value in simulations, is ill-determined. We addressed these problems by precise measurements and analyses, obtaining data at a temporal resolution of 5 kHz from minimally invasive recordings of individual sodium channels in the somatic membrane of pyramidal cells. We revealed that these sodium channels open much faster than widely used models suggest (e.g. [2]). Our tightly constrained model provided a quantitative match between predicted somatic action current and measured $dV/dt$ (Fig. 3.47). This, together with the direct measurement of single channel current and open probability, led to a lower bound for the surface density of sodium channels of 10 channels per $\mu m^2$ at the soma of pyramidal neurons. Importantly, even this lower bound is three times larger than the widely used estimates obtained from excised patches of somatic membrane [3]. Our results suggest that the arguments about axonal sodium channel densities and the basis of action potential generation ([4],[5]) are in parts based on inaccurate assessments of sodium channel kinetics and somatic surface density. Our findings cannot however be extended to the description of axonal channels and their control of action potential generation, as even our novel models fail to explain the encoding of high-frequency input. Studying spike encoding, from fluctuating input currents to fluctuating spike rates, during the maturation of neurons, we found evidence for two separate mechanisms that shape the transfer function (Fig. 3.48 and caption). The biophysical basis of these two mechanisms is now being explored using neurons from genetically altered mice and simulations of multi-compartment models.

TRANSPORT IN COMPLEX MEDIA

A complex medium consists of a variety of building blocks or has an organization that shows fluctuations and heterogeneities bridging several length and time scales. The mechanisms underlying transport phenomena in such complex media are not well understood although they occur in a wide range of physical, chemical, and biological systems. We study, for instance, how multiphase flows organize in porous or granular media and how extreme events and localized propagating waves emerge in random nonlinear media. We further address the transport of small objects (such as small molecules, micelles, colloids, particles or cells) in complex fluids (emulsions, liquid crystals, turbulent fluids) and their behavior under confinement. Another example is anomalous diffusion, which is relevant e.g. in cellular biochemical processes and animal behaviour.

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4.1 WETTING OF REGULAR SURFACE TOPOGRAPHIES

C. Semprebon, S. Herminghaus, M. Brinkmann

Despite the enormous amount of literature published on wetting of superhydrophobic surfaces the relationship between surface roughness and wetting hysteresis on generic surfaces is still poorly understood. One of the main reasons for the lack of a predictive theory is the large variety of rough surfaces encountered for natural and artificial materials. Experimental studies on regular arrays of posts [1] report high apparent contact angles on microstructured substrates and demonstrates the strong ability of these substrates to immobilize three phase contact lines even for a hydrophilic material contact angles. Several interfacial instabilities can lead to a depinning of the three phase contact line. Which of these instabilities govern the motion of the contact line is dictated by the geometry of the topographic features.

Figure 4.1 displays the spectrum of equilibrium configuration of a liquid meniscus pinned to a row of cylindrical posts obtained in numerical minimizations of the interfacial free energy. In a typical computation the apparent contact angle \( \theta \) is incremented in small steps, and each increment is followed by a sufficient number of minimizations steps. During this quasi-static increase of \( \theta \) a number of interfacial instabilities are observed. The apparent contact angle where the last local energy minimum has vanished defines the static advancing contact angle \( \theta_a \).

Figure 4.2 displays the results for material contact angle of \( \theta_0 = 50^\circ \) and \( \theta_0 = 60^\circ \). A comparison of the two diagrams reveals a dramatic change in the dependence of the advancing contact angle on the spacing of the posts although the material contact angle differs by only 10°.

For \( \theta_0 = 50^\circ \), the advancing contact angle \( \theta_a \) varies smoothly with the line fraction \( w \) and aspect ration \( h \) of the posts. At \( \theta_0 = 50^\circ \) one observes a steep increase of \( \theta_a \) from a very small value close to zero to almost complete immobilization at higher line fractions \( w \approx 0.9 \).

4.2 WETTING OF TRIANGULAR GROOVES

C. Semprebon, S. Herminghaus, R. Seemann, M. Brinkmann
C. Herrmann (Univ. des Saarlands)

The equilibrium shapes of droplets wetting linear surface structures typically show strong deviations from a spherical cap. Figure 4.3b) displays such a droplet shape on a periodic pattern of triangular grooves obtained from numerical minimizations of the interfacial energy. The apparent anisotropy of the shape observed both in experiments and numerical computations can be explained by the interplay between the liquid spreading into the direction of the linear surface features and pinning of the three phase contact line at acute edges of the surface topography.

Shapes of asymptotically large droplets wetting many grooves can be uniquely characterized by the largest local contact angle in the pinned segment of the contact line, \( \theta_p \), and an the longitudinal apparent contact angle of the droplet \( \theta_a \), measured in a side view perpendicular to the linear surface structures. As gravity is neglected in the model, the only relevant length-scale for a droplet wetting a sufficiently large number of linear surface features is set by the droplet volume \( V \). Indeed, it is observed in condensation experiments and corresponding numerical calculations (Fig. 4.4a) that a small growing droplet can attain a scale invariant shape with a constant eccentricity \( \varepsilon \equiv (L_{\parallel} - L_{\perp})/(L_{\parallel} + L_{\perp}) \) where \( L_{\parallel} \) and \( L_{\perp} \) denote the droplet extension into parallel and perpendicular direction of the grooves, respectively. However, if the ability of the linear surface structures to pin the interface is sufficiently high, any lateral movement of the contact line is suppressed and the liquid spreads solely into the directions of the linear structures. In this case, the width of the droplet does not increase and the eccentricity asymptotically tends to the value \( \varepsilon = 1 \).

The eccentricity \( \varepsilon \) of the droplet base can be obtained from a mapping onto equilibrium droplet shapes wetting a hydrophilic stripe of finite contact angle[1]. The color density plot in Fig. 4.4b) shows the base eccentricity \( \varepsilon \) of the droplet for given apparent longitudinal contact angle \( \theta_a \) and maximum pinned angle \( \theta_p \) in the limit of a droplet wetting infinitely many grooves.

Figure 4.3: a) Triangular grooves with wedge angle \( \psi \) and periodicity \( W \). b) Top view of a droplet obtained by numerical energy minimizations wetting \( \sim 30 \) triangular grooves.

Figure 4.4: a) Droplet eccentricity as a function of dimensionless droplet volume \( v \equiv V/W^3 \) for different wedge angles \( \psi \) and the same material contact angle \( \theta_\theta = 30^\circ \). b) Generic map of the droplet base eccentricity, \( \varepsilon \), as a function of the apparent, longitudinal contact angle \( \theta_a \) and the largest pinned contact angle \( \theta_p \) at the side.

4.3 TWO-PHASE FLOWS IN HETEROGENEOUS HELE-SHAW CELLS

R. Seemann, M. Brinkmann, J.-C. Baret, S. Herminghaus
M. Jung, M.S. de la Lama, T. Hiller, B. Semin

The forced displacement of immiscible fluids is studied in a microfluidic Hele-Shaw cell with circular obstacles for various wetting conditions. Transparent top and bottom walls of the Hele-Shaw cells allow imaging of the displacement process by optical high-speed microscopy, see Fig. 4.5. The invasion process could be quantitatively compared to the results of numerical simulations of 2d Darcy flow [1] based on Inoue’s Multi Particle Collisions algorithm [2]. Here, identical configurations of obstacles were used in simulations and the corresponding experiments.

For capillary numbers smaller or equal than \( Ca \leq 3 \times 10^{-3} \) (with respect to the more viscous fluid), the displacement process is independent on fluid viscosities or front velocity. In this regime interfacial tension dominates the process and both the emerging front shape and the residual oil saturation depend characteristically on the contact angle of the fluid interface with the cell walls [3]. Invading liquids with small contact angle display a stable front advance leaving almost no oil behind. For large contact angles, however, the front advance is localized in space and time. In this case, branched structures are formed by the invading fluid, entrapping a substantial amount of the displaced fluid. The transition between the stable and branched front advance is remarkably sharp, c.f. Fig. 4.6 a). This behavior is robust and widely independent on the packing geometry and confinement. This was demonstrated using porous matrices with different area fractions and device heights. The experimental results agree quantitatively with the numerical results as analyzed in terms of oil saturation and transient front length, see Fig. 4.6 b).

Figure 4.5: Time series of water dyed with erioglaucine \( (\theta \approx 125^\circ) \) flushed into a dodecane filled microfluidic matrix. 

Figure 4.6: a) Residual oil saturation as function of advancing contact angle of the invading phase for pillar arrays with 15% and 30% area density. b) Comparison of interfacial front length extracted from simulation (open symbols) and experimental results (closed symbols) for a complete wetting, neutral and complete non-wetting invading phase.

4.4 TWO-PHASE FLOW IN COMPLEX POROUS MEDIA

T. Hiller, M. Sanchez de la Lama, S. Herminghaus, J. Murison, M. Schröter, M. Brinkmann

Simulating immiscible two phase flows in porous media remains a challenging task. The complex interplay of fluid dynamic boundary conditions, the different affinities of the fluid phases to the pore walls, and a constantly changing topology of the fluid interface prohibits a single simulation method to study all relevant aspects of the flow. In recent years, a number of algorithms based on the idea of Multi Particle Collisions (MPC) were introduced as alternatives to Lattice Boltzmann or finite element methods [1, 2]. For the particular problem of forced immiscible displacement in chemically heterogeneous porous media, Inoue's MPC algorithm for multi-phase flow [3] had to be extended to account for different wettabilities.

One of the central aims of the MPC simulations is to compare the numerical results with the findings of time resolved X-ray tomography and the capillary pressure saturation curves for bead packings with mixed wettability conditions as presented in section 4.2. Three-dimensional simulations of immiscible displacement in beds of spherical beads provide access to residual fluid saturations, capillary hysteresis, and their relation to local packing geometry and controlled pore scale distribution of wettabilities.

Figure 4.7 displays snapshots of interfacial morphologies in three different bead packings at saturations of the displaced phase $S \approx 0.5$ during first imbibition. The volume fraction of the beads in the random packing is $\phi \approx 0.25$. To either sides of the cell, packings of hydrophilic or hydrophobic small spherical beads act as semipermeable membranes, analogous to the capillary pressure saturation cell described in section 4.2. A pressure gradient is applied in an inflow zone outside the packings and the pressure difference between the two connected phases is slowly ramped up. After each pressure increment, the liquid phases are given sufficient time to equilibrate to achieve a quasi-static advance. The distribution of invading fluid depends on the spatial distribution of the differently wettable surface domains. The size of these domains is characterized by the wetting correlation length $\xi$ which has values $\xi \approx d$ for the mixed beads, $\xi \approx 0.5$ for the janus beads, and $\xi \approx 0.16$ for the patchy beads, respectively.

As an example the simulated pressure saturation curve for a mixed bead packing is presented in Fig. 4.8. Similar to the experimental results, in the simulations the hysteresis opening $\Delta P_c$ increases with decreasing wetting correlation length $\xi$ (inset). This demonstrates the applicability of the MPC method in representing the physical relations observed in the CPS experiments (see section 4.2).

4.5 FORCED IMBIBITION IN BEAD PACKINGS

R. Seemann, S. Herminghaus
H. Scholl, K. Singh, A. Kabdenov M. DiMichiel (ESRF), M. Scheel (ESRF), A. Scheppard (ANU)

Forced multiphase flow, where an invading phase is forced into a porous matrix containing a defending phase, has many applications in processes: coating and impregnating of natural stones and concrete, soil de-contamination from organic spills, and oil mining. Despite the tremendous technical importance little is known about the process on the pore scale level. To shed light onto the underlying physical phenomena three dimensional fronts were imaged with ultrafast x-ray tomography (ESRF, Grenoble). As porous media bead packs of different size and wettability were used with various combinations of invading and defending liquids. For the tested bead packs and for capillary numbers \( Ca \leq 7.5 \times 10^{-8} \) the advancing contact angle could be shown to be the only relevant parameter to influence the liquid/liquid front shape and the residual oil saturation [1]. Figure 4.9 displays snapshots during imbibition for three different wettabilities.

![Image of cross sections through tomography images recorded in situ during the imbibition process. The advancing contact angles are a) \( \theta \leq 20^\circ \) b) \( \theta = (90 \pm 10)^\circ \) and c) \( \theta = (165 \pm 5)^\circ \).](image1)

The tomographic time series are analyzed in terms of oil saturation and interfacial area. Increasing the contact angle from about 85 to 125\(^\circ\), the interfacial areas of the emerging liquid/liquid front increase by about three times, see Fig. 4.10. The corresponding residual oil saturation for these samples increases from about 1% to about 10%.

![Image of quantitative analysis of the liquid/liquid fronts emerging in bead packs of different composition. The glass and basalt beads have contact angles of \( \theta = (125 \pm 15)^\circ \) and \( \theta = (85 \pm 15)^\circ \), respectively. The 'mixed' sample is composed from a half-half mixture of glass and basalt beads. left: Interfacial area of the liquid/liquid front. Right: Oil saturation curve.](image2)

4.6 WETTING CORRELATIONS

Julie Murison, Benoit Semin, Jean-Christophe Baret, Stephan Herminghaus, Matthias Schröter, and Martin Brinkmann

Wettability is a crucial parameter for multiphase flow in porous media [1, 2, 3]. The effect of spatial distribution of wetting domains has been neglected, and only dealt with by averaging contact angles [4, 5]. These approximations only hold for wetting heterogeneities larger than a pore.

![Figure 4.12: CPS curves for a range of wettability correlation length below and above the typical bead size. The top row shows tomography pictures of the samples used with the two wetting areas marked in blue and orange.]

We measure the effect of spatial wetting domains in porous media by creating tailored bead packings with bimodal wettability, constant in average but differing in wetting domain size. These domains are quantified by the lengthscale $\xi$, measured by X-ray tomography. (Figure 4.12).

Sample scale wettability is measured using Capillary Pressure Saturation (CPS) curves, obtained by pumping fluids in and out of a sample. The hysteresis loop opening $\Delta P_c$, measured between the secondary imbibition and drainage branches, monotonically decreases with increasing $\xi$ (Figure 4.11). $\Delta P_c$ corresponds to the dissipative work occuring during imbibition and drainage.

X-Ray tomography of the samples at intermediate saturations (Figure 4.13) show that the front morphology is smoothened at small values of $\xi$. Both observations are consistent with an increase of dissipation for small correlation length. To the best of our knowledge, it is the first time that a minimal descriptor of wetting heterogeneities is proposed and shown to influence flow behaviour in complex porous media.

4.7 LIQUID TRANSPORT IN WET GRANULAR MEDIA

C. Semprebon, S. Herminghaus, M. Brinkmann
R. Mani (ETH Zürich), H. Herrmann (ETH Zürich)

A description of the dynamics of wet granulates must include the transport of the wetting liquid. Redistribution of a non-volatile liquid inside a granular pile has, in principle, two origins. The first mechanism is simply based on the fact that liquid adhering to the grain surface gives rise to a transport coupled to the motion of grains. This applies, in particular, to partially wetting liquids that exhibit a high contact angle hysteresis on the heterogeneous grain surfaces. The second mechanism leading to transport are liquid flows on the grain surface, i.e., a relative motion of fluid to the grains [1]. These surface flows are driven, besides gravity, by interfacial energy and are observed in fluidization experiments with perfectly wetting liquids [2].

A first step to study transport of non-volatile liquids in realistic granular piles is to focus on the level of single grains and their surfaces. For the particular range of length scales occurring in a typical surface roughness one may assume a Darcy-type description of viscous flows in the wetting layer. The relation of the film morphology and the corresponding effective liquid mobility to the microscopic contact angle, average thickness of the wetting layer, and roughness is studied on non-flat model surfaces employing numerical minimizations of the interfacial energy, cf. Fig. 4.14. The redistribution of liquid on the scale of a single grain can be then described as a time dependent Darcy flow.

![Image](https://via.placeholder.com/150)

Figure 4.15: a): Example of the shape of the liquid interface of the film (color), and the underlying rough substrate (gray) from the numerical energy minimizations showing fluid collection in the valleys. The microscopic contact angle is $\theta = 10^\circ$. b): Corresponding flux density in the film in response to an externally applied pressure gradient. A number of 'back bones' of the flux are clearly visible.

To model the evolution of capillary bridge volumes reported in experiments [2], one can assume homogeneously rough spherical grains and quasi-stationary flows between the circular contact lines of the capillary bridges. Once a quasi-stationary flow has been reached the pressure distribution shown in Fig. 4.14 can be mapped onto solutions of the two dimensional Laplace equation with Dirichlet boundary data using the stereographic projection.

4.8 LIQUID CRYSTAL MICROFLUIDICS

Ch. Bahr, S. Herminghaus
A. Sengupta, U. Tkalec, B. Schulz
Ch. Pieper (Göttingen), J. Enderlein (Göttingen), M. Ravnik (Oxford/Ljubljana), J. M. Yeomans (Oxford), E. Ouskova (Aalto)

The rheological properties of nematic liquid crystals are fundamentally different from those of isotropic liquids because of the mutual coupling between flow, director orientation, and viscosity. In microchannels, we have to deal with the competing aligning effects of the flow and the anchoring of the director on the channel walls. We have developed [1] experimental techniques to provide the channel walls with different anchoring conditions and started a systematic study of the corresponding nematic flow behaviors.

For homeotropic anchoring on all channel walls, we observe with increasing flow rate a sequence of different, partly non-Poiseuille-like flow profiles [2]. The increasing effective birefringence with increasing flow rate (Figs. 4.16 a and b) enables a direct determination of the flow velocity field [3]. We have also studied the transient defect structures that appear in the nematic flow behind a pillar in the channel [4].

Hybrid anchoring conditions (homeotropic on three channel walls, uniform planar on the fourth wall) result in the generation of a line defect (disclination) in the nematic director field. We have demonstrated [5] how the disclination line can be threaded at will through the microchannel and used as a soft rail for the transport of colloidal particles or droplets (Figs. 4.16 c and d), paving the way to flexible micro-cargo concepts in microfluidic settings.

Figure 4.16: Polarizing micrographs of a diverging channel filled with 5CB in absence of any flow (a) and in the presence of flow (b) inducing a deformation of the director field resulting in an effective birefringence and the appearance of interference colors. The diverging width of the channel enables the simultaneous observation of different flow velocities. Scale bars: 300 µm. c) Colloidal chain of three silica particles being captured by a nematic disclination in the microchannel. Scale bar: 5 µm. d) Aqueous droplets being transported on a disclination. Scale bar: 50 µm.

Amphiphilic molecules play an essential role in natural systems and are
among others intensively used in the pharmaceutical, cosmetic, food,
and petroleum industries. Surfactant molecules are used for example as
detergents and dispersing materials, coating and foaming agents, emul-
sifiers and biocides, spanning a wide range of functions [1]. More than
two hundred years after the first observations reported by Benjamin
Franklin of the damping of waves by fatty acids [2], understanding the
dynamics of surfactant films remains a challenge, both theoretically
and experimentally. Interfacial rheology and adsorption dynamics are
key concepts to understand foaming, emulsification, and encapsulation
processes as well as dynamic properties of biological membranes.

Microfluidics offers controls for the manipulation of multiphase
systems in confined environments. The possibility to measure trans-
ient states at short timescales (~ ms) makes microfluidics especially
appealing as a new tool to quantitatively study the physics and physical-
chemistry of interfaces and emulsions [3, 4]. Microfluidic systems have
been developed to study interfacial properties [5]. The role of dynamic
processes in microfluidic emulsification has been recently elucidated [3],
but direct quantitative measurements of dynamic properties are still
lacking.

Here, we design a method to measure surfactant adsorption on
droplets in flow. We show for a perfluorocarbon surfactant that the
adsorption is transfer limited. In contrast, the dynamics of adsorption
of the perfluorosurfactant molecules in a pendent droplet experiment
diffusion limited: our microfluidic approach therefore provides a
new tool to determine the adsorption and desorption rate constants of
surfactant, relevant to understand emulsification and ageing processes.

We believe that our approach can be extended to the study of other
dynamic processes at interfaces, such as self-assembly of polymers or
polymerisation to gain deeper understanding of the dynamics and
micromechanics of thin shells upon formation and provide interfacial
rheology measurements.

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Molecular transport through membranes is an essential process in living systems as well as in technological systems. In cells, the porous properties of the membrane provides means to selectively exchange material in and out. This selectivity on the transported species is essential for technological development to control solvent (osmotic membranes), solutes (filters), and ions (batteries, fuel cells).

In emulsions, molecular transport provides means for the metastable system to reach a lower energy state by equilibrating chemical potential. As such, it is at the origin of the ageing processes such as coarsening by Ostwald ripening or solute equilibration in a heterogeneous emulsion. Practically, monodisperse emulsions are currently used as a large ensemble of microreactors for parallelized and miniaturized biochemical assays. At the core of this technology lies the assumption that individual droplets can be considered as closed microreactors. This assumption is not necessarily valid at all time-scales as mass transfer across the droplet boundary will eventually lead to leakage and cross-talk of molecules between droplets [1]. Such phenomena would be detrimental for drug-screening applications where incubations of compounds in droplets may be required for several days [2]. Although mass transport processes in emulsions have been investigated for many years, the lack of control on size distribution, spacing, and arrangement of droplets does not provide quantitative insights into the transport mechanism from the molecular description of the interface to the macroscopic scale of the emulsion.

Microfluidic tools allow calibrated emulsions to be produced with efficient stabilization methods [3]. A precise handling down to the single droplet level provides powerful platforms for quantitative studies not otherwise accessible [4, 5]. To immobilize droplets in a controlled way, local variations in confinement resulting in surface energy gradients can be used to trap droplets [6]. Accordingly an environment where droplets can buffer each other from one local minimum in surface energy to another is capable of immobilizing an alternating row of droplets with predefined spacing. We found that even though spatially separated, the exchange of fluorophores (model organic compound) occurs, even for fluorinated oils in which the solubility of organic molecules is typically very low. This counterintuitive fact is explained by surfactant molecules mediating solubility in the oil phase thereby influencing the partitioning of organic molecules. Surfactant molecules solubilized in the oil therefore play a crucial role in the exchange process. The equilibration process occurs as an exponential relaxation, as expected from simple arguments based on diffusive processes. For a three dimensional emulsion, we designed a microfluidic system for the automated analysis of the fluorescence of millions of individual droplets in order to obtain statistically relevant information. We found
that the surfactant acts linearly on equilibration time scale. The packing of the emulsion plays an essential role in the relaxation.

As droplets are randomly arranged, the system does not relax exponentially but with a power-law in the late kinetics. This relaxation process is recovered in a minimal model based on a diffusion process between nodes of a regular lattice. In this case, we also recover exponential relaxations for the eigenmodes of the discrete Laplace operators. The smallest eigenvalue (fastest mode) is obtained for an alternating arrangement of filled and empty droplets, the three dimensional version of our microfluidic one-dimensional array.

Our method and analysis provides means to relate macroscopic relaxation to the microscopic details of the exchange process. We experimentally found that partitioning between the oil and the water favors the exchange. By adding proteins in the droplet, the partitioning favors the aqueous phase which in turn slows down the exchange process. Additives – be it surfactant in the oil or proteins in the aqueous phase – therefore control the rates of exchange in the emulsion. We are currently using the microfluidic control of the droplet in order to gain additional insights on the transport mechanisms at the droplet interface, but also through thin polymer shells (see section Active & Reactive Interfaces).


Figure 4.21: Modelling the exchange in an emulsion. Considering diffusion processes across membranes leads to a discrete diffusion equation. The relaxation of the concentration in the late kinetics is given by the sum of all eigenmodes of the Laplace operator leading to the power law behavior experimentally observed.

Figure 4.22: Reproduced from [5] with permission from RSC.
4.11 OPTIMIZING MICROFLUIDICS

H. Schrobsdorf, Q. Brosseau, J.-C. Baret, T. M. Schneider

In droplet-based microfluidics chips are often designed to generate, merge, and sort droplets that are transported along channels, see Fig. 4.23. Designing efficient custom-tailored chips for applications currently revolutionizing many biochemical essays, requires an accurate quantitative understanding of the multi-phase flow underlying droplet formation and transport [1]. Analytical approaches are mostly limited to unrealistically simplified geometries and even the fundamental question of how fast a droplet is transported through a channel can only be analytically assessed in the asymptotic limit of a long droplet in a cylindrical channel at small Capillary numbers [2]. Thus, accurate numerical simulation tools are required for design and optimization purposes.

We thus aim at developing adequate tools for simulating viscous free-surface flows in complex geometries. The numerical method needs to accurately represent interface curvature, allow for surface tension gradients and take into account potentially non-newtonian fluid response. One promising option are Volume Of Fluid (VOF) methods, which also locally conserve the volume of all phases exactly and thereby keep droplets from numerically evaporating, see Fig. 4.24.

As a first step we are aiming at adapting Gerris [3] an implementation of free-surface VOF methods by Stéphane Popinet, originally aimed at inertia dominated flows, to microfluidic settings. Besides reliable conservation of volume and access to all physical parameters of the system, Gerris provides advanced tools for parallel computations. Such a fast accurate solver allows for parameter studies. Additionally, in combination with advanced mathematical optimization tools, new essays can be designed.

As an example for a microfluidic experiment, we consider the deformation of droplets in expansions used to determine surface tension (see Section 4.11). Our approach will enable optimal flow geometries to be designed for accurate measurements and finally reduce the amount of experimental calibration required for dynamic measurements. As an extension, we will attempt to model the Marangoni stresses ultimately leading to tip streaming in flow (Fig. 4.25). Modeling Marangoni stresses is in general of relevance to better describe coalescence or emulsification. Finally, more complex problems dealing with droplet self-assembly in flow will also be considered [4] (Fig. 4.23).

The mechanical stability of two-row droplet arrangements are studied experimentally in a quasi 2d microfluidic setting [1, 2] and theoretically by minimizing the free surface energy [1, 3]. Droplets of different size were generated and a compressive stress could be applied quasi statically to the droplet packings. Depending on their confinement in the microfluidic channel the droplet packings are mechanically stable and reorganize continuously from a zigzag arrangement into a bamboo arrangement upon compression or are mechanically unstable and discontinuously reorganize from a zigzag structure into a staircase arrangement [2, 3], see Fig. 4.26.

Figure 4.26: Experimentally applied compression force $F_c$ respectively analytically calculated rescaled elastic force $f = F_c \cdot 4/\pi \gamma H$ as function of the self-adjusting area fraction $\phi$ of 2d droplet packings for several confinement values. (a) For large confinements ($A_d/W^2 \geq 0.525$ exp. and $\geq 0.471$ theo.) reversible transitions during a compression-decompression cycle are found. (b) For small confinements ($A_d/W^2 \leq 0.46$ exp. and $< 0.471$ theo.) hysteretic transitions are observed. Top and bottom filled symbols correspond to a compression and decompression cycle, respectively [2].

In a dynamic situation when the droplets move slowly along a straight microfluidic channel and the pressure drop in the flow direction is equivalent to the quasi statically applied pressure, the resulting droplet arrangements are identical. The mechanically unstable droplet arrangements decay into a strictly periodic series of stable packing geometries that border the unstable region. Increasing the flow velocity above a certain threshold causes the emergence of compression and de-compression waves resulting in mechanically unstable droplet arrangements.

Microcompartmentalization is an essential feature of living organisms. At an early stage in evolution, microcompartments provide means to link genotypes and phenotypes required for systems to evolve when the functional macromolecules are distinct from the encoding molecules. Microcompartments presumably played a role at an earlier prebiotic stage. Synthesizing large molecules from smaller ones is an unfavorable process due to the loss of entropy. Microcompartments such as aerosol droplets have been proposed as means to circumvent this penalty by increasing concentration of compounds in the course of evaporation [1].

In these compartments, interfaces play a major role. We have shown that a simple chemical reaction between an amine and an aldehyde favors product formation when performed in micron-sized droplets. The process does not require any size modification of the droplet. We show through an adsorption-reaction-diffusion model that even with low binding affinity of the molecules to the interface, the equilibrium constant of the reaction and the forward rate constant are inversely proportional to the droplet size [2]. This process is presumably universal as it does not require specific binding at the interface and might have played a role in prebiotic chemistry.

Interfacial reactions are then a key to control the formation of microcapsules that can be used as formulation tools, encapsulation vectors or microreactors with solid walls to control the adhesion of cells. We are now studying the in situ polyurea shell formation in microfluidics to generate a series of microreactors with controllable elastic and permeation properties. In addition, we also use simple acido-basic interfacial reactions to measure the dynamics of surfactant adsorption at very short time-scales (in the case of carboxylic acids) and we propose new bio-inspired interfacial reactions to create self-propelled biomimetic reactors based on the Marangoni instability studied in the department of Stephan Herminghaus.

Active and reactive soft interfaces provide novel means to program functions at the scale of microreactors and will become an essential part in synthetic biology to prepare functional compartments made of soft matter.

4.14 INERTIAL PARTICLES IN TURBULENCE

G. P. Bewley, E. Bodenschatz, H. Xu
J. Bodenschatz, H. Capelo, D. Ivanov, S. Lambertz, S. Risius, H. Xi,
J. Bec (Nice, France), M. Cisse (Nice, France), L. R. Collins (Cornell,
USA), A. Daitche (U. Münster, Germany), M. Gibert (Grenoble,
France), G. H. Good (Cornell, USA), P. J. Ireland (Cornell, USA),
A. Johansen (Lund Observatory, Sweden), S. Malinowski (U. Warsaw,
Poland), E.-W. Saw (Nice, France), R. A. Shaw (Michigan Tech. U.,
USA), H. Siebert (IfT Leipzig, Germany), Z. Warhaft (Cornell, USA)

Turbulence transports and mixes matter very effectively, much more so than diffusion. It also produces violent localized agitations.
These aspects of turbulence have unexpected consequences when a flow carries particles. This is particularly true when the particles are big enough or heavy enough to have their own life in addition to the one imbued by turbulence. In our experiments we have observed how turbulence sometimes causes particles to un-mix, rather than to mix, or how it triggers collisions between particles more frequently and violently than typical conditions would suggest. We survey these results, and others, in what follows.

Clouds are beautiful examples of inertial particles. Clouds are water particles mixed by vigorous atmospheric turbulence. They are also the primary source of uncertainty in climate predictions, in part because we lack an understanding of the strong coupling between turbulence and the growth and decay of cloud particles [2]. It has long been suggested that this coupling bridges the gap between the observed water droplet growth rates in warm clouds and theoretical predictions [3]. A convincing demonstration of this hypothesis is however lacking, due to the difficulty in performing realistic numerical simulations and in observing real clouds from aircraft. We perform both laboratory experiments and field observations of clouds, which offer the unique opportunity to make detailed measurements that resolve the dynamics of individual cloud droplets.

When cloud droplets are small enough, they move with the turbulent air in the cloud. On the other hand, as droplets become larger their inertia affects their motions, and they move differently than the air. Falkovich et al. describe theoretically a specific, new dynamical mechanism called the “sling effect” by which extreme events in the turbulence cause small groups of cloud droplets to break free from the airflow, even while most droplets follow the flow [4]. The sling effect thereafter causes the trajectories of these droplets to cross each other, which increases the chance of collisions that form larger droplets. In a laboratory “soccer ball” experiment, we combined experimental techniques that allow for precise control of a turbulent flow with three-dimensional tracking of multiple particles at unprecedented resolution. In doing so, we observed both the sling effect and crossing trajectories between particles, as seen in Fig. 4.29 [1]. The results provide the necessary support for a theoretical framework that predicts the collision rate of particles, and so the evolution of their size distribution.

Figure 4.29: The sling effect (adapted from [1]). We show the tracks of 19 $\mu$m cloud droplets, with their positions marked at intervals of 67 $\mu$s in a frame with dimensions of about $0.7 \times 0.7 \times 0.5$ mm. These length and time scales are small relative to those of the turbulence. When their inertia is irrelevant, droplets follow each other along parallel trajectories. Here we see instead that inertial droplets moved in two distinct directions, distinguished by the two colors. The yellow spheres mark the positions of the droplets at a given time.
During field campaigns over the last three summers at Zugspitze, the highest mountain in Germany with an altitude of 2940 m, we advanced laboratory image-based techniques for field observations of mountain-top clouds. Fig. 4.30 shows two photos of a laser-sheet slicing into the clouds. In clouds with large droplets, many “holes” were visible which were not present when the droplets were smaller. Droplets may have been absent in these holes because their inertia caused them to avoid vortices in the cloud. This phenomenon has been observed in numerical simulations at low Reynolds numbers and was postulated to happen also in real clouds. Our observations are the first visual evidence of this. This kind of “preferential concentration” of cloud droplets, and the associated dynamics, could have a large impact on the collision and coalescence rate of cloud droplets.

The dynamics of inertial particles gains additional complexity when gravity is relevant. As particles fall, they transit turbulence structures: does this cause them to fall more quickly or more slowly? We addressed the question with both numerical simulations made possible by the expertise of collaborators at Cornell University, and with the “soccer ball” experiment, making this the first truly comprehensive study of its kind. In the experiment, we used cutting-edge techniques like shadow-imaging and an ultrasonic-nozzle to form water droplets to investigate an unprecedented parameter range. Among the new, manifold results is the confirmation that particles can fall either more quickly or more slowly in turbulence, depending on the relative strengths of the characteristic time and velocity scales of the particles and turbulence.

Modeling the forces on a particle moving in a turbulent flow remains an unsettled problem. In nearly all theoretical or numerical analyses, the history forces \([5]\) are ignored, even without proper justification. Other theoretical studies indicate that this could result in large errors \([6]\). To find out the truth, we measured particle motions in a vibrating fluid \([7]\). In comparison with previous experiments, the advantage of ours was that we could independently adjust the dimensionless vibration frequency and the Reynolds number. As seen in Fig. 4.31, we found that history forces are needed to correctly describe the particle motion, even for very small Reynolds numbers \((Rep < 0.2)\). For larger Reynolds numbers, we observed in the data interesting deviations from theoretical predictions. How to incorporate the apparent interplay between finite Reynolds number effects and the history forces is an interesting and ongoing aspect of the work.

The interaction between particles and turbulence underlies planet formation in protoplanetary disks (PPDs). In this setting, micrometer-sized particles are embedded in the gases of the PPDs, and turbulence causes collisions. While sticking after collision can lead to particle growth up to the millimeter size range, particles with larger sizes usually fragment after collisions, which hinders further size increases. Moreover, meter-sized particles in PPDs lose their momentum quickly due to drag and drift radially toward the central star within a timescale much shorter than the typical planet-formation time \([8]\). Currently, the most favorable theory of planet formation is that particles with sizes of centimeters or below form loose clusters due to hydrodynamic
Figure 4.31: Measurements of the amplitudes of particle motions, $A_p$, normalized by those of the fluid, $A_s$, as a function of dimensionless vibration frequency $S$. The particle Reynolds numbers, $Re_p$, are written next to each data point. The legend includes the diameters of the particles used in the experiments.

Figure 4.32: Trajectory of a big particle and tracer particles swirling around it in a turbulent flow. The jet colormap encodes the particles' velocities. The particles were about 1 cm in diameter, or 100 times larger than the small scale, $\eta$, of turbulence.

Interactions. The clusters grow sufficiently large for gravity to take over, which leads to collapse and aggregation of the particles into km-sized planetesimals, the building blocks for planets. Numerical simulations have supported this scenario [9], but no experiment has so far been published. In an apparatus that we recently built in our lab, we study gas-particle dynamics under conditions close to those in PPDs in order to check both the assumptions made in the theory and their quantitative predictions.

Particles can not only be heavy, but also large relative to the scales of motion in the turbulence. It is presently impossible to model the forces on large particles, since the flow surrounding them is not smooth. To make progress, it was necessary not only to follow the motions of big particles, but simultaneously also the fluid motions around them. We overcame this experimental challenge with an advanced particle-tracking system [11]. To isolate the effect of size, we developed a method to track in three dimensions large, density-matched particles in turbulent water. Using the techniques, we measured both the translation and rotation of big particles, and the trajectories of surrounding tracer particles. From data like those shown in Fig. 4.32, we then characterized the boundary layers near the surface of the big particles, and the wakes behind them. This is the most advanced experimental result in the field, which helps to clarify the two-way coupling between particle and flow. We are continuing the work by increasing the number density of particles to quantify their impact on turbulent structure over a wide range of scales.

Over the last decades there has been a growing interest in non-equilibrium systems exhibiting anomalous kinetics. Of particular interest (e.g.) in biology are subdiffusive processes that are characterized by a sublinear growth of the mean squared displacement \(\langle q^2(t) \rangle \sim t^\delta\) with \(0 < \delta < 1\). In many experiments, the subdiffusive behavior can be attributed to trapping events whose duration, \(T\), follows a scale-free waiting time distribution, \(\Psi(T) \sim T^{-(1+\delta)}\) with \(0 < \delta < 1\), where the time that a diffusing quantity spends in a specific state can be of the order of the observation time. The standard model to describe such systems is the Continuous Time Random Walk (CTRW) and its scaling limit, which is described by the Fractional Fokker-Planck equation (FFPE) and subordinated Brownian motion (see Fig.4.33). The CTRW is arguably the most popular mathematical model to characterize subdiffusive processes and has been successfully applied to model experimental data in systems ranging from the classical example of dispersive transport in disordered semiconductors to the diffusion of lipid granules in living yeast cells [1].

![Diagram showing Continuous Time Random Walk (CTRW) and Random Walk](image)

Figure 4.33: In contrast to the standard random walk model, where only the transitions are random, in the Continuous Time Random Walk (CTRW) model the waiting times between two consecutive transitions are also assumed to be random. Mathematically, a CTRW can be described in terms of a standard random walk whose displacements are executed at the events of an independent renewal process. This method, which is referred to as subordination, allows for a consideration of individual sample paths of the process.

The advent of modern single-particle-tracking methods has triggered an increasing interest in the diffusive properties of microscopic tracer particles or single molecules in living biological cells and complex fluids, often revealing anomalous diffusion and weak ergodicity breaking. A theoretical concept that is particularly useful from this point of view is subordination (see Fig.4.33), because it allows for an investigation of individual sample paths of CTRWs, which can be compared with subdiffusive experimental trajectories [1]. The usefulness of the concept of subordination can also be seen in the examples below [2, 3]. A goal of our research is therefore the development of a concept of subordination that also allows us to assess superdiffusive trajectories. We found that this can be achieved by extending the CTRW to a phase space and subordinating the velocity instead of the space coordinate. We have shown that this idea provides a framework to create sample
trajectories also of other superdiffusive processes such as Lévy Walks [2].

Another delicate and open problem concerning CTRWs is the determination of their response behavior to external perturbations. The ability to calculate it is extremely important from an experimental perspective, since response functions play a principal role in promoting the communication between theory and experiments in non-equilibrium systems. To tackle this problem analytically, we have set up the functional representation of CTRWs, which considers the time-inhomogeneity of the process by the inclusion of an additional field that takes the renewal process into account [3]. This representation, from which a path integral formation for fractional Fokker-Planck equations can be derived, serves as a tool that allows one to calculate averages of path-dependent observables, such as multi-point correlation functions.

In the ecological field of foraging animals one focuses prevalently on two-dimensional properties of stochastic processes. Of particular interest in this context is the convex hull of a planar trajectory, defined as the minimal convex polygon that encloses all points of its trajectory (see Fig. 4.34), which often provides a good estimate for the home-range of foraging animals. Since many animals are believed to follow Lévy Walk strategies when searching for food, we have investigated the convex hull of this process by numerical means to quantify their habitat size. Recently, it has been observed that fish trawlers in the Mediterranean Sea influence the foraging behavior of certain seabirds, forcing them to adopt a CTRW-type strategy. With this motivation in mind we were able to analytically calculate the average area and perimeter of the convex hull of general subdiffusive CTRWs by the application of novel subordination methods [4].

If the product of a chemical reaction is the result of a complicated multistep process or if the reaction is catalyzed by a fluctuating environment, the reaction times are usually non-exponentially distributed. Employing a coarse-grained description, such a reaction can be approximated by a one-step process with a waiting time distribution and can therefore be described by a CTRW in chemical space. An example of such a process is the production of mRNA in gene transcription. It is however well-known that mRNA also degrades at a constant rate. Thus, to describe the number of mRNA molecules, a stochastic process has to be considered where the state of the process is affected by normal and anomalous kinetics, simultaneously. We have developed a theory to analyze such stochastic processes and have shown that the time evolution of the mean number of molecules crucially depends upon the explicit form of the waiting time distribution and cannot be described by considering mean waiting times alone [5].

Wave propagation in random media — this might sound abstract but is in fact very tangible and almost omnipresent in science and everyday life. A common example of such random waves in our scientific and everyday environment are surface water waves such as wind-driven ocean waves; light, sound, electrons, tsunamis, and even earthquakes are however also waves that typically propagate in a natural environment through complex media. Due to this complexity, the medium is best described as random, with examples including the turbulent atmosphere, complex patterns of currents in the ocean, translucent biological tissue or a semiconductor crystal sprinkled with impurities.

In recent years, it has become clear that even very small fluctuations in the random medium, if they are correlated, lead to strong fluctuations in the wave intensities that have pronounced, branch-like spatial structures (an example is shown in Fig. 4.35). This branching has been reported for electron, light, sound, and water waves. For the latter, it has been shown to be a possible mechanism for the formation of giant freak waves that are known to be a serious hazard for seafaring ships. Branching leads, however, to strong intensity fluctuations with heavy-tailed distributions in all the wave systems mentioned above (and not only those), of relevance as well, e.g., for remote sensing or communications. It is thus of high theoretical and practical interest to find the intensity distributions of branched flows and their dependence on the parameters characterizing the random medium.

The basic mechanism of branching is the formation of random caustics in the corresponding trajectory or ray flow [1, 2]. Random caustics are expected to cause power-law tails in the wave intensity distribution. These, however, will only be observable when the wavelength is many orders of magnitude smaller than the typical spatial scale of the disorder. For more realistic wavelengths, the intensity distribution of the waves in the branching regime remains an open problem because of the multiple mechanisms influencing this distribution. Thus, while the correspondence of theory and experiment is well established qualitatively, a quantitative comparison allowing us to confirm the underlying mechanisms and to predict wave intensity distributions in applications was still missing. We were recently able to take several important steps to approach this goal.

One of the most fundamental predictions of theory is the typical scale along the propagation direction at which random caustics occur and its scaling with the disorder parameters. We could recently establish, both numerically and experimentally, that the ratio of the variance to the squared mean of the intensity fluctuations, i.e. the scintillation index (SI), is an adequate quantity to assess the spatial scale of branched wave flows [3]. The SI exhibits a pronounced peak at the onset of branching, as illustrated in Fig. 4.36. As shown in Fig. 4.37a,
the position of this peak exhibits the same scaling behavior with the fluctuation strength of the medium, $\varepsilon$, as with the random caustic statistics (even for a wider scaling range). This shows that branching leads to its own fundamental length scale of wave propagation in random media.

The peak of the SI defines the **strong fluctuation regime**, where the fluctuations are much stronger and their distribution much more heavy-tailed as in the **saturated fluctuation regime**, where the intensities follow the exponential Rayleigh’s law and the SI becomes 1. The bottom panel of Fig. 4.36 shows examples of rogue waves with two cuts along a branched wave flow that exhibit fluctuations up to approximately 10 times the mean intensity! While the derivation of the full distribution of intensities in the strong fluctuation regime is very difficult and still elusive, we were able to derive the probability distribution of the highest waves and their scaling with the parameters of the medium [4], as illustrated in Fig. 4.37b.

In the saturated regime, wave intensities are exponentially distributed. We have recently shown, that in branched flows this regime can be reached long before the mean free path [5], due to the superposition of an exponentially increasing number of branches. Ray flows were conjectured to show a log-normal intensity distribution in this regime and we could show that this conjecture is indeed correct. Wave flows, however, do not exhibit log-normal behavior, even for the smallest wavelength, but we demonstrated that decoherence allows us to explain the semiclassical limit and we derived the intensity distribution for arbitrary degree of coherence, as shown in Fig. 4.37c.

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4.17 THE PATH TO SELF-TRAPPING OF BOSE-EINSTEIN-CONDENSATES

Ragnar Fleischmann
Holger Hennig (Cambridge, USA), Thomas Neff

Bose-Einstein condensates (BECs) trapped in periodic, optical potentials have proven to be an invaluable tool to the study of fundamental and applied aspects of quantum optics, quantum computing and solid state physics. In the limit of large atom numbers per well, the dynamics can be described well by a mean-field approximation which leads to a lattice version of the Gross-Pitaevskii equation, the discrete nonlinear Schrödinger equation (DNLS). One of the most intriguing features of the dynamics of such nonlinear lattices is that excitations can spontaneously and stably localize even for repulsive nonlinearities. This phenomenon of discrete self-trapping (ST), also referred to as the formation of discrete breathers (DB) or intrinsic localized modes, is a milestone discovery in nonlinear science that has sparked many studies. DBs have been observed experimentally in various physical systems such as arrays of nonlinear waveguides and Josephson junctions, spins in antiferromagnetic solids, and BECs in optical lattices.

Many experiments do not allow the detailed control of the initial condition necessary to directly excite the ST solutions, and more generally we need to understand the interplay of ST with extended complex dynamics. It is thus an important question, how self trapped and long term stable states can become excited by general initial conditions. This fundamental question, however, had remained mostly unanswered. We have recently made progress in understanding two important mechanisms of ST in BECs, that also carry over more generally to the other systems described by the DNLS. One mechanism, which leads to a very complex ST scenario, is self-localization (SL), where homogeneously extended or thermalized initial conditions can excite self trapped states in the presence of local dissipation (e.g. boundary dissipation). An example is shown in Fig. 4.38. We were able to derive an explicit prediction of the nonlinearity strength at the SL transition, explaining earlier numerical work, and we have shown that SL persists beyond the mean field approximation [1].

Another approach to create ST states is to study how generic localized wave packets can excite ST. In a seminal work from 2001, Trombettoni and Seferis developed a variational approach to study the mean field dynamics of Gaussian wave packets of BECs in optical lattices which has become a standard reference in the field. However, numerical simulations show strong deviations from the variational dynamics. We have therefore numerically calculated a detailed dynamical phase diagram that separates ST from the diffusive and a solitonic regime by defining suitable order parameters and we were able to derive an explicit analytic expression for the ST transition making use of the concept of the Peiers-Nabarro energy barrier [2].

DISORDER IN SPACE AND TIME, STOCHASTICITY

Disorder, random fluctuations and stochasticity govern the dynamics of many complex systems in biology and physics. They can be either due to external noise or are intrinsically created by an out-of-equilibrium system. For chaotic systems such as turbulent fluid flow, disorder and fluctuations are defining features and in biology many mechanisms require fluctuations to function. We study paradigms and develop general tools for describing stochastic dynamics as well as for extracting information from measured noisy signals.

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## 5.1 Crackling Noise in Percolation

Jan Nagler, Malte Schröder, S. H. Ebrahimnazhad Rahbari (Azarbayjan Shahid Madani University, Iran)

Many systems crackle when pushed slowly. Examples include the crumpling of paper, earthquakes, solar flares, and the magnetization of slowly magnetized magnets. For a piece of wood in fire one can even hear crackling noise without special equipment. Across all systems that display crackling noise, the order parameter exhibits randomly-distributed, discontinuous jumps, and these discrete, spontaneous events span a broad range of sizes. The magnification of the hysteresis curve of a magnetic material in a changing external field, for instance, reveals that the magnetization curve is not smooth, but rather exhibits small discontinuities. This series of correlated, discontinuous jumps is called the Barkhausen effect, which is a standard example for crackling noise in physics (see Fig. 5.2(a)).

![Figure 5.2: Crackling noise. a) Barkhausen effect in ferromagnets: the hysteresis curve shows tiny discontinuities b) Crackling noise in percolation. The evolution of the largest component is displayed. The control parameter, f, determines the magnitude of the discontinuities that, importantly, survive in the thermodynamic limit.](image)

Fragmentation processes where homogeneous parts break up into smaller ones (see Fig. 5.1(a)), are ubiquitous and have been studied intensely. An important observation is that the size of the fragments are of the same order of magnitude as the parent pieces. Thus the case where one fragment is microscopic while the size of the other fragment is substantially larger is rare. We have modeled this by systematically suppressing asymmetric breakups. This suppression suggests a fractional increase of clusters that is time-reversed fragmentation (see Fig. 5.1(b)).

![Figure 5.1: a) Fragmentation and b) fractional percolation. In the process of fragmentation, clusters split up into parts of a certain fraction. We have studied the reverse dynamics, fractional percolation.](image)

With a single event analysis [1, 2] we could show that (i) a fractional growth mechanism, (ii) a threshold mechanism, and (iii) a mechanism that amplifies critical fluctuations account for the main features of crackling noise. The framework allows us to derive macroscopic features from the underlying micro-dynamical mechanisms and exposes connections between the seemingly unrelated concepts of percolation, fragmentation, and crackling noise [3].

5.2 EVOLUTION OF DROPLET SIZE DISTRIBUTIONS

T. Lapp, M. Rohloff, B. Hof, J. Vollmer
M. Abel (Potsdam), G. Bewley, M. Wilkinson (Milton Keynes)

In nature and technology one commonly encounters situations where a mixture is subjected to a slow temperature change which drives it deeper into the phase-coexistence region. Continuously heating a binary fluid mixture can lead to an oscillatory response of precipitation (Fig. 5.3 a) [1, 2, 3, 4]. These oscillations can be followed in the size distribution [2, 4] and turbidity [1, 4]. The temperature ramps are chosen such that the temperature induced change of droplet volume fraction, $\xi$, is constant. We model the emerging precipitation cycles as alternation of two growth regimes [4]. Small droplets mainly grow by diffusively collecting supersaturation. Large droplets sediment and grow by collisions with smaller droplets. For intermediate droplet radii both growth modes are inefficient. This bottleneck sets the timescale $\Delta t$ for the precipitation period. We deduced a non-trivial scaling, $\Delta t \sim \xi^{-3/7}$, with a prefactor which contains the relevant, temperature-dependent material parameters of the mixture. It faithfully describes the period (Fig. 5.3 b). The improved understanding obtained from this quantitative description of precipitation will find applications in low temperature physics [5], material science, and to the modeling of atmospheric precipitation on earth and other planets.

In parallel to the growth of droplets in the bulk we also considered their growth and coalescence on substrates [6]. Remarkably, the observed size distributions are selected by the physics characterizing the small-scale droplet growth, Fig. 5.4 d) and e), rather than by a universal scaling description.


Figure 5.3: a) The demixing of isobutoxyethanol and water for $\xi = 2.5 \times 10^{-2}$s$^{-1}$. The space-time plot shows the time evolution of vertical turbidity profiles. For different composition and $\xi$ the oscillation period, $\Delta t$, varies over more than two orders of magnitude. b) All data collapse on a single master curve when plotting $\Delta t \xi^{-3/7}$ as a function of the reduced temperature $\theta$. The lines provide our theoretical predictions [4].

Figure 5.4: Rescaled size distribution of droplets on a plate [6] for a) a numerical model, and b) water droplets on polyethylene film. c) A data collapse $f(s/S) = n(s) s^{-5/3} (s/Y)^{1/3} / \xi (s)$ is achieved by accounting for different microscopic droplet growth d) and e), and a fractal arrangement of the droplets characterized by the non-universal exponent $\alpha$. 
5.3 CRISIS AND CHAOS IN SHEAR FLOWS

T. Kreilos, T. M. Schneider,  
B. Eckhardt (Marburg)

In linearly stable shear flow’s turbulence spontaneously decays over a characteristic transient lifetime, $\tau$. The lifetime sharply increases with Reynolds number, $\text{Re}$, such that there is a possible divergence marking the transition to sustained turbulence at a critical point; this has been discussed, yet the mechanism underlying the increase has not been understood. We demonstrate a mechanism by which the lifetimes increase: a locally attracting orbit forms a turbulent pocket via a route-to-chaos sequence of bifurcations, followed by a boundary crisis in which the chaotic attractor turns into a chaotic saddle. The complexity of the turbulence-supporting saddle hence increases and it becomes more densely filled with unstable periodic orbits, increasing the time it takes for a trajectory to leave the saddle and decay to the laminar state. We demonstrate this phenomenon in the state space of plane Couette flow and show that as a result, characteristic lifetimes vary non-smoothly and non-monotonically with Reynolds number.

In a small, periodic domain, the emerging chaotic saddle is visualized for successively growing $\text{Re}$ in Fig. 5.5. The first known coherent structures are created in a saddle-node bifurcation, with an attracting upper branch whose basin of attraction (small, dark-red region in (a)) is separated from the attracting laminar state by the stable manifold of the lower-branch. The fixed-point undergoes a series of bifurcations that result in a chaotic attractor (b). At $\text{Re} = \text{Re}_{cr}$, the chaotic attractor collides with the lower-branch state, leading to boundary crisis where it turns into a chaotic saddle (c). At higher $\text{Re}$, a complex saddle has formed (d).

At higher $\text{Re}$, the same mechanism creates further new pockets embedded in the chaotic saddle (Fig. 5.6). Once the local chaotic attractor undergoes a boundary crisis it joins the surrounding saddle at a discrete $\text{Re}$. This sudden expansion of the chaotic saddle allows for longer transients quantified by an increased $\tau$. Consequently, a growth of the saddle via discrete bifurcations is associated with non-smooth and non-monotonic variations of the lifetime [2]. Smooth variations are only recovered in a statistical sense.

5.4 STATISTICAL MECHANICS OF GRANULAR MEDIA

M. Schröter, S. Zhao
R. Stannarius (Uni Magdeburg)

This project tries to answer the scientific question whether static granular packings can be described with a statistical mechanics based approach as suggested in [1]: assuming the existence of a periodic driving protocol which explores all mechanically stable states with equal probability, a configurational entropy $S$ can be defined as the logarithm of the number of these states for a given volume $V$. Then a configurational temperature, named compactivity $X$, can be defined as $\partial V/\partial S$. This approach is far from being an established theory. Several basic questions, like the role of ergodicity, or even how to measure $X$ are still open issues. For a recent review see [2].

In the last three years we tested this statistical mechanics approach using packings of binary discs (c.f. Figure 5.7). Our two main results are shown in in Figure 5.9: I) The Voronoi volumes associated with the individual particles are correlated, these correlations decay exponentially even in dense systems [3]. II) We compare experimentally three alternative suggestions to measure $X$ from volume distributions. Due to the volume correlations all three become intensive only for clusters with more than 150 particles. Moreover, only two of them agree in their numerical values; the third one can be shown to fail also with regard to other granular phenomena [4].

In ongoing work we study together with Ralf Stannarius the role of configurational entropy in the segregation of binary granular mixtures.

Figure 5.7: Binary disc packing, prepared with flow pulses in an air-fluidized bed.

Figure 5.8: Voronoi tessellation of a disc packing as in Figure 5.7. The hexagonal wheel picks pairs of particles at a distance $L$; the correlation between their volumes is shown in the left panel of Figure 5.9.

Figure 5.9: Left panel: The correlation between two Voronoi volumes as a function of their distance $L$ (measured in units of small disc diameters $d_s$). Dense packings exhibit anti-correlations for $L \geq 2.5 d_s$. From [3]. Right panel: Comparison of three different ways to compute compactivity for single discs and clusters of 150 particles [4]. In all three cases $X$ of a single particle is smaller than that of a larger cluster. $X_{OH}$ and $X_{VF}$ agree quantitatively, $X_{\Gamma}$ is about an order of magnitude smaller.

5.5 FOUNDATIONS OF STOCHASTIC THERMODYNAMICS

B. Altaner, S. Herminghaus, M. Timme, J. Vollmer
L. Rondoni (Torino), S. Grosskinsky (Warwick)

Stochastic Thermodynamics is the quest for understanding the emergent macroscopic thermodynamic behavior of complex systems that are modeled by stochastic dynamics [1]. Such models are mesoscopic descriptions, and their apparent random behavior has its origin in deterministic-chaotic dynamics at the microscopic level [2, 3]. Different notions of entropy and entropy production have been introduced for different types of models that address the description of the dynamics with different resolution. We address the question of thermodynamic consistency: When and how can entropies and entropy production be related that arise in the context of different models? How does this connect to the notions of entropy and dissipation in equilibrium thermodynamics? Results obtained during the report period include:

1. The connection of macroscopic thermodynamic currents in nonequilibrium steady states to cycles in mesoscopic stochastic models [4].

2. A thermodynamically consistent, fluctuation-sensitive coarse-graining algorithm for stochastic, mesoscopic models [5]. The potential of this method was demonstrated by simplifying a well-known model for the motor protein kinesin (see Figure 5.10).

With our Master student A. Wachtel we presently look systematically at the structure of emergent macroscopic fluctuations in the framework of large deviations theory.

Moreover, we address the microscopic-mesoscopic connection: How do entropy changes in dynamical systems (KS-entropy, Lyapunov exponents) relate to the entropy production identified for a stochastic process generating the time-series of coarse-grained observables? To answer these questions we devised network multibaker maps as a versatile model system to understand different types of dynamical systems [6]. Preliminary results hint at a new understanding of local equilibrium as a requirement for thermodynamic consistency.

5.6 LIFE AFTER SEX: THE AMEIOTIC GENOME OF THE BDHELLOID ROTIFER ADINETA VAGA

J.-F. Flot, O. Hallatschek

Bdelloid rotifers are microscopic animals that are considered ‘ancient asexual scandals’ because they have persisted and diversified for at least 40 million years in the apparent absence of sexual reproduction and meiosis [1]. This runs contrary to the common view of asexuality as an evolutionary dead end for animals (notably because of Muller’s ratchet, i.e., the accumulation of deleterious mutations due to genetic drift, which is essentially irreversible in the absence of recombination), causing doubts as to whether bdelloids are really asexual.

To bring a definite answer to this question, we used next-generation, whole-genome sequencing to search for genomic signatures of sex (or lack thereof) in the bdelloid rotifer, *Adineta vaga* [2]. Genome assembly turned out to be particularly challenging, since laboratory crosses could not be performed to reduce this organism’s natural heterozygosity: hence, a novel approach had to be devised to separately assemble the haplotypes of this species.

Intragenomic comparison of the reconstructed haplotypes allowed us to distinguish alleles from ohnologues (i.e., paralogues resulting from whole genome duplication). At local scale, the genome of *Adineta vaga* turned out not to be markedly different from the one of a sexually reproducing species: notably, there was no genome-wide allele sequence divergence (the so-called Meselson effect supposed to occur when mutations accumulate in the absence of recombination), as the divergence between allelic gene versions was 4.4%, a value similar to the ones measured in sexual species of ascidians and urchins. At chromosome scale, however, we detected numerous genome rearrangements between alleles, making meiotic pairing of chromosomes nearly impossible (Fig. 5.11). In twenty cases, allelic regions comprising of

Figure 5.11: Circular plot representing the connections between alleles found on av1 (the largest assembled fragment of the genome of *Adineta vaga*) and other genome fragments. In a sexually reproducing species all of the genes of av1 should have their other alleles arranged in the same order on another genome fragment. In the case of *Adineta vaga*, however, local colinearity between allelic regions of the genome does not extend to chromosome scale, a situation incompatible with meiotic pairing.
tens to hundreds of genes were found to be physically linked to one another on the same assembled genome fragments, which appear to be incompatible with meiotic segregation of alleles into haploid gametes; in seventeen of these cases, allelic regions were arranged in palindromes (inverted segmental repeats), reminiscent of the genome structure of cancer cells and of the ‘amplionic’ structure of the Y chromosomes of mammals and flies (Fig. 5.12). Hence, we propose that the lack of chromosome-scale homology and the presence of large genomic palindromes are general signatures of ameiotic evolution.

Other notable features of the genome of Adineta vaga include a high percentage of putative, horizontally transferred genes of non-metazoan origin (10% of the total gene set), as well as strong signatures of interallelic gene conversion events (that seem to be at least one order of magnitude more frequent than point mutations). Both horizontal transfer and gene conversion probably result from the frequent cycles of desiccation and rehydration experienced by bdelloids in their natural environments (mosses, lichens, ephemeral ponds, ...) and may explain how bdelloids have been able to thrive over geological timescales in the absence of meiotic recombination.

Figure 5.12: Circular plot of the twenty assembled genome fragments where allelic regions were found to occur on the same chromosome.

In three cases, the two allelaid regions had the same orientation (direct repeats, shown in pink), whereas in the seventeen other cases they were inverted (palindromes, shown in purple). Additional local allelic relationships between assembled genome fragments are shown in violet.

5.7 ACTIN DYNAMICS AND MOTILITY STATISTICS OF AMOEBOID CELLS


The actin cytoskeleton, a dynamical, cross-linked biopolymer scaffold at the inner side of the plasma membrane is essential for many biomechanical properties of eukaryotic cells. Examples that rely on the rapid rearrangement of the actin cytoskeleton in response to external chemical cues are found in wound healing, in the morphogenetic development of an embryo, or in the metastatic spreading of cancer cells in the body [1]. One of the most convenient and well-studied eukaryotic model organisms is the social amoeba *Dictyostelium discoideum*, a single-celled eukaryote that exhibits chemotactic responses in gradients of extracellular cAMP [2].

In a recent study, we have exposed single chemotactic *Dictyostelium* cells to well-controlled temporal stimuli of cAMP [3]. Short pulses and periodic pulse trains were generated using microfluidic flow photolysis, an approach that is based on the light-induced cleavage of caged cAMP in a microflow [4]. Single cell responses of the actin system to a short stimulus of cAMP included short, strongly damped responses of the actin machinery, as well as slowly decaying, weakly damped oscillations. In a small subpopulation, even perpetual autonomous oscillations in the cortical actin density were observed. These findings suggest that the actin machinery of chemotactic *Dictyostelium* cells operates close to the onset of oscillations. Stimulation with periodic sequences of cAMP pulses confirmed these results. When monitoring the actin response as a function of the stimulation frequency, we found a resonance at a stimulation period of around 20 s. Our findings can be explained in the framework of a generic model that captures the time delay in the regulatory network of the actin system. By using cell lines that expressed GFP-tagged fusion proteins as well as knockouts of actin-binding proteins that enhance the disassembly of actin filaments, we were able to confirm our model.

When placed in a gradient of cAMP, receptor-mediated signaling pathways translate the external signal into an asymmetric pattern of actin activity inside the cell. A clear leading edge is formed in the gradient direction, where enhanced actin polymerization pushes the membrane forward to induces pseudopod formation. At the same time, the lateral formation of membrane protrusions is suppressed and the rear of the cell contracts, so that, overall, a chemotactic motion arises, where the cell’s center of mass is displaced in the direction of the chemical gradient [5]. In general, chemotaxis of eukaryotic cells may depend both on the gradient steepness and on the average ambient concentration of the chemoattractant. In a recent theoretical work, it was predicted that the efficacy of chemotaxis is determined...
by a single control parameter only, namely, the signal-to-noise ratio (SNR) [6]. The SNR depends on fluctuations related to the binding event of the chemoattractant molecule to the transmembrane receptor and on fluctuations at the level of receptor-induced intracellular second messenger production. We have quantitatively tested this prediction based on a systematic analysis of Dictyostelium chemotaxis in stationary linear gradients of cAMP using microfluidic tools in combination with automated cell tracking [7]. Examples of chemotactic trajectories from this study can be seen in the upper part of Fig. 5.14. Our analysis showed that the theory correctly describes the experimental findings for a SNR equal to or smaller than one. For a larger SNR, deviations from the theoretical predictions were observed due to additional events downstream in the signaling cascade. This is illustrated in the bottom part of Fig. 5.14, where the chemotactic index (CI) is displayed as a function of the SNR at the level of the G protein for different average cAMP concentrations. For SNR\(_G\) ≤ 1, both curves collapse, whereas for SNR\(_G\) > 1, the CI saturates at a concentration-dependent value.

Apart from global measures like the chemotactic index, we have focused on detailed descriptions of the chemotactic motion in terms of stochastic differential equations. In particular, we have extended our previous work on non-directed random motion of Dictyostelium cells and derived a statistical model that quantitatively captures the chemotactic motion in a chemical gradient [8, 9]. Our Langevin-type model equation describes directional motion as the interplay of deterministic and stochastic contributions. We performed angle-resolved conditional averaging to extract the form of this equation directly from our data. It is characterized by a quadratic damping term and by multiplicative noise. In the presence of a gradient, the deterministic part shows a clear angular dependence leading to an effective directional force term in the equation of motion. With increasing gradient steepness, this force passes through a maximum that coincides with maxima in both speed and directionality of the cells. The stochastic part, on the other hand, does not depend on the orientation of the directional cue and is independent of the gradient steepness. We have thus provided a probabilistic description that will serve as a starting point to quantify differences in the motion patterns of mutant cells in order to characterize the role of different signaling molecules and cytoskeletal regulators in the directed locomotion of eukaryotic cells.

5.8 HOW DID THE FIRST SPECIES EVOLVE? – STATISTICAL PHYSICS OF EARLY EVOLUTION

H. Arnoldt, J. Nagler, M. Timme
S. Grosskinsky (University of Warwick, UK), O. Hallatschek

Core aspects of evolutionary dynamics crucially depend on stochastic events coming from, e.g., random mutations and interactions, stochastically changing environments or number fluctuations in finite populations [1, 2]. It remains an outstanding problem how the first species could have evolved, particularly in the highly stochastic environments of early evolution that are thought to be dominated by horizontal gene transfer.

Speciation in early evolution by horizontal gene transfer? We were analyzing the impact of horizontal gene transfer on evolutionary dynamics, with a specific focus on the emergence of speciation in early evolution. Horizontal gene transfer (HGT) is the transfer of genetic material between organisms within their lifetimes. Today, HGT is basically active in certain simple organisms, but is assumed to have been prominent during the early stages of life on earth [3]. High HGT rates, however, are thought to induce a high rate of mixing between genomes amongst the organisms and thereby to imply an evolutionary state with a collection of organisms exhibiting a continuous variety of genomes, sometimes called the “reactive soup.” It therefore remains unclear how evolution in the presence of dominant HGT could have created separate species of organisms with (almost) identical genomes.

Our theoretical studies on the impact of HGT on stochastic evolutionary dynamics suggest that such a “reactive soup” state may actually coexist with a state where selection dominates and populations may evolve to become fitter (cf. Figure 5.15). Stochastic switching between these two types of states seems viable such that exploring genome space at high HGT rates alternates with increasing fitness (in the sense of being better adapted to the given environment). In the selection-dominated state, the population may then acquire reduced competence levels, such that the organisms are less inclined to participate in HGT. Repeated switching between selection-dominated and HGT-dominated states may then yield separate yet appropriately adapted (fit) species (Arnoldt et al., in preparation).

Hypernetwork dynamics – progress on the general theory of network dynamics. Mathematically, the possible genetic changes due to horizontal gene transfer constitute an important example for the dynamics of hypernetworks. To date, studies on the nonlinear or stochastic dynamics of networks in general still largely focus on systems with two-point interactions, likely because pairwise coupling prevails in classical subfields of physics. Hypernetworks are networks with “links” or interactions simultaneously defined by more than two nodes. Scientists now increasingly recognize that three-point and higher order interactions govern the dynamics of many networked systems in nature, in social and in engineering systems.

Figure 5.15: Population dynamics switch between a “reactive soup” state and a selected state. The more the population is distributed in genotype space, the higher the population entropy $S$ (a) and the smaller the average fitness $f$ (b). In the “reactive soup” (high $S$) state, HGT dominates, whereas in the low-$S$ state, selection dominates, thus increasing fitness. (c) The potential $V(S)$ of the entropy dynamics exhibits a bifurcation from a switching to a selection-dominated state upon decreasing the competence of the individuals for HGT.
In biological evolution, such hypernetworks naturally arise through interactions mediated by HGT: in a single HGT event, genetic material from one organism (say, A) is transferred into the genome of another (say, B) such that the latter becomes a new organism (say, C) with a genome different from that of B. This constitutes a particular three-point interaction among organisms A, B, and C, where A specifically influences the transition of B to C. In our studies of stochastic evolutionary dynamics in the presence of HGT, we have now contributed towards mathematically formulating this dynamical problem of hypernetworks, having numerically simulating it and are currently working towards analytically defining its relations (“projections”) to standard network dynamics in a general setting (Timme et al., in preparation).

5.9 STOCHASTIC POPULATION DYNAMICS

S. Eule, T. Geisel, D. Lamouroux, C. Kirst, J. Nagler, V. Belik

From ensembles of molecules in chemical reactions to groups of organisms in large ecosystems, populations are permanently exposed to random fluctuations. These fluctuations originate either from the finiteness of the population or from a randomly changing environment. Often they influence the fate of a population significantly and can lead to such dramatic events as the extinction of a species and the loss of biodiversity. We are specifically interested in the effect of migration on the preservation of an ecosystem. To this end, we have investigated the influence of random movement in a model of three species under cyclic competition, which is equivalent to the well-known rock-paper-scissors game. Intrinsic fluctuations eventually lead to the loss of a species and ultimately only one species survives. If migration is included into the model, this loss of biodiversity is significantly slowed down due to the formation of spatial spirals. To vary the population size independently from the spatial extent, we have introduced a carrying capacity. We found that it is a crucial parameter to determining a critical mobility below which the system becomes almost stable [1].

If a population is exposed to a randomly changing environment, small changes in the amplitude of the fluctuations can have drastic effects on the evolution of the population and lead to so-called noise-induced phase transitions. In contrast to the commonly studied stationary probability distribution of the population frequency, we are interested in the statistics of the extrema of the frequency, as they influence the fate of the population most. We have studied a standard model of population dynamics with birth and death rates switching randomly between two values. For the paradigmatic case of a memoryless switching behavior with exponentially distributed waiting times, we were able to find a full, analytical solution [2].

Spatially varying environments on the other hand have up to now attracted astonishingly little attention in population dynamics. To study the effect of geographic heterogeneity in epidemic models, we considered a model of two spatially separated populations with differing infection rates. While they each have a well-defined endemic state if separated, we were interested in what happens if one allows for migration between the two populations [3]. Below a critical traveling rate we found the counterintuitive result that migration decreases the level of infection even further in the healthier population while it increases the level in the other one. This finding demonstrates that conventional prevention and control strategies may even be harmful if disease properties vary spatially.

5.10 CLASSIFYING AND PREDICTING EVENTS IN COMPLEX SYSTEMS

S. Hallerberg, M. Timme, J. Nagler
F. Noriega, N. Sharafi, X. Zhang, H. Gutch, D. Hofmann, Y. Radstake, M. Zetzsche K. Hammerschmidt (German Primate Center, Göttingen), H. Vester (OceanSounds, Norway), A. S. de Wijn (Stockholm, Sweden) C. Kühn, (Vienna, Austria)

Classifying and predicting events generated by a system with complex dynamics are challenging tasks, in particular, if the system exhibits chaotic or transient dynamics in high-dimensional phase space.

One example for events that form such a challenge for classification are the vocalizations of social whales such as dolphins, killer whales (see Fig. 5.17) and pilot whales. Their vocal repertoire consists of a variety of sounds such as calls, whistles, clicks, and buzzes and there are also observations of these sounds being used in systematic combinations (see Fig. 5.18). If and how these acoustic patterns are used to transmit information within a group of whales is largely unknown. We study distributions of acoustic features of ensembles of killer whale vocalizations depending on behavioral context. Computing Kullback-Leibler-divergences, we find significant qualitative and quantitative differences between sound features produced in different behavioral contexts. In particular, distributions of sound features during salmon hunting and feeding [1] and in non-feeding contexts are substantially different. We further estimated the social structure of a group of killer whales using photographs of their dorsal fins (see Fig. 5.19). Analyzing the time stamps of the photos reveals which whales associate.

Apart from complexity, a special challenge for classification and prediction consists in events which are rare and far different from the average behavior of the system under study. As examples for these extreme events we consider here critical transitions in multistable systems, short time anomalous movements in molecular dynamics and rare events in spatio-temporal chaos.

Critical transitions in multistable systems have been discussed as models for a variety of phenomena ranging from the extinctions of species to socio-economic changes and climate transitions between ice-ages and warm-ages [2, 3]. From bifurcation theory we expect a critical transition to be announced by a decreased recovery from external perturbations [3]. However, it is not clear, whether corresponding changes in observation variables are statistically relevant such that they could be used as predictors for critical transitions. We therefore quantify the predictability of critical transitions in bistable systems under the influence of external noise.

We also study how rare and extreme events are reflected in the dynamical properties of systems exhibiting spatio-temporal chaos and how this information can be used to develop better predictions of extreme events.

Finally, we use prediction algorithms in the spirit of Granger causality [4, 5], to reveal links between discrete events and variables of a
high dimensional dynamic systems. Recent studies highlight the existence of a connection between the short term anomalous movements in the diffusion of molecules and the dynamics of their internal degrees of freedom [6]. We apply statistical inference to reveal connections between energy fluctuations in specific internal degrees of freedom and short-time anomalous movements in surface diffusion, i.e., long ballistic jumps (see Fig. 5.20). We also verify that it is possible to predict and manipulate the diffusion of the simulated molecule by deliberately triggering the indicators [7].


Figure 5.20: Anomalous nano-motion: ballistic jumps in simulated trajectories of benzene molecules on a graphite surface.
5.11 RECONSTRUCTION AND PREDICTION IN CORRELATION NETWORKS

Annette Witt, Theo Geisel, Jan Nagler, Magdalena Kersting

Complex networks consist of many interacting units, which are idealized as nodes. A given interaction between two nodes is usually represented by a link. We consider correlation networks (cornets) where the $i$-th node is associated with the temporal development of an observable, $x_i(t)$. The undirected link between two nodes is defined by their cross-correlation function, $C_{ij}(\tau)$, which depends on the time lag $\tau$.

An example for this abstract structure is given by a set of temperature time series at different locations, $i$ and $j$ (the nodes), and their set of linear, two-point correlation functions (the links). Cornets have been exploited for quantifying the interactions that underly the dynamics in many heterogeneous networks. Examples include the interactions in gene expression networks, the activity of brain areas, the dynamics in climate networks and collective behavior in socio-economic systems.

In many cases the cornet under study is sparse and thus incomplete. As cornets carry essential information about the underlying system it is thus an important question if and how missing parts of a cornet can be reconstructed, and if and how an observable can be predicted.

To each network node we assign a stochastic process, $P_i$, and a set of realizations of this process, $\{x_i(t)\}$. We call the complete set of all $P_i$ a $P$-cornet and a single set of realizations an $R$-cornet.

Based on spectral matrix factorization [2] we have developed an algorithm that generates $R$-cornets and their associated multivariate time series for a given $P$-cornet [3]. Furthermore, for $R$-cornets we have identified the conditions for the reconstruction of the entire linear cross correlation structure from a subnetwork which contains the same nodes but only a fraction of the links. Remarkably, certain loop structures of the subnetwork determine the reconstructability; the subnetwork must either contain a loop with an odd number of links, or a self-link. Fig.5.11 shows examples of subnetworks which allow a complete $R$-cornet reconstruction.

For a given $P$-cornet we have developed a parameter-free tool for generating $R$-cornets and their associated time series [3]. These consistent ensembles of multivariate time series allow for hypothesis tests such as a significance test for the presence of nonlinear correlations [4], or a test for stationarity.

5.12 DYNAMICS OF NEURONAL ACTION POTENTIAL ENCODING

F. Wolf, A. El Hady, A. Neef

(a) Schematic representation of the ongoing synaptic drumfire to which neurons in the CNS are typically exposed. Sparks represent active synapses. Cortical pyramidal neurons will typically receive synaptic inputs at a rate of several kilohertz. (b) & (c) Two alternative experimental approaches to emulate the resulting input fluctuations and register the fluctuation-driven activity in-vitro: whole cell current injection (b) and CoDyPs (c), here depicted for a neuron cultured on a circular extracellular electrode. In contrast to the whole cell stimulation/recording, CoDyPs offers extended recording and stimulation/recording of multiple neurons simultaneously.

Figure 5.22: Two ways to study in-vivo-like fluctuation-driven action potential activity under controlled conditions.

The ability of neuronal populations to rapidly encode varying stimuli and respond quickly to abrupt input changes are crucial for basic neuronal computations, such as coincidence detection, grouping by synchrony, and spike-timing-dependent plasticity, as well as for the processing speed of neuronal networks. Our theoretical and computational analyses predicted [1, 2, 3, 4, 5] that these abilities are linked to the fast-onset dynamics of action potentials. Using a combination of whole-cell recordings from rat neocortical neurons [6], analytically tractable non-equilibrium statistical mechanics models [3] and computer simulations [5, 7], we recently provided the first experimental evidence for this conjecture and proved its validity for the case of action potential initiation in the axon initial segment, typical for cortical neurons [7]. We found neocortical neurons with rapid-onset of action potentials capable of phase-locking their firing to signal frequencies up to 300 – 400 Hz [6, 7]. Populations of a few thousand neurons are capable of responding within 1 – 2 ms to subtle changes in their input current. We found that the ability to encode high frequencies and response speed were dramatically reduced when action potential onset was slowed by experimental manipulations or was intrinsically slow due to an immature action potential generation mechanism [7]. Multi-compartment conductance-based models reproducing the initiation of spikes in the axon initial segment could encode high frequencies only
if action potential onset was fast at the initiation site (e.g., attributable to cooperative gating of a fraction of sodium channels as previously predicted by us from biophysical observations), but not when a rapid onset of somatic action potential was produced solely by lateral currents. These findings indicate that rapid-onset dynamics are a genuine property of cortical action potential generators. Furthermore, it strongly suggests that they are essential for high bandwidth computation and information transfer in cortical circuits.

Although our results clearly verify our previous theoretical predictions and establish an unexpected temporal accuracy of action potential initiation and encoding, the biophysical and molecular basis of this phenomenon remains elusive. Studies of single neuron computation that preserve natural operation conditions so far rely on invasive stimulation methods that are severely constrained by limited recording duration and low yield. Combining noninvasive optogenetic stimulation with multichannel multi-neuronal recordings promises to overcome these fundamental limitations and to open up an avenue to effectively investigate the encoding dynamics of neurons under different conditions. The characterization of single neuron computation, however, requires a precise knowledge of the input in order to compute, for instance, quantities like the spike-triggered average or covariance of the input, or to describe correlation gain and firing rate adaptation in the dependence of the stimulus properties. An optical, noninvasive stimulation approach would be instrumental for such studies, but only if (1) the induced conductances are highly reproducible with correlation times suitable to mimic fluctuating synaptic conductances, (2) waveforms can be precisely designed and predicted, and (3) conductance waveforms can be stably induced in long-term experiments. In order to study dynamical encoding properties effectively using optogenetics, we have developed and characterized continuous dynamic photostimulation (CoDyPs), a novel approach to mimic in-vivo-like input fluctuations noninvasively in cells transfected with channelrhodopsins [8]. Even during long-term experiments, cultured neurons subjected to CoDyPs generated seemingly random, but highly reproducible action potential patterns. In voltage-clamped cells, CoDyPs induced highly reproducible current waveforms that could be precisely predicted from the light-conductance transfer function of the channel. When combined with non-invasive spike-detection, CoDyPs allows the acquisition of orders of magnitude larger data sets than previously possible, opening the way for studies of dynamical response properties of many individual neurons.

The control of dynamical systems is a major challenge in nonlinear science, with applications in physics, biology, engineering, and medicine. Under the topic ‘control’ we show that collective network dynamics may enable reliable computations based on “imperfections” of natural systems including chaotic and unstable dynamics or random failure. In microfluidic systems we demonstrate control of multiphase flow with potential applications to high-throughput quantitative biology. In biomedical applications we study the control of multiple vortex-like rotating waves underlying the spatial-temporal complexity of electrical turbulence in the heart, which may open the door towards painless and non-damaging termination of life-threatening cardiac arrhythmias.

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6.1 HIGH-THROUGHPUT QUANTITATIVE BIOLOGY

J. Lim, P. Gruner, D. Pekin, J.-C. Baret
M. Konrad, C. Karamistos (MPI-bpc); A. Griffiths (ESPCI); V. Taly
(Université Paris Descartes)

Droplet-based microfluidic systems have an enormous potential for applications in the field of quantitative biology. The ability to parallelize and automatize assays is for example key in drug screening applications, providing reliable and statistically relevant measurements to discover new drugs [1]. For molecular diagnostics, we have shown that the sensitivity of detection of mutant DNA sequences in normal sequences can be increased by more than three orders of magnitude using droplets as microreactors providing new tools to detect cancer in patients at very early stage [2]. Such a system is of practical relevance as the success of a treatment is, in a large part, related to the timing of the diagnosis. Another area of interest for droplet microfluidics is the ability to select specific variants in a population at very high throughput [3]. Microfluidic tools are therefore used for directed evolution and protein engineering [4] in which large libraries of mutants are screened and selected for their improved properties.

We are developing microfluidic tools for directed evolution of enzymes of therapeutical interest related to cancer research (see side Figure). L-asparaginase (L-ASNase) is an enzyme currently used as a treatment for Acute Lymphoblastic Leukemia. However, the bacterial origin of the L-ASNase makes it prone to trigger immunoreactions which results in the interruption of the treatment, very often fatal for the patient. The human version of ASNase – less immunogenic – is at present not active enough to be used as a drug. We propose to use directed evolution in microfluidics to improve the enzyme efficiency. We developed a three-step fluorogenic assay to detect L-aspartate produced by hydrolysis of L-asparagine by L-ASNase. For purified enzymes, the kinetic measurement of the L-ASNase activity in droplets, are in agreement with those observed by the standard spectrophotometric assays. For cells expressing enzymes – which will be used in the directed evolution experiments – no activity was detected when the enzyme is expressed in the cytoplasm. By displaying the enzyme at the membrane of the bacteria, we recover quantitatively the activity level showing that the transport of reagents and products through the cell membrane is here a key to be considered (see also section 7.1).

Driven by technological developments, it is clear that increasing the throughput of assays is beneficial. We have demonstrated methods to parallelize fluorescence detection based on microfabricated microtens array, interfaced with microfluidic channels. Ultra-High throughput is then now accessible with our system exceeding 100 000 droplets/sec [6], larger than the throughput of commercial flow cytometers. We demonstrated the detection of single bacteria in droplets through a model enzymatic reaction: the β-galactosidase activity of E.coli cells is here detected in 100 pl droplets. Such a throughput is at least 10 fold larger than those demonstrated so far with biological systems in microfluidics.

Figure 6.1: Detection of Asparaginase activity based on a fluorogenic assay. (a) Principle of the assay. (b) On chip measurement of enzymatic activity in droplets for purified enzymes. (c) Cell-based assay: we developed a display technique to circumvent the transport through the inner cell membrane.
Figure 6.2: Parallelisation of fluorescence detection with lens array. (a) Scheme of the microfabrication process for both the micro-lens array and the microfluidic channels. (b) Example of multicolor fluorescence detection for droplets. (c) Reinjected emulsion in a parallelized system made of 100 micro-lenses. The signal is recorded on a high-speed camera and post-processed to measure enzymatic activities of single cells in droplets. The throughput reached in the case of the β-galactosidase activity was larger than 100 000 droplets per second.

Beyond the technological aspects, droplet-based microfluidics has a tremendous potential for synthetic biology. We have demonstrated several cell-free platforms for protein expression and single gene amplification in compartment that provide new tools to miniaturize biochemical assays [5]. At the same time, making use of soft matter properties such as controlled transport or self-propulsion, we can transform the so far passive microcompartments into active, out-of-equilibrium, functional microcompartments made of simple soft-matter ingredients. It becomes possible to assemble minimal cells from bottom-up in a synthetic biology approach.

6.2 INTELLIGENT DYNAMICAL SYSTEMS AND NATURAL COMPUTING

G. Weber, F. Fix

How can bio-inspired dynamical systems process information? Theoretical concepts of neural and neuro-inspired computations often rely on stable dynamics and see irregular and transient unstable dynamics and the absence of a central clock as problems to be avoided to achieve a desired computation. Over the last 15 years, several alternative, distributed ways of computation have been suggested. Yet, most of these approaches come with particular limitations, including limited robustness and limited controllability. Our work on natural information processing now demonstrates that several “imperfections” of natural systems such as chaotic and unstable dynamics, random failure, and sensitivity to parameter mismatch, may serve as constructive support for reliable computations by collective network dynamics [1, 2, 3].

Self-organized coordination of sensor networks

Many technical systems require synchronization of its dynamical elements to ensure proper function. Distributed sensor systems constitute important examples. When networks of interacting units are set up and need to communicate, e.g., in wireless embedded sensor networks, they often have no central control or clocking available. Yet, the units need to agree on a common timing in order to send and receive information packages reliably.

We have now designed networks of oscillators that stochastically communicate via pulses and exploit their stochastic features to mathematically guarantee global synchronization [4]. In particular, features of unreliable pulse emission and stochastically varying delays are used to derive a certificate for synchronization. Numerical complementary studies show clear evidence that the time scales to achieve synchrony may well be small enough for real-world implementations. The class of systems we propose guarantees global synchronization from arbitrary initial conditions, independent of the interaction topology of the network and include distributed and stochastic delays in communication as well as temporally varying network topologies. Our mathematical work is currently complemented by an extension to include a lower bound for the actual delays in the system, thus enabling practical application in real sensor networks (Klinglmayr et al., international patent protection [4]).

Universal heteroclinic computing via high-dimensional control signals

A heteroclinic connection in a dynamical system is a distinguished trajectory that links two saddles in state space. It occurs if unstable directions of one saddle are contained in the stable manifold of a second. A sequence of such connections linking several saddles cyclically
is called a heteroclinic cycle. If a dynamical system of coupled units exhibits a certain symmetry, complex heteroclinic networks consisting of interconnected heteroclinic cycles emerge in a robust way. Heteroclinic networks are of high current mathematical interest. Simultaneously, their specific dynamical features – supporting repetitive switching close to the saddles – pose a promising challenge for the study of information encoding and computation, in particular in artificial neural systems.

Within the last two years, we have introduced a new paradigm for natural computation based on switching close to heteroclinic networks of saddle states [5]. In such systems, symmetry-breaking external signals naturally induce cyclic switching dynamics close to what has been a heteroclinic cycle in a symmetric system. Our analysis shows how to exploit such dynamics to execute universal logic operations. Already for small systems, such as five coupled oscillators, a variety of functions may be executed, including arbitrary unary, binary and ternary operations as well as sets of up to three binary functions within the same system setting. Another interesting feature of such systems is that the number of function “results”, and thus the number of inputs that can be distinguished by the system increases exponentially with system size, i.e., the number of coupled units.

By construction, heteroclinic processing of input signals does not rely on the exact system setup, but only on the abstract heteroclinic network of states a system realizes (see Fig. 6.4). As a broad range of systems exhibit saddle states that are dynamically linked via heteroclinic connections to form complex networks, this new paradigm of heteroclinic computing may be tested in electrical, optical, and electronic systems, among others.

**Dynamics on networks of states as novel research field**

The above studies offer an interesting hint towards new perspectives on what network dynamics actually is. So far, network dynamics has mostly been studied as the dynamics of networks of coupled units. Already for certain Markov processes, the dynamics on abstract networks of states and transitions between them becomes of relevance. The new paradigm of computing via switching across heteroclinic networks of (saddle) states now also exploits controlled (essentially deterministic) state switching but endows the emerging spatio-temporal dynamics with a computational meaning. Thereby, studying transient dynamics of defined transitions among states might become its own subfield of network dynamics.

6.3 FORCES OF CELLULAR GROWTH AND DIVISION

J. Hartung, H. Toncروا, S. Herminghaus, O. Hallatschek

Most microbial species have the ability to form surface attached multispecies communities that are extremely robust to antibiotics or mechanical perturbations. Gaining control over the formation of such biofilms is of tremendous socio-economic interest because they are implicated in many diseases and cause significant industrial costs (e.g. through clogging) [1]. While a paradigm shift has spurred intensive research efforts to uncover the unique biology of biofilms, still little is known about physical constraints on the formation of biofilms. In this project, funded by the SFB 937, we investigate the response of biofilms to spatial constraints. When microbes grow in dense clusters they exert mechanical forces to incorporate new cell material. When these forces become large they may slow down microbial cells and modify the growth environment. In order to test this hypothesis, we have constructed microfluidic devices made of a silicone rubber, which enabled us to entrap yeast cells, monitor their growth and proliferation, and measure the mechanical pressure exerted on the surroundings and the corresponding growth rate in vitro.

Fig. 6.5 shows an image of a typical experiment with a space filling yeast population. Interestingly, the cells do not flow out of the chamber like a liquid but instead the population builds up a pressure of about 0.8 MPa, which is driven by the jamming of cells observable at the marked position. Typically, these jamming events only last for a limited time followed by an avalanche of cells escaping the channel until cells jam again. We hypothesize that these stick slips are analogous to what is observed in granular matter under quasi-static shear flow [2].

In future research, we will augment our studies by exploring the stresses and strains produced by growing biofilms in model cohesive granulates, consisting of glass beads bound together by rubber capillary bridges made of cross-linked silicon oil. The great advantage of this material is that we can precisely control its properties, such as the distribution of pore sizes, elastic response, and fracture yield stress. We have performed initial tests using budding yeast, and the results look promising, in the sense that they reproduce self-organized jamming and crack propagation similar to our microfluidic experiments.

![Image of S. cerevisiae cells trapped in a PDMS device. The mechanical pressure inside of the growth chamber is equal to 0.8 MPa. Pressure is created by jamming of the sheared cell packing, which suggests to analogies to granular matter.](image)

6.4 CONTROL OF SPATIAL-TEMPORAL CHAOS IN THE HEART

P. Bittihn, D. Hornung, T.K. Shajahan, U. Parlitz, S. Luther
V. I. Krinsky, G. Luther, E. Bodenschatz, F. H. Fenton (Atlanta, USA), A.
Pumir (Lyon, France), M. Hörning (Kobe, Japan), G. Hasenfuss
(Göttingen, Germany), R. F. Gilmour Jr. (Charlottetown, Canada)

Spatially extended non-equilibrium systems display spatial-temporal
dynamics that can range from ordered to turbulent. Controlling such
systems is one of the central problems in nonlinear science and has
far-reaching technological consequences. Few examples of successful
control with applications in physics and chemistry have been demon-
strated [4]. In biological excitable media, the systems’ complexity makes
successful control challenging. This difficulty applies in particular to
electrical turbulence in cardiac tissue, known as fibrillation (Fig. 6.6).
During fibrillation, synchronous contraction of the muscle is disrupted
by fast, vortex-like, rotating waves of electrical activity [5]. The loss
of synchronous contraction of the ventricles, i.e. the main chambers
of the heart, results in a loss of pumping function and is immediately
life threatening. In the European Union, an estimated 700,000 cardiac
deaths per year are associated with ventricular fibrillation (VF).

Controlling the complex spatial-temporal dynamics underlying
life-threatening cardiac arrhythmias such as VF is extremely difficult,
because of the nonlinear interaction of excitation waves in a heteroge-
neous anatomical substrate. In the absence of a better strategy, strong,
globally resetting electrical shocks remain the only reliable treatment
for VF. However, high-energy shocks (typically 1kV, 30 A, 12 ms) have
significant side effects including tissue damage and intolerable pain,
indicating a substantial medical need.

We have established a relationship between the response of the
tissue to an electric field and the spatial distribution of heterogeneities
in the scale-free coronary vascular structure. We show that in response
to a pulsed electric field, \( E \), these heterogeneities serve as nucleation
sites for the generation of intramural electrical waves with a source
density \( r(E) \) and a characteristic time, \( \tau \), for tissue depolarization
that obeys the power law \( \tau \propto E^n \). These intramural wave sources
permit targeting of electrical turbulence near the cores of the vortices
of electrical activity that drive complex fibrillatory dynamics. We have
shown in vitro that simultaneous and direct access to multiple vortex
cores results in rapid synchronization of cardiac tissue and therefore,

![Figure 6.6: Spatial-temporal complexity in the heart. (Top)
Numerical simulation of vortex-like rotating in a rabbit ventri-
cle. (Bottom) Spatial-temporal chaos associated with ventricu-
lar fibrillation.](image)

![Figure 6.7: Low-Energy Anti-Fibrillation Pacing (LEAP).
(Left) Termination atrial fibrillation in vivo using LEAP.
(Right) LEAP requires 80-90% less energy than conventional
defibrillation. Figure from [1].](image)
efficient termination of fibrillation [1, 2]. Using this control strategy, we demonstrate low-energy termination of fibrillation in vivo (Fig. 6.7).

Our results give new insights into the mechanisms and dynamics underlying the control of spatial-temporal chaos in heterogeneous excitable media and provide new research perspectives towards alternative, life-saving low-energy defibrillation techniques. The Biomedical Physics Group has received the GO-Bio Award 2012 (Gründungsoffensive Biotechnologie) from the German Ministry for Education and Research, which supports further development of LEAP towards clinical application.

To further develop and optimize the control of spatial-temporal chaos in the heart, the fundamental biophysical and dynamical mechanisms underlying the interaction of electric fields with cardiac tissue need to be further explored. We developed a theory that predicts the response of tissue boundaries to electric fields depending on their shape (Figure 6.8) [8]. We found high sensitivity of convex tissue regions, a finding which was confirmed in cell culture experiments. For weak electric fields, the anatomy of the cardiac muscle therefore leads to distinct locations of wave emission that can potentially be used as control sites. The anatomical features responsible for the success of LEAP were found to be the internal tissue boundaries created by the cardiovascular tree penetrating the tissue. The size distribution of these heterogeneities obtained from the analysis of cardiovascular µCT data was found to follow a power law and could be mathematically linked to the activation patterns observed experimentally using optical mapping. The presence of the same scaling behavior of cardiovascular sizes in other species such as pigs suggests that the physiological basis for LEAP is universal. We expect that combining the growing knowledge of arrhythmia initiation, the characterization of undesired activation patterns and the mechanisms of wave induction via electric fields bears the potential for novel and highly optimized low-energy control strategies of chaos in the heart.

One route to chaos well-known from nonlinear dynamics is via a period-doubling cascade, a mechanism that has also been proposed for the heart in the form of so-called alternans: a beat-to-beat variability of the response of cardiac tissue to periodic stimulation. In a recent experimental study in canine hearts, we showed that the alternans amplitude, defined as the difference in action potential duration (APD) between the current and the preceding stimulation, has a complex spatial pattern that is highly sensitive to pacing site location and stimulation history [6]. These findings lie outside the scope of the current theoretical understanding and therefore stimulate further investigations of the underlying causes.

Once turbulent activity has developed in the muscle, the success of tailor-made control strategies will depend critically on adequate quantitative measures characterizing the malignant dynamics. We studied how nonlinear dynamics tools such as Lyapunov stability analysis [7] can help to quantify the stability and complexity of arrhythmias and therefore allow for the systematic study of the influence of global parameter changes or heterogeneity on the characteristics of spatial-

Figure 6.8: Boundary shape determines sensitivity to electric fields. Snapshots of two-dimensional numerical simulations on left ventricular geometry (rabbit; µCT slice; dark gray = muscle tissue).

Color indicates membrane potential response to homogeneous electric-field stimulation (field left to right; pulse duration 5 ms). Activation of only one protrusion on the endocardium (0.2 V/cm; top), the endocardial boundary (0.4 V/cm; middle), blood vessels (1 V/cm; bottom), cf. arrows.
temporal chaos in the heart. Numerical simulations revealed that substrate heterogeneity can result in hitherto unknown emergent effects on chaoticity [8]. Figure 6.9 shows an extreme case where chaos is completely suppressed by patches of low excitability, although a homogeneous decrease in excitability throughout the medium would lead to more turbulent dynamics.

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*equal contribution
6.5  E-FLOW FOCUSING AND THE MICROFLUIDIC JUKEBOX

S.H. Tan, F. Maes, J. Vrignon, B. Semin, J.-C. Baret

With the advances in technology, we are now able to generate music electronically without relying solely on physical instruments. Here, we demonstrate a musical interpretation of droplet-based microfluidics as a form of novel electronic musical instruments.

First, we have shown that electric fields can be used to modulate droplet size at a flow focussing junction. The principle is the modulation of the interfacial tension by the Electrical Maxwell stress. The droplet volume being classically controlled by the Capillary Number, we derive an effective capillary number controlling the droplet size in the dripping regime. Phenomena such as the dripping to jetting transition and the destabilization of jets when the conductivity increases are however not captured by this simple picture and relate to the stabilization of liquid structures in electric fields [1].

To demonstrate the high-throughput switching capability and the control of droplet frequency, we designed a new musical instrument to play songs in real time. The transduction of the droplet frequency into sound is achieved by labelling the droplets with fluorescein and recording the fluorescence signal from photomultiplier tubes directly on a computer sound card. Our system provides sharp transitions between notes and several songs have been played. The accuracy of the system is mainly limited by the standard hydrodynamic variability linked to the stability of pumps, especially close to the dripping to jetting transition [1].

![Figure 6.10: Electroactuation at Flow Focusing. (a) Microfluidic chip (b) Size modulation by electric field.](image)

![Figure 6.11: The Microfluidic Jukebox: using musical scores available on-line (a), we program a series of voltages to be applied to our chip (b) according to a preliminary calibration (c). The frequency of the droplet production is modulated in real time and the optical signal recorded from photomultipliers provides an electrical signal recorded through the computer audio card. The example of ‘Ode to Joy’ is displayed here (d).](image)

PATTERNS AND INSTABILITIES

Spatially extended nonlinear systems can spontaneously generate ordered patterns by dynamic interactions among their constituent parts. Research at the MPIDS investigates fundamental processes of dynamical pattern formation in systems from physics and biology. Hydrodynamic systems such as shear flows represent core paradigms of the nonlinear science of pattern formation. Biological systems studied in the MPIDS utilize processes of pattern formation to set up and maintain architectures of cells and organs to best serve the needs of the organism or to fulfill vital functions. Examples include traveling electromechanical waves in cardiac tissue, transport systems such as patterns of veins in plant leaves, or the complex spatial structures in which neuronal circuits are laid down in the brain. Our research in both living and inanimate systems is designed to uncover the fundamental features essential for the generation and functionality of paradigmatic patterns. To achieve this aim we are developing new experimental techniques for the precise quantitative assessment of dynamic patterns as well as advanced mathematical concepts and tools to accurately and transparently represent the essential interactions underlying their pattern formation dynamics.

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Some of the fundamentally most important shear flows, such as pipe, channel, Couette and boundary layer flows become turbulent though the laminar state is linearly stable. The transition process occurring in these flows has turned out to be much more complicated than in linearly unstable situations like Rayleigh Benard convection or Taylor Couette flow. Because of its fundamental and practical importance, pipe flow is probably the most prominent example amongst those linearly stable shear flows. Even for this simple geometry it has not been possible to clarify some central and seemingly simple questions regarding how turbulence first arises. It has already been noted in the pioneering study of Reynolds [1] that turbulence does not arise through a linear instability and that the perceived transition point strongly depends on disturbances present in a given set up. Following these observations Reynolds postulated that a 'real critical point' exists below which flows will always return to laminar even if subject to a strong perturbation initially. The existence of such a critical point was the basis of the Reynolds number concept introduced in his 1883 paper [1]. In a subsequent attempt to determine the exact value of this transition point Reynolds introduced the so called ‘Reynolds decomposition’ [2] which is widely regarded as the starting point of modern turbulence research. However the method was unsuccessful in determining the critical point. Even in the following 125 years it has not been possible to resolve its value or the nature of the transition process.

Figure 7.1: Space time plots from direct numerical simulations of Couette flow. Turbulent regimes are shown in yellow, laminar ones in black. Left: Below the critical point all turbulent stripes eventually decay. Right: Above critical turbulent stripes multiply.

A main difficulty is the spatio-temporal nature of flows in the transitional regime and the extremely long time scales involved. In linearly stable shear flows turbulence first appears in the form of localised spots surrounded by laminar flow. A first key observation allowing us
to determine the critical point was that spots are transient in nature and exhibit a memoryless decay\cite{3, 4, 5}. Turbulent spots can however also nucleate new ones in their vicinity and by this process increase the turbulent fraction. Turbulence then becomes first sustained when the spreading outweighs the decay and hence the turbulent fraction increases \cite{6}. While in Figure 7.1 (left) laminar turbulent intermittent flow (here in Couette flow) is shown just below critical in Figure 7.1 (right) a case above critical is displayed \cite{7}. In the subcritical case all the turbulent spots (yellow/red) disappear over time (top to bottom) while above critical the spreading clearly dominates and the turbulent fraction increases while each individual spot remains localised and surrounded by laminar fluid (black). Close to the critical point the time scales for flow patterns to approach equilibrium (i.e. either laminar or a finite turbulent fraction) are extremely long and cannot be easily resolved in experiment or simulations. We hence had to use a different method to determine the critical point. Instead of a direct measure the time scales of the decay and spreading process were determined independently. Since both turned out to be memoryless processes they are given by a characteristic time scale. Figure 7.2 (left) shows the characteristic times for spot decay (left branch) and those for spot spreading (right branch) obtained in experiments and simulations of pipe flow. The critical point is then simply the intersection point of the two and hence at $Re=2040$ \cite{6}. Similarly for Couette flow simulations the analogous result is shown in Figure 7.2 (right) and here the critical point corresponds to $Re=325$ \cite{7}.

The sustainment of turbulence here is a consequence of the increasing spatial complexity and in contrast to the classical view that turbulence arises purely from an increase in temporal complexity (as proposed by Landau and Ruelle-Takens). This transition type is akin to critical phenomena in model systems such as coupled map lattices and directed percolation. These systems display scale invariance at the critical point and are characterized by universal critical exponents. Having developed a method to determine critical points for the onset of turbulence in shear flows offers a unique opportunity to elucidate the very nature of the transition process and to probe if it is equally characterized by universal exponents. In order to show that the inter-
Figure 7.3: Distribution of sizes of laminar gaps in spatio-temporally Couette flow simulations. Far above the critical point size distributions are exponential and hence have a characteristic scale. As the critical point is approached the distributions become scale invariant (black data points).

The section point indeed corresponds to a second order phase transition, and we investigated the spatio-temporally intermittent flow patterns in Couette flow. As the phase transition point is approached, flow patterns should exhibit scale invariance: in the present case the laminar gaps interspersing turbulent domains should lose any characteristic length so that at the critical point laminar gaps of any (arbitrary large) size can be found. Detailed simulations [7] where great care had to be taken that the flow patterns had reached a stationary state indeed confirm this prediction: As shown in Figure 7.3 the size distributions which far above the critical point scale exponentially and hence have a characteristic length, change to a power law close to critical (power laws are scale invariant). In our ongoing studies we attempt to determine the critical exponents for pipe, Couette, and Taylor Couette flow. At the same time we investigate the transition for localised turbulent structures to fully turbulent flow.

7.2 LOCALIZATION AND PATTERNS IN SHEAR FLOWS

T. Kreilos, P. Subramanian, H. Schrobsdorff, T. M. Schneider
E. Brandt (UNH), W. Pesch (U. Bayreuth), J. F. Gibson (UNH)

In the past decade, ideas from nonlinear dynamics in combination with advances in numerical simulation techniques have laid the foundation for a new approach to study turbulence. A connection between dynamical systems and turbulence has been the subject of conjecture since the 1940s [1]. Only recently, however, has concrete progress allowed dynamical systems to be truly established as a new paradigm to study turbulence. This progress is based on the discovery of exact equilibrium and traveling-wave solutions to the full nonlinear Navier-Stokes equations. These exact solutions, together with their entangled stable and unstable manifolds, form a dynamical network that supports chaotic dynamics, so that turbulence can be understood as a walk among unstable solutions [2, 3].

Turbulence often does not fill the whole available domain. Instead, it coexists with laminar flow, giving rise to localized laminar-turbulent patterns. Despite its success in other areas, the emerging view of turbulence as a dynamical system has not yet been able to address the full spatiotemporal dynamics of turbulent flows. One major limitation is that exact solutions have mostly been studied in small computational domains with periodic boundary conditions. The small periodic solutions cannot capture localized spatial structures such as turbulent spots (Fig. 7.4) that are triggered by a localized perturbation and then grow by invading the surrounding laminar flow. Generalizing the dynamical systems picture of turbulence to the spatiotemporal aspects of flows in extended domains thus requires the existence of localized exact solutions.

Such spatially localized exact solutions were recently constructed for plane Couette flow (PCF), the flow between two parallel plates moving in opposite direction. These solutions are localized versions of the spatially periodic Nagata equilibrium [4]. They share the topology of periodic solutions previously shown to play key roles in the transition to turbulence and are related to their periodic counterparts by homoclinic snaking – a pattern-forming bifurcation scenario well studied for simpler PDE models such as the Swift-Hohenberg equation (Fig. 7.5). The snaking solutions are localized in one spatial dimension. Flow structures underlying localized spots however need to be localized in two dimensions. Constructing those fully localized solutions requires developing advanced numerical tools for parameter continuation in large domains (Ch. 7.3). Preliminary results indeed indicate the existence of a fully localized invariant solutions (Fig. 7.6).

Patterns are a generic feature of transitional flows in various geometries. In boundary layers – one of the technologically most relevant flow situation – turbulence emerges in a localized spot that, as in PCF, invades the laminar domain. While pure DNS of boundary layers can nowadays be performed, an analysis of invariant solutions is not yet feasible with current computer infrastructure. Thus, we focus on the
asymptotic suction boundary layer (ASBL), where a constant suction through a porous plate keeps the boundary layer thickness from growing. The ASBL captures many features of a full boundary layer yet due to the spatial homogeneity of the base flow, it is easier to treat numerically. We developed suitable simulation techniques [6] and currently study localized invariant solutions in the ASBL.

Guided by the striking similarity between the bifurcation structure of localized shear flow solutions and well-understood patterns in simpler PDE models, we aim to derive effective amplitude equations for the turbulence intensity. Standard methods for constructing amplitude equations however fail in shear flows where spatiotemporal features emerge while the base state of the governing equations remains linearly stable. This is in stark contrast to buoyancy driven flows where the mechanism generating spatiotemporal patterns is considerably better understood and linked to an instability of the unpatterned base state. In inclined layer convection (ILC), i.e. convection in a channel that is inclined to the horizontal, we obtain a smooth transition between the two scenarios. For small inclination the system shows the typical buoyance-driven patterns. For higher inclination, buoyancy drives a flow of warm and cold fluid along the plates setting up a linearly stable shear flow supporting patterns similar to those observed in PCF (Fig. 7.7). Thus ILC allows to exploit methods relying on the linear instability of the flow to construct exact solutions at small inclinations and then follow them into the shear-dominated regime. Together with new experimental studies in the Bodenschatz department our continuation studies thereby aim at explaining the rich variety of states in ILC [7] and are an important step towards elucidating the general mechanisms underlying laminar-turbulent patterns. In 1986 Pomeau envisioned to describe transitional turbulence as a nucleation phenomenon in some non-equilibrium generalization of equilibrium phase-separation concepts [8]. Our work will ideally provide a mechanistic foundation for this approach.

7.3 HIGH-PERFORMANCE CONTINUATION SOFTWARE

H. Schrobsdorff, T. Kreilos, D. Fliegner, T. M. Schneider
J. F. Gibson, E. W. Brand (UNH)

Identification and elucidating the bifurcation structure of stationary flow fields is key to understanding laminar turbulent patterns in transitional flows, see Ch. 7.2. We therefore follow invariant solutions $\tilde{u}^*$ satisfying the fixed point equation $0 = N(\tilde{u}^*, \varphi)$, with $N$ the Navier-Stokes operator for varying continuation parameters $\varphi$. Due to the nonlinearity of the governing PDEs and the large number of degrees of freedom required to represent a velocity field, efficiently computing roots of the fixed point equation in arclength continuation schemes is non-trivial and requires iterative matrix-free Krylov-Newton methods. While structures in rather small periodically continued domains can be continued using serial implementations [1], more complex structures in larger domains are represented by $10^7$ to $10^8$ coupled degrees of freedom so that parallel distributed-memory computations are necessary.

Taking advantage of unrestricted and direct access to dedicated high-performance compute clusters (Fig. 7.8) we developed adequate MPI-based parallel continuation tools. These are based on Channelflow, a custom coded, serial spectral Navier-Stokes solver [2], see also www.channelflow.org. The developed code scales extremely well with an almost linear speedup. The communication overhead is constant leading to an almost constant parallel efficiency.

The developed software together with flexible in-house computer infrastructure greatly improves our simulation capabilities and allows for studies that had been out-of-reach of previous serial computations. For the continuation of the equilibrium solution discussed in Ch. 7.2, numerically represented by approximately 6.3 million coupled degrees of freedom, we observe a speedup by a factor of almost 60 for the continuation so that computations that took two months can now be performed in a day (Fig. 7.9).

While the continuation methods are initially tailored towards following invariant solutions of the Navier-Stokes equations, we currently generalize the techniques to allow for continuation studies and the bifurcation analysis of other multi-dimensional nonlinear partial differential equations. Applications include extensions of the Navier-Stokes equations describing active fluids and boyancy driven flows but also mechanical problems such as the response of elastic shells. As a long-term goal we aim at developing a flexible software package that can easily interface with existing PDE solvers. This requires further improving the robustness of numerical algorithms but also poses new challenges in terms of software design and engineering.

7.4 CHIMERA STATES IN MECHANICAL OSCILLATOR NETWORKS

Erik A. Martens, Shashi Thutupalli, Antoine Fourrière, Oskar Hallatschek

The synchronization of coupled oscillators is a striking manifestation of self-organization that nature employs to orchestrate essential processes of life, such as the beating of the heart. While it was long thought that synchrony or disorder were mutually exclusive steady states for a network of identical oscillators, numerous theoretical studies over the last 10 years revealed the intriguing possibility of ‘chimera states’, in which the symmetry of the oscillator population is broken into a synchronous and an asynchronous part. Even if such a symmetry breaking in a network of identical oscillators is quite counterintuitive, chimera states now represent a very robust theoretical concept. Yet, a striking lack of empirical evidence raises the question of whether chimeras are indeed characteristic to natural systems, like synchronization itself.

We devise a simple experiment with identical mechanical oscillators coupled in a hierarchical network with two subpopulations and obtain a palpable realization of chimera states without any fine-tuning. By varying the effective spring coupling between the subpopulations, \( \kappa \), and the nominal metronome frequency, \( f \), we identify a wide spectrum of complex states, encompassing and extending the set of previously described chimeras. We show that chimeras emerge naturally from a competition between two antagonistic synchronization patterns.

Our mathematical model reproduces the experimental observations and shows that the self-organization obtained in our experiments is controlled by elementary dynamical equations from mechanics that are ubiquitous in many natural and technological systems. The symmetry breaking mechanism revealed by our experiments may thus be prevalent in other diverse systems exhibiting collective behavior and we argue that chimeras and their relatives should be considered as the rule rather than the exception in complex systems.

7.5 DYNAMICS OF CRACK PATTERNS

L. Goehring, E. Katifori, P. Nandakishore

In nature, ordered crack patterns are found in situations ranging from cracks in garden mud, to the snouts of Nile crocodiles or the vast polygonal networks that stretch across the polar deserts of Earth and Mars. To a degree these patterns can also be controlled, as in the artistic craquelure of paintings and pottery. More precise control can be made by the imprinting of memory in vibrated pastes or the lithographic templating of nanoscopic crack patterns, for example. The physics of these patterns is captured by an energy balance as the cracks grow. Unlike many other physical problems, however, crack growth involves only a local energy minimization, at the point and time that a crack is growing, rather than the global minimisation of some functional. Since energy can be released by the widening of a crack anywhere along its path, whereas to a good approximation energy is only spent in a small region immediately around a growing crack tip, the entire history of the crack affects how it will grow at any instant. This means that although the highly practical question of whether a crack will grow or not (and hence, whether a bridge will fall down, or an airplane wing snap off) is solved, one cannot accurately predict the direction that a crack will grow in any but the simplest cases. We are investigating the dynamics of cracks in thin sheets, with two general long-term goals:

- Predicting how a crack will grow in an arbitrary situation, and
- Designing/templating structures to give a desired crack pattern.

To this end, we study a number of simple model systems, many inspired directly by nature. These involve cracks in curved surfaces, cracks over patterned substrates, wavy cracks in colloidal films, and crack patterns that evolve through cycles of cracking and healing.

The growth of leaf veins closely resembles how crack patterns form in drying films. This apparent similarity leads to many questions regarding fracture induced pattern formation. Is this similarity just superficial, or is it due to homologous morphogenetic mechanisms? We are developing an experimental program to look at fracture in thin curved films, which resemble the conditions under which leaves develop, that will hope to provide quantitative answers to these questions, and determine if leaf veins are indeed mechanically the same as cracks.

Cracks in thin layers can also be affected by what lies beneath their surface. This applies to cracks that cluster around a buried crater, or cracks in Renaissance paintings that reflect the grain of the wood over which they were painted, or cracks in films spin-coated over microscopic patterns etched into silicon. The pattern of surface cracks should not depend on the absolute size of the features, as fracture mechanics has no inherent length scales. Rather, as we are finding, the patterns only depends on the relative wavelength and amplitude of the substrate features, and fall into a small number of broad classes.

Wavy cracks in colloidal films is one system in which we have made progress predicting how cracks grow [1]. Here, cracks advance...
Cracks in thin layers can be affected by the shape of their substrate. For a sinusoid substrate, as the dimensionless layer thickness decreases, the crack pattern first aligns with the underlying features, then develops secondary instabilities. Although these images show dry mud cracks, ~10 cm across, the results should scale to both planetary-scale features, and microscopic cracks.

directionally, across the film. A wavy crack can appear between two existing straight cracks. The flanking cracks preferentially release stress normal to their surface, and so the wavy crack would gain energy by curving towards either one. However, as it approaches one, it must advance into a region with a lower total strain energy density. A balance between these effects predicts a path that continuously curves towards the local direction of maximum strain energy release rate, which accurately describes the shape of the wavy crack, and its scaling.

Finally, we have learned how cracks can evolve when they are allowed to break and heal, over and over [2]. These experiments are inspired by polygonal terrain, extensive landscapes of crack patterns that cover the permafrost regions of Earth and Mars. We know these landscapes are evolving, but the dynamics are too slow to see directly. We have studied crack patterns in mud that is repeatedly dried and rewetted, and can explain the resulting patterns (and by extension, the permafrost) by a few simple general assumptions of crack behaviour.

![Figure 7.14](image1.png)  
**Figure 7.14:** Polygonal terrain (a) is common in permafrost soils. The pattern is dynamic, but the timescales of resurfacing are millennia, at least. Similar dynamics can be studied in clay layers, when they are repeatedly dried and rewetted [2]. The crack pattern evolves from one dominated by rectangular pieces, to one with hexagonal tiles (now, over only weeks). This behaviour can be predicted by assuming that cracks appear near the positions of old cracks, but that the order of cracking is different in each cycle.

![Figure 7.15](image2.png)  
**Figure 7.15:** (a) Wavy cracks in drying colloidal latex films form when a secondary crack tries to advance between two pre-existing straight cracks. (b) A crack path prediction that requires cracks to curve towards the direction of maximum strain energy release rate accurately predicts the relationship between wavelength $\lambda$, film thickness $h$, and the distance between the bounding cracks, $2b$.

7.6 LIQUID-SOLID TRANSITION IN DRYING COLLOIDS

L. Goehring, J. Vesaratchanon, S. Javadi, P.-C. Kiatkirakajorn
B. Cabane (ESPCI), J. Li (ESPCI), L. Pauchard (Paris-Sud), F. Boulogne
(Paris-Sud), F. Giorgiutti-Dauphiné (Paris-Sud), R. Botet (Paris-Sud),
R. Schweins (ILL), M. Sztucki (ESRF)

There are several routes for solidifying materials. For homogeneous
materials such as metals the liquid-solid transition can result from a
drop in temperature, as intermolecular forces cause atoms or molecules
to settle into equilibrium positions. For particulate materials such as
photonics, ceramics and coatings, the usual route is through the liquid-
solid transition that is caused by evaporation from a dispersion of solid
particles in a volatile solvent. One often sees this transition as being
driven exclusively by the loss of free volume, and thus the solvent
‘disappears’ from the description, and equilibrium phase diagrams
can be calculated. However, there are many cases where flow during
solidification plays a role that is important and counterintuitive. For
example in the transport of particles to the edge of a drying drop
dilute dispersion, or in the formation of drying fronts in more
concentrated colloidal films [1, 2]. In these cases, the dispersion rapidly
changes from a liquid, to a soft solid, to a hard solid. Meanwhile the
flow of solvent breaks the orientational symmetry of the dispersion,
leading to a structural anisotropy that affects the mechanical and optical
properties of the solid [3]. In fact, the forces driving these transitions
represent a balance between the drag of the fluid past the particles, and
a buildup of pressure or stress in the network of particles, and can also
cause macroscopic deformations like cracks, wrinkles, or shear bands.
We are attempting to build a coherent theory of the transport, dynamics,
and structure-forming physics of solidifying colloidal dispersions.

Figure 7.16: Directional solidification of a colloidal dispersion
in (a) a Hele-Shaw cell. Neutron scattering patterns (b-d) reflect
the evolving arrangement of the colloidal particles [3],
and are used alongside optical measurements [1] of (e) structural color,
(f) shear bands and cracks and (not shown) particle tracking, to determine how a
drying dispersion changes from a liquid to a solid.

7.7 PLASTICITY AND FRACTURE IN DRYING COLLOIDAL FILMS

L. Goehring
W. J. Clegg (Cambridge), A. F. Routh (Cambridge)

Colloidal dispersions, for example many paints or coatings, often crack as they dry. Diverse patterns can be seen, such as regular parallel cracks, wavy cracks, star cracks, and spiral cracks. Typically, interpretation of these patterns is made by the well-established framework of elastic fracture mechanics. However, we still lack any direct measure of the fracture properties, or inherent toughness, of colloidal films, and any proof that the films are indeed behaving elastically.

Elastic fracture mechanics assumes that strains are linear, elastic and reversible. We tested these assumptions in films of a hard latex by intermittently blocking evaporation over a drying film, thereby relieving the film stress [1]. We found that although the deformation around a crack tip has some features of brittle fracture, only 20–30% of the crack opening is relieved when it is unloaded. Atomic force micrographs of crack tips also show evidence of plastic deformation. By measuring the shape of the crack tips, we have also made the first direct measure of the fracture toughness of this class of material, and the energy required for fracture. Surprisingly, over 90% of the fracture energy is consumed in irreversible plastic processes. Through a scaling argument showing that the yield stress of a colloidal film is generally comparable to the maximum pressure it experiences during drying, we further conclude that such plasticity will normally be significant. This suggests a counterintuitive method to increase the toughness of colloidal coatings by decreasing the adhesion between particles and encouraging plastic losses until the cost of cracking is too high to occur.

![Figure 7.17: Directional drying of colloidal dispersions leads to the development of a series of drying fronts. (1) A liquid dispersion like paint first (2) orders, then (3) solidifies. The solid (4) cracks, and ultimately (5) drains of water, forming the final dry solid porous film. The solid regions (3–5) are usually modelled as elastic materials, whereas most of the energy in fracture is actually lost through plastic processes, which can be controlled to toughen the film.]

![Figure 7.18: (a) The shape of a crack is parabolic, very close to its tip. The opening shape for different film thicknesses (different colours), can give us the ratio of fracture toughness to Young’s modulus, $K_C/E$. (b) The film’s toughness is raised by plastic deformation, features of which (micro-cracks, dislocations, and particle rearrangement) can also be seen by AFM of the film surface during drying.]

7.8 MECHANICS AND VASCULAR PATTERNING IN THE DEVELOPING LEAF

Eleni Katifori
J. Dawson, F. Ditengou and Klaus Palme (Freiburg), Irina Kneuper and William Teale (Freiburg)

Photosynthetic capacity in leaves is closely tied to their vascular architecture; therefore understanding how plants form their vein patterns can provide insight into their high performance capabilities. However, there is no consensus yet regarding the actual mechanisms of the vein architecture development, despite a wealth of studies and the discovery of a number of genes that control vascular formation [1].

The main leaf vein appears very early in the leaf development. The cells that will differentiate from the young mesophyll cells (leaf interior) to xylem and phloem (leaf veins) can be seen by labelling the expression of genes controlling the production of the plant hormone auxin and the protein PIN1 (Fig. 7.19(A)). For this reason, these two molecules are thought to control the vascular tissue formation. The auxin canalisation hypothesis, the cornerstone of most models, stipulates that high auxin flow in cells induces cell changes by the polarisation of the PIN proteins along the cell wall. These changes promote the flow of auxin, eventually draining the surrounding tissue from this morphogen. Finally, high auxin flow is believed to induce cell differentiation to vascular tissue. These models have been able to explain many experimental observations but suffer from certain pitfalls. Without fine-tuning (e.g. phantom morphogens) auxin canalization models do not form closed loops, a basic feature of living vascular structures. In addition, mutants where the expression of PIN has been reduced, still form vascular tissues.

A major element missing from the current vein patterning models is mechanics. Mechanical forces have been shown to play a role in various other aspects of plant development. In collaboration with the experimental group of Frank Ditengou at Freiburg, we are exploring the interplay between mechanics and auxin production and diffusion and their effects in vascular development in the growing leaf. We adapt a cell based computational model [2] and simulate tissue growth driven by inter-cellular diffusion of the plant hormone auxin, created in special auxin producing cells. We show how auxin concentration based modulation of the cell mechanical properties during the leaf tissue growth influences the early stages of leaf vein patterning. We find that auxin production and auxin concentration, coupled with tissue growth and mechanics can predict the formation of the main vein. Tools developed for this project can help us explore how mechanics affects the cell patterning and distribution of cell sizes in the growing floral organs.

7.9 CURVED ORIGAMI: FOLDING OF STRUCTURES WITH NON-ZERO GAUSSIAN CURVATURE

E. Katifori
E. Couturier (USACH, Chile), E. Cerda (USACH, Chile), J. Dumais
(Univ Adolfo Ibanez, Chile)

Origami, the Japanese art of paper folding, is a popular topic for mathematical studies and a continuous inspiration for engineering applications, such as deployable structures and medical stents. Nature also frequently exploits basic origami principles to implement ingenious solutions to a number of biological problems, as for example the efficient packing of developing leaves in the bud or the folding of retracted insect wings. More generally, large scale deformations of flat sheets (e.g. wrinkling) are quite relevant for biological applications and their mathematics have been well developed [1]. However, relatively little is known about the large scale deformations or folding of shells with intrinsic curvature. A major impediment to progress in this direction is the inherent difficulty in obtaining analytical expressions for the deformed shapes.

Thin curved shells that undergo large deformations are very common in biology, manifesting in structures such as seed pods or pollen grains. When released from the anther, pollen dehydrate and their outer wall deforms to accommodate this volume loss (see Fig. 7.20). This folding process needs to be reversed when the pollen reaches a new flower and its success is crucial for the biological fitness of the pollen grain. In past work we have studied this process in detail by modelling the outer wall as a deformable thin shell [2]. We have found that successful and reversible folding requires proper design of the aperture, an area on the pollen wall where the mechanical stiffness becomes very small.

Inspired by the biology of pollen grains, we asked a more general question: how do curved things with one opening (aperture) deform? In particular, what is the behavior of a thin spherical shell with an opening (aperture) of n-fold axial symmetry when compressed? We address this question via a series of experiments (3D scanning of compressed ping-pong balls), theory (geometry of constant gaussian curvature surfaces) and simulations (tethered mesh algorithms) [3].

We analytically derived a two-parameter family of approximately isometric, constant positive Gaussian curvature (quasi-CGC) shapes (shown in Fig. 7.21) that is in excellent agreement with our experimental results of deformed shells and the tethered membrane simulations minimizing the stretching and bending energy. The analytic solutions that describe those shapes have n-symmetrically arranged curvature singularities which correspond to cusps of the folded shape. We examined the properties of the folded shells and observed that in the analytic solutions isometric closure is more easily achieved when the singularities lie away from the center of the aperture. We found that when allowed by the geometry of the aperture and the nature of the load, physical shells expel the curvature singularities into the aperture.

Figure 7.20: Hydrated and dehydrated form of typical pollen grains. (A)-(C) Examples of aperturate pollen grains showing the hydrated morphology with the aperture exposed (left) and the sealed geometry (right). The pollen grains of Lilium grandiflorum (A) and Dianella caerulea (C) have a single aperture; while the pollen grains Euphorbia milii (C) have three apertures. (D) The inaperturate pollen grain of Aristolochia gigantea illustrates a typical configuration in the absence of mechanical inhomogeneity (mirror inversion). (Length scale for (B)-(D): 30-35μm and for (A)100μm). For ease of view, the aperture margin in (C) has been marked with a dashed black line. The apertures in all cases except in (C) left are shown directly facing the reader.
Additionally, we observed that the deformed shape of the shell opposite the opening is independent of the exact shape of the aperture.

Figure 7.21: A two-parameter family of quasi-CGC surfaces. The geodesic distance between the singularities and the lower pole increases with $\mu$ while the deformation increases with $\lambda$ ($\lambda = 0$ is a sphere). Dark and light blue regions indicate where the Gaussian curvature deviates from $K = 1$ by less than 5% and more than 5%, respectively. Insets show lateral views for each of the surfaces, and their deviation from a circular (undeformed) cross-section.

These findings open the way to more interesting questions. Can our methodology be generalised to describe large scale deformations of more general shapes? Similar to the finite number of origami basic folds, it may be possible to find a number of building blocks for curved surfaces that will allow us to construct good approximate solutions for large scale deformations of doubly curved shapes. Understanding how to analytically describe large scale deformations of curved structures will pave the way for the design of curved structures with prescribed functions.

Solids of complex 3D shapes emerge in many natural settings including icicle and stalactite growth [1], geothermal hot springs [3], chimneys of deep see hydrothermal vents – so called “black smokers” –, and silica biomorphs, i.e. biologically inspired shapes that emerge in an inorganic chemical system [4]. How do surface growth mechanisms form shapes of a complexity rivaling biological systems? The fundamental problem of diffusion-dominated surface growth was first analyzed exactly 50 years ago in the now classic work of Mullins and Sekerka. Nevertheless, as more recent investigations show, even the simplest growth process of an object in a supercooled melt or a supersaturated solution is still far from understood (see e.g. [2]). The intriguing complexity of the system stems from the fact that the growth depends on the diffusion field which in turn is coupled to the overall shape of the surface in a non-local fashion. The problem becomes even more interesting if one extends it, either by generalizing the transport mechanism of the field, e.g. to diffusion plus convection, or by considering multi-species systems within a chemical reaction network.

We develop a simulation code to investigate different growth mechanisms. For the classical diffusion-dominated surface growth one is only interested in the normal component of the diffusive flux at the surface. Therefore, a boundary integral method is appropriate. Instead of discretizing the full volume around the growing object to solve for the diffusion field, we only need to discretize the object’s surface. The modern approach used to solve the boundary integral equations is the so-called symmetric Galerkin boundary element method, being basically a FEM method for integral equations [5].

In an exemplary numerical simulation we follow the time evolution of a 2D (slab-symmetric) randomly shaped object growing through precipitation. The surrounding diffusion field is bounded by the unit circle on which a constant concentration is prescribed. The snapshots in Figure 7.22 show the evolving surface color coded by local curvature. The complex dendritic shapes arise through the interplay of the destabilizing diffusional growth and the stabilizing surface tension.

Currently we are generalizing the methods to take into account multiple species related by chemical reaction networks and develop a 3D simulation code. Together with theoretical considerations these simulations will eventually elucidate how shapes in silica biomorphs - coral like structures formed through precipitation processes in an inorganic chemical system - can be controlled.

7.11 KINNEYIA: A HYDRODYNAMIC INSTABILITY IN THE FOSSIL RECORD

K. Thomas, S. Herminghaus, L. Goehring
H. Porada (Göttingen)

Kinneyia is a fossilised biofilm, which can be found on exposures of ancient seashores and is characterized by clearly defined ripple structures, a few millimetres apart. It usually forms as the capping layer of a major storm deposit, or other violent event. Although Kinneyia has been known of for a century, its mechanism of formation has remained elusive so far. It occurs in the fossil record from the Archean to Jurassic periods, spanning half of the Earth’s total existence, but interestingly Kinneyia-like wrinkles are not seen in the more modern record.

We propose that the key mechanism in the formation of Kinneyia is a Kelvin-Helmholtz type instability of a viscous film under flowing water. Biofilms and biomats consist of microbes held together by a gel-like matrix of extracellular polymeric proteins. The rheology of this matrix is similar to that of a polymer solution, and the mat behaves in many ways as a viscoelastic fluid with a relaxation time of a few minutes. The linear stability analysis of a viscoelastic film under shear from superficial flow predicts that the film’s surface is unstable to wrinkling on a wavelength about 4-5 times the thickness of the film [1].

Analogous experiments using polymer solutions as mats confirm our prediction: under flowing water ripples spontaneously form at a wavelength 3-4 times the thickness of the film, and grow at this wavelength to reach a saturation amplitude [1]. Fossils and casts of fossils were also collected from exposures of Precambrian Kinneyia in Namibia, and scanned to produce a 3-D height profile. The ratio of wavelength to amplitude matches the experimental observations, and while we do not know the thickness of the original mat (as we preserve only a fossil of a sediment’s imprint over the mat), the thickness inferred from their wavelengths matches those of typical modern mats [1].

The robustness of the wrinkling mechanism suggests that similar structures should be seen in modern mats. However, Kinneyia is linked to storm deposits, which are infrequent. Additionally, grazing animals and rapid bioturbation since the Cambrian have rendered conditions for biomats increasingly unfavourable; they are relatively scarce today. Thus, Kinneyia may have become so rare as to not enter the fossil record. Another line of thought concerns rheology: biomats are active matter, and we know that active mechano-response is well conserved at least in modern eukaryotes. As we do not know the history of this response, the microbial mats may well have evolved an active motion to counteract the wrinkling instability. We are developing biotic experiments to check these possibilities, either of which would profoundly impact how we interpret these fossil clues to the history of life on Earth.

Smectic liquid crystals easily form freely suspended films which are ideal model systems for two-dimensional liquids. We have started, using single molecule tracking, to study the diffusion behavior and its dependence on film thickness, temperature, and near phase transitions between different smectic phases. The most prominent result is a pronounced increase of the diffusion coefficient $D$ with decreasing thickness (Fig. 7.24a), describable by an empirical function of the form $D = D_{\infty}(1 + A/h)$, where $h$ is the film thickness, $D_{\infty}$ the diffusion coefficient of the bulk phase, and $A$ a constant. Molecular dynamics simulations provide a quantitative description of the observed behavior (inset in Fig. 7.24a). We have also continued our studies [1] of ultrathin smectic films on solid substrates, exploring the manipulation of the porous film structure on the molecular scale using the different modes (contact/tapping) of an atomic force microscope. These findings may lead to new nanolithography applications.

The second emphasis of this project is on surfactant-laden liquid crystal interfaces. We have focused on surfactant layers which change their structure in response to external stimuli. Gibbs films of semifluorinated alkane molecules on the surface of organic liquids show a first order transition between a dilute and a dense state. We have explored the influence of this transition on the anchoring and ordering behavior of liquid crystal phases in contact with the Gibbs film [2] and found that the transition in the Gibbs film induces an anchoring transition in the liquid crystal phase. We also conducted the first in situ AFM study [3] of these films, revealing the presence of surface micelles in the dense state of the Gibbs film (Fig. 7.24b).

Figure 7.24: (a) Diffusion coefficient $D$ in freely suspended smectic-A films as a function of film thickness. The inset shows the results of a numerical simulation. b) AFM height image ($0.5 \times 0.5 \mu\text{m}^2$) of a Gibbs film of semifluorinated alkane molecules formed on the surface of a liquid crystal droplet, demonstrating the hexagonal array of surface micelles.

7.13 ACTIVE EMULSIONS: PATTERN FORMATION AND ARTIFICIAL SWARMING SWIMMERS

Ch. Bahr, S. Herminghaus
K. Peddireddy, S. Thutupalli, P. Kumar

During our studies of surfactant-laden liquid-crystal/liquid interfaces, we observed that droplets of common thermotropic mesogens exhibited an interfacial instability when immersed into aqueous phases containing ionic surfactants at concentrations above the critical micelle concentration. The instability results into the spontaneous formation of a microemulsion, i.e., the liquid crystal molecules are transferred from the parental droplet into the surfactant micelles in the aqueous phase and the initial liquid crystal droplet finally completely dissolves. During the solubilization process, we observe [1] interesting transient structures and dynamical phenomena which strongly depend on the type of the liquid crystal phase.

Figure 7.25: a) Thermotropic myelin tube ejecting a thinner tube (arrow) forming a coiled structure. b) Series of micrographs (crossed polarizers) showing two self-propelling nematic droplets (diameter ≈ 50 μm, velocity ≈ 5 μm/s) moving in glass capillary (square cross-section). The two droplets approach each other, encounter and reorient, and move in the respective opposite direction (arrows indicate the direction of motion). c) Cross section and director field of a nematic droplet with homeotropic surface anchoring at rest (left) and with internal convection (right).

Smectic droplets develop at their surface elongated tube-like structures which resemble the myelin figures which have been known for decades in lyotropic systems. The thermotropic myelins exhibit new features, such as a hierarchical formation of the myelins tubes (thinner tubes are growing from the surface of thicker tubes) and the formation of coiled superstructures (Fig. 7.25a). Nematic droplets retain their shape (apart from slowly shrinking) but show a convective flow pattern inside (Fig. 7.25c) and a self-propelled motion (Fig. 7.25b) which render the droplets a promising new type of artificial microswimmer: their preparation is exceptionally simple and microfluidic methods enable the generation of a large number of identical droplets which makes this system especially suited for studies of collective behavior.

Spiral waves represent a very prominent example of a self-organization in quite different active distributed systems including the colonies of Dictyostelium discoideum, the chemical Belousov-Zhabotinsky reaction, the heart muscle, the eye retina, the CO oxidation on platinum single crystal surface, and many others.

The most general features of the spiral wave dynamics can be reproduced by a two-component reaction-diffusion system [1]

\[
\frac{\partial u}{\partial t} = D \nabla^2 u + F(u, v), \quad \frac{\partial v}{\partial t} = \epsilon G(u, v),
\]

(7.1)

where the local kinetics of an activator \(u\) and an inhibitor \(v\) is specified by the nonlinear functions \(F(u, v)\) and \(G(u, v)\).

In the case of excitable dynamics a supra-threshold stimulus generates a propagation of the excitation front at a velocity \(c_p\) which depends on the inhibitor value \(v\) near the front and on its local curvature \(k\). Based on the assumption that these two relationships are linear, the existence of two limits of the spiral wave dynamics has been demonstrated relating to the trigger-trigger (TT) and trigger-phase (TP) waves [2, 3]. In both of the limits, a dimensionless parameter \(B = 2D/(d_u c_p^2)\), where \(d_u\) is the excitation pulse duration, completely determines the spiral wave parameters [3, 4, 5].

However, there is a strong quantitative difference between the relationships predicted for TT and TP waves [3].

In our study [6] the free boundary approach is applied to demonstrate the existence of a smooth transition between TT and TP spiral waves. We introduce a modified Barkley model which enables us to study this transition by varying of a single model parameter. In addition we show that this parameter can be determined experimentally.

In order to reproduce a transition between pure TT and TP waves we introduce a modified Barkley model with the kinetic terms containing an additional parameter \(v_m\)

\[
F(u, v) = \begin{cases} 
  u(1 - u)(u - \frac{v + b}{a}), & \text{if } v \leq v_m, \\
  -0.3u, & \text{if } v > v_m,
\end{cases} \quad G(u, v) = u - v.
\]

(7.2)

If \(v_m\) is sufficiently small, the autocatalytic dynamics will be switched to the passive one, when the growing inhibitor value \(v\) exceeds \(v_m\). This results in an appearance of a phase wave at the wave back, namely in its part where the inhibitor value reaches \(v_m\).

Note that this induces also a nonlinearity of the relationship \(c_p = c_p(v)\) shown in Figure 7.26 (a) which changes the spiral wave dynamics essentially. We demonstrate that for given \(v_m\) the dimensionless angular velocity \(\Omega = \omega D/c_p^2\) is uniquely determined by the parameter \(B\), but is strongly affected by \(v_m\), as shown in Figure 7.26 (b). Here red solid, dash-dotted, dashed, dotted and blue solid lines are relating to \(v_m/v^* = 2.0, 1.5, 1.0, 0.5\) and 0.1, correspondingly.
Figure 7.26: (a) Planar front velocity $c_p$ vs the inhibitor value $v$ near the front obtained for the model (1), (2) with $v_m = 0.15$. At the Maxwell point $c_p(v^*) = 0$. (b) The dimensionless angular velocity $\Omega$ vs the dimensionless parameter $B$.

It is important to stress that when $v_m/v^* \to 2$ the obtained function $\Omega(B)$ approaches the relationship found earlier for TT waves [5] (red solid). In the limit $v_m/v^* \to 0$ the function $\Omega(B)$ approaches the relationship we found earlier for pure TP waves [3] (blue solid).

In order to verify the selected relationships, direct numerical integrations of the modified Barkley model have been performed with different $v_m$ values, as shown by separate symbols in Figure 7.27(b).

Figure 7.27: The normalized pulse duration as a function of the normalized propagation velocity computed for the model (1), (2) with $a = 1, b = 0.4$, (a) $\epsilon = 0.00035, v_m/v^* = 1.5$ and (b) $\epsilon = 0.00015, v_m/v^* = 0.5$. Dashed lines represent analytical predictions. Dotted green lines correspond to TT waves.

We demonstrate also that the parameter $v_m/v^*$, which controls the detected transition from TT to TP waves can be determined from the observation of a pulse train propagation in a given reaction-diffusion system. To this aim we represent the normalized pulse duration $d_u/d_0$ as a function of the normalized pulse velocity $c_p/c_0$, as shown in Figure 7.27. If $1 < v_m/v^* < 2$ the slope of the relationship has a jump at $c_p/c_0 = C_m$, as shown in Figure 7.27 (a), and $v_m/v^* = 1 + C_m$. If $v_m/v^* < 1$ the relationship is passing through the points $(C_s,0)$ and $(1,1)$ as shown in Figure 7.27 (b), and $v_m/v^* = 1 - C_s$. In contrast to both of these cases, the relationship for TT waves is linear and connects the points $(0,0)$ and $(1,1)$.

Our results open perspectives not only in theoretical studies, but also in some important applications, like screening of antiarrhythmic drugs, since the similar measurements of wave trains are quite usual in cardiology.

7.15 INTRACELLULAR, INTERCELLULAR AND CELL-SUBSTRATE DYNAMICS


Complex dynamics and pattern formation underly eukaryotic cell motility, polarity, and tissue development on the single cell as well as on the cell population scale. To understand these biomechanical processes we focus on the model organism *Dictyostelium discoideum* (*D. d.*), which, after six hours of starvation, migrates chemotactically towards increasing concentrations of the signaling molecule cAMP. With microfluidic devices, advanced microscopy, electrical impedance spectroscopy and theoretical modeling we investigate the signaling dynamics, reorganization of cytoskeletal biopolymers in the cell cortex and oscillatory behavior. Further studies are concerned with biomechanical impact of flow, electric fields, and surface curvature on intra- and intercellular, amoeboid and mammalian cell dynamics. Finally, to understand the cell-substrate interaction, we experimentally study *D. d.*’s adhesion apparatus with force microscopy.

One essential feature of cell migration is pseudopod formation, where the cell membrane is locally pushed out by actin polymerization. Here we study the dynamics and pattern formation in the cortex of *D. d.*. For eukaryotes it is known that the protein super-family of Ras regulates processes like cell division and polarization. In *D. d.*, especially, Ras-G is responsible for cAMP dependent chemotaxis. We are particularly interested in the physical and biochemical processes and patterns of Ras-G within the cell cortex. With two fluorescent labels, we visualize and compare the initial upstream chemotactic signaling with actin polymerization and relate it to pattern selection processes. We extract the cell contour with image processing tools from confocal images, calculate its curvature (curv.) and correlate it with the fluorescence intensities, hence with Ras-signaling and pseudopod extension. The results of all three different measures are shown exemplarily in Figure 7.29.

Besides signaling pathways of directional sensing and motility, chemotaxis includes polarity, a breaking of the symmetry that gives the cell a leading an retracting edge. In a theoretical analysis we have

![Figure 7.28: Simulated traveling waves of PIP3 (green) and PTEN (red) are indistinguishable from the experimental observations by Gerisch et al. [1].](image)

![Figure 7.29: Non-normalized cross correlations extracted from kymographs. Left: Ras-G and LimE, Middle: Curv. and Ras-G, Right: Curv. and LimE: black dots (no shift in either direction), black crosses (highest correlation). No time shift can be observed on the whole cell level.](image)
studied the pattern formation of cell polarity. During spontaneous cell polarization of \(D. \text{ d.}\) cells, phosphatidylinositol (3,4,5)-triphosphate (PIP$_3$) and PTEN (phosphatase tensin homolog) have been identified as key signaling molecules, where randomly triggered excitable PIP$_3$ waves regulate PTEN concentration (Figure 7.28). Our analysis shows that this requires switch-like dynamics of the overall membrane bound PTEN concentration, which in turn necessitates a combination of two species of PTEN (PTEN*, PTEN**) with differing dephosphorylation rates. Our quantitative model with a coupled reaction-diffusion system shows excellent agreement with experimental results and predicts a ratio \(\sigma\) of dephosphorylation rates acting on PIP$_3$ of \(\sigma \approx 80 \sim 100\) [2]. It suggests that surface-attached, cell membrane spanning PIP$_3$ waves are necessary for resetting the global actin network (Figure 7.30).

As described above \(D. \text{ d.}\) synchronizes itself during the cell signaling phase with waves of cAMP. We have quantified these collective phenomena on the intercellular level by applying for the first time electric impedance measurements. We showed that \(D. \text{ d.}\) seeded on micrometer-sized electrodes provoke impedance oscillations [3]. We record time dependent correlation of Electrical Cell-substrate Impedance Sensing (ECIS) signals [4, 5] and changes in height detected by TIRF-microscopy by comparing light intensity of substracted BF images from both assays. A high impedance signal \(|Z|\) is found to correlate with a high fluorescence intensity and thus with a small cell-surface-distance (Figure 7.31).

The arrangement of \(D. \text{ d.}\) analyzed on bright field images reveals synchronous formation of cell aggregates contributing to impedance oscillations (Figure 7.31 B), while a decrease of circularity \(<C>\) occurs
out-of-phase. Modeling calculations show that cells in united structures generate higher impedance values than the same number of isolated cells [6]. In addition, we analyze starving cells in microfluidic devices in combination with an impedometric assay (no flow) [7]. The results provide a quantitative understanding of the overall cell morphology during early starvation (Figure 7.32).

To investigate the influence of symmetry breaking on the signaling dynamics, we studied, in collaboration with O. Steinbock, the influence of a advecting flow on the wave dynamics. We loaded starved cells into a straight millifluidic device (30 mm x 2 mm x 100μm), allowed the cells to settle for 15 min in order to adhere, started a laminar flow, and observed the cAMP induced contraction waves with dark-field microscopy (Figure 7.33 A).

Figure 7.33 b shows flow-driven instability waves for the averaged flow velocity of \( V_f = 2 \) mm/min, while a space-time plot and phase maps are shown in Figure 7.33 c-f. We observed that waves i) develop in the channel due to a convective instability, ii) are propagating only in flow direction, and iii) have curved wave fronts that resemble the parabolic flow profile. Experiments at different flow rates show that both \( V_w \) and \( \lambda_w \) are proportional to the flow velocity while the period \( T \) is independent. We obtained a more detailed understanding of this flow-induced instabilities by comparison with the Martiel-Goldbeter model.

Exogenous and endogenous electric fields can also play a role in cell physiology as a guiding mechanism. Electrotaxis of cells is a directional response found in several cell types. We found that \( D. d. \) also exhibits electrotactic behavior in electric field gradients. First experiments show a electrotactic response not only to direct but also to oscillating electric fields. Further investigations are on its way for studying the electric sensing mechanisms of \( D. d. \) in single channel microfluidic devices.

Although very heterogenous forest soil is the natural environment of \( D. d. \), all migration experiments are done on flat surfaces like cover slides or petri dishes. To our surprise we found that \( D. d. \) shows what we call curvotaxis. Our experimental observations show that cells prefer to migrate along the curved axis, as shown in cell tracks (Figure 7.34 A) and migration angle histogram (Figure 7.34 B). This behavior was unknow so far and we are currently identifying the underlying biomechanical processes.

Figure 7.33: (A) Side view of the experimental setup. (B) Top view of flow-driven instability waves. (C) Space-time plot. (D) Phase map of signaling patterns before and (E) during flow-induced wave propagation. (F) At high flow velocity, single wave fronts can cover the entire channel length.

Figure 7.34: Cells on fiber overlayed with cell tracks. Trajectories are mostly parallel to the curved axis.

Figure 7.35: SCFS assay. Side view of cell attached to cantilever. Below: Force-separation curve.
Cell-substrate adhesion of eukaryotes still remains to be fully understood. As D. d. lacks integrins, it is ideally suited to study alternative adhesion properties reflective of eukaryotic evolution. In Single Cell Force Spectroscopy (SCFS, Figure 7.35) we attach single D. d. cells to a cantilever and probe quantitatively cell-substrate adhesion. We find that substratum adhesion is dramatically reduced during the first 6 hrs of development, resulting e.g. in reduced work of adhesion $W_{adh}$ (Figure 7.36 A). This decrease fails to occur in cells lacking the cAMP receptor (cAR-) and so can be considered developmentally regulated. In collaboration with the UCSD we compare null mutants of adhesion transmembrane proteins SadA (Sad-) and SibA (Sib-) to wild type cells after 6 h of development and find no difference (Figure 7.36 B) suggesting that neither play a significant role in the adhesion. Cytoskeleton plays a more critical role, as controls with Latrunculin A (LatA, Figure 7.36 A) and Talin null (Tal-) mutants show.

In collaboration with the Max Planck Institute for Biophysical Chemistry we recently extended our investigations of biomechanics to a mammalian brain cell model capable of actively creating flow. The mammalian brain is characterized by ventricles which are interconnected cavities filled with cerebrospinal fluid (CSF). In humans, the ventricles contain up to 150 ml of CSF that is turned over several times every day. CSF flow is mediated by beating cilia, i.e. tiny rod-shaped organelles protruding from the surface of ependymal cells lined up in ventricles. Cilia activity is believed to regulate sleep/wake cycle, appetite, and brain repair. Hormones and cytokines of the CSF exert effects in distinct regions of the brain. Our fluid flow and ciliary beating studies in mouse ventricles show that the brain ventricles are characterized by a complex pattern of liquid flow driven by cilia (Figure 7.37).

7.16 SELF-ORGANIZATION AND OPTIMIZATION IN THE EVOLUTION OF VISUAL CORTICAL CIRCUITS

F. Wolf, W. Keil, L. Reichl, and J. D. Florez Weidinger
D. Coppola (Randolph-Macon College), M. Kaschube (U Frankfurt), Z. Kisvarday (U Debrecen), S. Löwel (U Göttingen), G. M. Schnabel (U Chicago), M. Schottdorf, L. White (Duke U)

(A) Overview of the evolutionary invention of neocortex and its likely transformation during the evolution of modern mammals. Primates and rodents differ fundamentally in the layout of orientation selective neurons in their primary visual cortex. In primates neurons are arranged in columns and maps. Rodents show an interspersed layout without any discernible spatial organization. As mesozoic mammals were small brained and nocturnal they presumably lacked orientation columns as do all small brained modern mammals. Neocortical tissue receiving ascending thalamic afferent innervation presumably originated with the invention of the neocortex in the first mammals about 200 million years ago.

(B) Schematic representation of key processes during the self-organization of orientation selective cortical circuitry. Individual neurons can dynamically reorganize their orientation selectivity but do so under the influence of the extensive cortical circuit in which they are embedded. (C) Different types of intracortical interactions lead to qualitatively distinct types of emerging spatial arrangements of orientation selective neurons.

Response characteristics of orientation-tuned neurons in the visual cortex appear to be similar in mammalian lineages widely separated in evolution. The spatial arrangement of preferences across the cortex, however, shows fundamental differences. While in primates and carnivores orientation preferences form orientation maps, in rodents they are spatially interspersed. The developmental processes and evolutionary origins of these two opposite layout-types remain enigmatic. We discovered that columnar orientation maps realize an apparently quantitatively universal, common design [1, 2, 3, 4] that naturally emerges by activity-dependent self-organization of large scale neuronal circuits when orientation selective long-range interactions are present [1, 6, 7, 8, 9]. In particular we performed comparative studies of visual cortical orientation columns and pinwheels in mammalian species whose evolutionary paths separated more than 65 million years ago [1, 3]. We found that statistical measures characterizing the spatial layout of pinwheels from the scale of hundreds of microns to the entire primary visual cortex (V1) were virtually identical, agreeing with an accuracy of a few percent. To understand how distinct evolutionary lineages can independently evolve this common design, we examined a broad set of mathematical models for the developmental self-organization of orientation columns [1, 6, 7, 8, 9]. We found that models from a symmetry-defined class, exhibiting a universal (i.e.,

Figure 7.38: Self-Organization in the Evolution of Visual Cortical Architecture.
model-independent) solution set, robustly and specifically predict every aspect of the common design when suppressive long-range interactions are dominant [1, 8] (see [1, 5] for evidence that the developmental reorganization orientation columns depend on long-range interactions). This suggests that developmental network self-organization has canalized the evolution of neuronal circuitry underlying orientation maps in these species into the common design that was not present in their last common ancestor. A predicted signature of this mechanism is a pinwheel density close to the mathematical constant $\pi$. Confirming this prediction, we found that mean pinwheel density was indeed statistically indistinguishable from the predicted value with a potential deviation of only up to 2%.

To understand the origin of the qualitative difference between the two design types found in primates and in rodents, we then investigated whether cortical circuit self-organization can also explain the rodent layout type in a unified model. We demonstrate a direct transition from quasi-periodic arrays of orientation columns to interspersed organization. An interspersed organization is actively generated when local circuits are predominantly suppressive. Numerical simulations show that the final arrangement of orientations shows a weak negative correlation between nearest neighbours and that it suffers from a substantial dynamical lability of neuronal selectivities compared to columnar architectures. Interspersed layouts in general exhibit superior stimulus coverage but cause higher wiring costs to maintain a selective like-to-like connectivity. We thus examined models in which cortical organization is assumed to optimize a composite cost function that penalizes reductions in stimulus coverage and excessive wiring length depending on cortex size. In these models we found a transition from interspersed layouts to columnar architecture above a critical area size. Our results suggest that neuronal circuit self-organization played a critical role in the evolution of cortical functional organization and that the invention of orientation columns was driven by the emergence of large brains.

7.17 **HIGH-RESOLUTION IMAGING, SIGNAL ANALYSIS, AND DATA DRIVEN MODELING OF THE HEART**

S. Luther


The development of detailed physiological models of the heart, the availability of large quantities of high-quality structural and functional experimental data, and ever-increasing computational power have significantly enhanced the understanding of cardiac dynamics and hold the promise of new clinical applications for the diagnosis and treatment of heart disease [1]. However, the systematic integration of experimental data into high-dimensional, multi-scale models and their subsequent evaluation, validation and analysis remains a major challenge. Therefore, we are developing a data driven, integrative strategy that combines high-resolution imaging techniques with state of the art numerical modeling through innovative state estimation methods.

**High-resolution Cardiac Imaging.** Physiological cardiac modeling requires detailed structural, functional, and dynamical characterization of the heart. The Research Group Biomedical Physics develops high-resolution fluorescence imaging techniques (optical mapping) for intact, Langendorff-perfused hearts (see Fig. 1). Techniques from computer vision research are applied to reconstruct the three-dimensional shape of the heart from multiple silhouettes. We combine optical mapping with motion tracking, which permits, for the first time, fluorescence imaging of contractile, moving cardiac tissue. This unique experimental technique enables the simultaneous measurement of membrane voltage, intracellular calcium, and surface strain.

The dynamical characterization of cardiac tissue is based on the restitution relations of action potential duration and conduction velocity, obtained from optical mapping. This functional data is complemented by structural information, including coronary vasculature and fiber orientation obtained from micro-computed tomography, diffusion-tensor magnetic resonance imaging, and histological data. Measurements on cellular and subcellular level, including patch clamp, sharp electrode patch, and STED microscopy [1], are available through our research partners and complement the experimental techniques developed by the Biomedical Physics group.

![Figure 7.39: 3D reconstruction of excitation wave propagating on a mouse heart during left ventricular pacing.](image-url)
**State and Parameter Estimation.** Many physical models contain parameters whose values are not known and difficult to measure. These parameters can be identified by adapting the model to experimental data using synchronization of optimization methods, for example. With the synchronization approach the model of interest is driven by the available time series and parameters are estimated by minimizing the synchronization error. As an example for synchronization based data assimilation, we developed a scheme for synchronizing extended excitable media [2] and an approach for sparse observations [3]. Optimization-based methods also aim at reproducing the observed time series by means of the corresponding model output. However, since no synchronization is employed, one additionally has to make sure that the underlying temporal evolution of the state variables fit the model dynamics. This can be achieved by including (deviations from) the dynamical equations in the cost function [4]. By employing efficient optimization methods and automatic differentiation [5] unknown state variables and parameters can be estimated even for high dimensional systems [6].

Figure 7.40 shows as an example the reconstruction of the dynamics of hyper-chaotic Mackey-Glass system [5]. In general, not all parameters of interest may be accessible with the given time series. This issue of “observability” is independent of the estimation method chosen [7].

**Classifying cardiac biosignals using ordinal pattern distributions.** The performance of (bio-)signal classification strongly depends on the choice of suitable features (also called parameters or biomarkers). We have investigated the discriminative power of ordinal pattern statistics and symbolic dynamics in comparison with established heart rate variability parameters applied to beat-to-beat time series. Fig. 7.41. Using an example of patients suffering congestive heart failure, we demonstrate the feasibility of this approach for efficient classification [8] and for system identification [9].

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7.18 DYNAMICS OF FLUID AND BIOLOGICAL INTERFACES

O. Bäumchen

The newly established experimental research group studies the dynamics of complex liquids and biological objects at interfaces.

On small length scales, the flow of complex liquids is purely driven by intermolecular capillary forces. Starting from any liquid surface exhibiting nonconstant curvature, a thin liquid film approaches its flat equilibrium state: Levelling processes of topographic perturbations like single steps [1, 2] or trenches [3] reveal characteristic micro- and nanofluidic features emerging from local Laplace pressure gradients. In the regime of intermediate asymptotics, i.e. after passing an initial transient regime, self-similarity and scaling laws are discovered, both in excellent agreement with analytical models [3, 5] and numerical calculations [4]. The complete description of the dynamics is a powerful tool to address key questions of fluid mechanics on small length scales: Can liquids slide? Does confinement alter the mobility of complex liquids? The insights can be applied to gain precise control of minute amounts of liquids in lab-on-a-chip devices.

We also take advantage of the opposite effect: Destabilizing forces and the surface minimization of initially unperturbed systems can lead to liquid instabilities such as the Rayleigh-Plateau instability. This phenomenon can not only be observed for water flowing out of a faucet, but also e.g. for thin liquid films on flat substrates and on micro-fibers.

By transferring concepts like capillarity, elasticity and ideas from fluid mechanics to the mechanics of biological systems, the research group aims at bridging the gap between polymeric and biological systems. Novel experimental techniques open fascinating pathways for a quantitative description of the dynamics of biological matter like vesicles, cells and active micro-organisms, in particular at interfaces.

Figure 7.42: (a) Schematic of the initial condition of a topographically perturbed film surface. The schematic is not to scale: the trench width is on the order of microns, its depth is about 100 nm. (b) AFM image of a trench in a polystyrene (PS) film (image size: 30 µm, height scale: 115 nm) [3].

Figure 7.43: (a) AFM profiles h(x, t) of a trench (a = 1.6 µm, h₀ = 2d₀ = 206 nm) in a thin PS film at time t. (b) Normalized profiles (a = 2.5 µm, h₀ = 611 nm, d₀ = 59 nm) show self-similarity in t^{1/3} and agreement with the analytical solution (dashed line) of the linearized equations. The ratio of viscosity η and surface tension γ is the only fit parameter [3].

By transferring concepts like capillarity, elasticity and ideas from fluid mechanics to the mechanics of biological systems, the research group aims at bridging the gap between polymeric and biological systems. Novel experimental techniques open fascinating pathways for a quantitative description of the dynamics of biological matter like vesicles, cells and active micro-organisms, in particular at interfaces.

Figure 7.44: Optical micrograph of a lipid vesicle (attached to a micropipette) near a wall.

7.19 ELECTROMECHANICAL WAVES AND INSTABILITIES IN CARDIAC TISSUE

J. Christoph, M. Chebbok, S. Stein, T. Baig, U. Parlitz, S. Luther
G. Hasenfuss (University Medical Center, Göttingen)

Intramural Electromechanical Wave Imaging

Self-organized dynamics of vortices or scroll waves underlie complex spatio-temporal pattern formation in many physical, chemical and biological systems [1, 2, 3]. During life-threatening cardiac fibrillation, the pairwise formation and annihilation of filament-like phase singularities associated with three-dimensional rotating waves and their nonlinear interaction with the complex anisotropic and heterogeneous multicellular substrate results in self-sustained electromechanical turbulence [4, 5]. Understanding the mechanisms underlying the onset, perpetuation, and control of fibrillation requires imaging of wave propagation deep inside cardiac tissue. However, the visualization of spatial-temporal dynamics inside cardiac tissue that relates cardiac structure and function evades experimental realization. We have shown that (i) high-speed, high-resolution ultrasound imaging of tissue strain permits the visualization of complex transient spatial-temporal dynamics of cardiac fibrillation deep inside the ventricular wall; (ii) the dynamics of intramural phase singularities can be obtained from tissue strain, which are found to be co-localized with electrical activation in simulations of cardiac electro-mechanics; and (iii) the analysis imaging reveals detailed tissue structure including local fiber orientation [8]. Our findings may provide novel perspectives for diagnostic and therapeutic strategies.
In cardiac tissue, excitation-contraction-coupling (ECC) refers to a physiological process that converts an electrical stimulus (action potential) into a mechanical response (contraction) mediated through the intracellular release of Ca\textsuperscript{2+} (Figure 7.47). The propagation of waves of electrical excitation results in mechanical tissue contraction which is associated with characteristic spatial-temporal patterns of compressile and tensile strain. High-resolution ultrasound enables us to visualize the spatial-temporal pattern inside cardiac tissue, permitting for the first time the visualization of intramural vortex wave dynamics.

We have applied ultrasound imaging to Langendorff-perfused intact rabbit hearts. In B-mode (2D imaging mode), we have visualized mechanical tissue deformation at frame rates of 309Hz at a spatial resolution of 30\textmu m (VisualSonics Inc., Vevo 2200). The imaging plane is located inside the ventricular wall, approximately parallel to the epicardial surface, as illustrated in Figure 7.45. During arrhythmia, tissue strain obtained from the mechanical deformation shows complex spatial-temporal patterns. Figure 7.46 shows vortex-like rotating strain wave patterns. Intramural ultrasound recordings are complemented by epicardial optical measurements of the membrane potential using voltage-sensitive fluorescent dye. The optical membrane potential recording shows a single spiral wave meandering on the surface of the ventricle.

**Simulations of Electrical and Mechanical Waves in Cardiac Tissue**

Numerical simulations have been developed to study the spatial-temporal dynamics of electrical excitation and mechanical contraction of the heart. The simulation of tissue mechanics is based on a discrete particle approach using a mass-spring-system consisting of tetrahedral volume elements. The model takes into account anatomical tissue anisotropy including muscle fiber direction [1]. An example of ventricular fibrillation in an intact rabbit heart is shown in Figure 7.48. Multiple vortex-like rotating waves of electrical excitation cause the tissue to develop corresponding wave patterns of contractile motion. Currently, it is investigated whether the topological structures of both, electrical and mechanical patterns, retain similar properties [8].

This research is supported by the Deutsche Forschungsgemeinschaft (SFB 1002: Modulatory Units in Heart Failure), and the German Center for Cardiovascular Research (DZHK e.V.), by the European Community’s Seventh Framework Programme FP7/2007-2013 agreement HEALTH-F2-2009-241526 (EUTrigTreat) and by the Max Planck Society.

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[8] J. Christoph et al. (manuscript in preparation)
MAGNETIC RESONANCE IMAGING IN REAL TIME

J. Frahm, M. Uecker, S. Zhang, D. Voit, S. Schaetz

The invention of fast low-angle shot (FLASH) gradient-echo MRI in 1985 with its at least 100-fold gain in acquisition speed vastly broadened the spectrum of clinical MRI and even allowed for preliminary studies of dynamic processes such as turbulent flow – though at still very limited temporal resolution [1]. Recent progress now overcomes these problems by combining modified FLASH sequences with advanced mathematical concepts for image reconstruction [2]. The new method provides real-time images (i.e., MRI movies) at so far unsurpassed spatiotemporal resolution and thus offers new scientific and clinical applications [3] - [7].

Low flip-angle gradient-echo sequences are used because of their insensitivity to tissue-dependent susceptibility differences and their ability to continuously acquire data at high speed without violating RF power deposition limits. However, the conventional rectilinear (Cartesian) coverage of data space is replaced by a radial encoding scheme which avoids motion artifacts (due to the absence of a phase-encoding gradient) and, even more importantly, is tolerant to moderate undersampling. In fact, high speed or sufficiently accelerated acquisitions are only achieved by extreme data undersampling, so that conventional reconstructions by inverse FFT have to be replaced by iterative image estimations. We therefore defined the image reconstruction as the solution of a nonlinear inverse problem. In contrast to computationally simpler linear approaches, the nonlinearity allows for a simultaneous optimization of the image and all sensitivity profiles of the many independent receive coils that are commonly employed in a modern MRI system. To further improve the ill-conditioned mathematical problem by constraining the range of possible solutions (i.e., image estimates that are in agreement with the few acquired data) we took advantage of a temporal regularization strategy which exploits the inherent redundancy in a time series of images by penalizing the difference to the preceding frame. Finally, the high computational burden has been
solved by the development of a parallelized algorithm on a server with multiple graphical processing which then has been integrated as a bypass into a commercial MRI system. The current version achieves online reconstruction rates of more than 20 frames per second.

A most promising application is cardiovascular imaging [3], [6], [7] as real-time MRI studies of the heart may be performed without breath holding and even without ECG synchronization (see Figure). Moreover, the ability to analyze individual heartbeats for the first time offers access to the variances of functional parameters (e.g., ejection fractions and stroke volumes) and the immediate physiologic responses to exercise and stress. Real-time acquisitions are also a prerequisite for the examination of aperiodic phenomena such as arrhythmia or turbulent blood flow that both are chaotic in nature and therefore not amenable to synchronized data acquisitions from multiple cardiac cycles.

The “tropical limit” of an \( n \)-soliton solution of the Korteweg-deVries (KdV) equation represents it as a piecewise linear graph in (two-dimensional) space-time (Fig. 7.50 shows an example), with values of the dependent variable assigned to the lines. The interaction of solitons is described in this limit by creation and annihilation of “virtual solitons”. A corresponding graph is completely determined if we know the branching and merging events, which can indeed be computed in terms of the parameters entering the general \( n \)-soliton solution. The complexity of the problem can be reduced by taking higher KdV hierarchy variables – related to symmetries of the KdV equation – into account, but a complete classification of the possible graphs beyond the 3-soliton case is out of reach [1].

The Kadomtsev-Petviashvili (KP-II) equation generalizes the KdV equation to a nonlinear PDE in three space-time dimensions which, in particular, describes stable networks formed by line-like waves, e.g., on shallow water ([2] and references therein). At a fixed value of time, the tropical limit of a corresponding exact line soliton solution lives on a graph in two-dimensional space. A complete classification of the possible evolutions, in the abovementioned sense, seems to be impossible. But for the class of (rooted binary) tree-shaped KP-II line soliton solutions such a classification has been achieved for arbitrary soliton number [3]. For fixed soliton number, any such evolution corresponds to a maximal chain of a Tamari lattice, see Fig. 7.51. Tamari lattices are partially ordered sets that form polytopes called associahedra (see [4]). The step from a vertex to the next is a rightward application of the basic associativity law. It corresponds to a right rotation in the realization in terms of rooted binary trees (cf. Fig. 7.51). The evolution of tree-shaped KP-II line solitons is simply governed by the familiar associativity law!

As shown in [5], the tree-shaped KP-II line soliton solutions also realize higher Tamari orders, which can be constructed from higher Bruhat orders, introduced by Manin and Schechtman in 1986 and associated with generalizations (“simplex equations”) of the famous Yang-Baxter equation that underlies quantum integrable models. In a similar way, higher Tamari orders determine generalizations of the so-called pentagon equation ([5] and work in preparation). In particular, the exploration of soliton interactions in the tropical limit revealed unexpected relations with well-known structures in (geometric) combinatorics.

NETWORKS

From vascular networks in plants and animals to route networks in public transport, from neural circuits in the brain to power grids spanning entire continents – systems with fascinating complex webs of interactions permeate every aspect of our lives. Understanding how these networks are organized and how they behave dynamically constitutes a challenging endeavor of current cross-disciplinary research and bears a growing potential for applications. Complex webs constitute a major thrust at the MPIDS and are represented by a wide variety of projects, ranging from the applied, such as novel approaches to distributed public transportation, the leaf venation or neural network function, to the more abstract, such as the study of precursory fluctuations in percolation theory.

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8.1 LEAF SIZE AND OPTIMALITY OF PLANT VASCULAR NETWORKS

E. Katifori

H. Ronellenfitsch, J. Liesche and A. Schulz (Copenhagen), K. H. Jensen and N. M. Holbrook (Harvard), Sara Puijalon (Lyon)

All vascular plants are endowed with two separate systems of conductive tissue, the xylem and the phloem, allowing them to transport energy (sugars), nutrients, water and signaling molecules within their body. The architecture of the vascular networks of modern leaves evolved from primitive dichotomously branching structures, still seen in living fossils like gingko, to the elaborate reticulate webs of most modern flowering plants (Fig. 8.1(A)). It allowed the precursors of modern plants to outcompete their ancient relatives and quickly dominate most ecosystems. The vein architecture in all leaves exhibits some dominant trends, the products of convergent evolution, but also considerable diversity [1]. In order to understand the reasons behind these dominant trends we examine a number of network optimization models.

In Ref. [2] we explored the function of the xylem (the plant vascular network that distributes water to the leaves to replenish what is lost by transpiration) and the emergence of loops in modern leaves. We modelled the water flow in the xylem of the leaf blade and inquired what network architecture is optimal for water distribution under spatially fluctuating loads or damage. We found that nested reticulate structures are optimal in both cases. We are currently expanding this work and further exploring the space of optimisation functionals for the flow in the leaf xylem. We study cases where the transpiration on the leaf blade is not uniform (as one would find in leaves where the stomata density decreases close to the leaf margin) and investigate the optimal architectures under various implementations of damage, as would be inflicted by cavitation due to drought, fungal or insect attacks (see Fig. 8.1(B) for a typical network optimized for random localized damage).

The phloem vascular system in leaves collects and redistributes the products of photosynthesis and facilitates transport of signaling molecules in plants, thus permitting growth and long range communication within the organism. The flow is driven by osmotic pressure, generated by differences in sugar concentration between distal parts of the plant. Like the xylem, over the course of evolution the phloem will tend to attain a form optimal for its function, under relevant natural constraints [3]. Little is is known about the network structure, regulation and diversity of the phloem system. We modeled the phloem in the simplest possible geometry: a one-dimensional leaf, found, for example, in the needles of conifer trees (Fig. 8.2). We found the optimal sieve tube (phloem vein) distribution for various physiologically relevant optimising functionals. In collaboration with experimental groups at Harvard and Copenhagen, we compared our predictions to measurements of the phloem structure in four tree species representing a diverse set of habitats and needle sizes, from 1 cm (Picea omorika)
to 35 cm (Pinus palustis). We showed that the phloem shares common traits across species, habitats, and orders of magnitude of needle length. The minimal model accounting for these traits takes into account the transport strategy and natural constraints. In our model, the system can be described by a single dimensionless "phloem number" $a$ that reflects how the phloem varies in shape along the needle. Against the current paradigm, we found that conserving energy (minimising dissipation) is more important than maximizing volumetric flow in needles.

The phloem and the xylem function in conjunction in the leaves of vascular plants to create a complex web of interactions that are difficult to decouple. For example, phloem loading depends on the water pressure in the mesophyll, which in turn is contingent on xylem function. To test our phloem models in a simplified setting, we need to examine phloem function in isolation. This is possible in aquatic plants that have reduced, or completely absent xylem. In collaboration with the experimental group of Sara Fujalon in Lyon, expert on the biology of aquatic plants, we are measuring phloem anatomy in aquatic plants with linear leaves.

To go beyond phloem structures in one dimensional leaves, we generalized the pine needle model to more complex two dimensional networks. Among other questions, we are currently looking into how phloem anatomy and function influence leaf size. Our ultimate goal is to have a unified understanding of the microfluidics, xylem and phloem together, of a broad leaf blade.

Figure 8.2: (A) Z-stack of lateral cross-sections of a pine needle. The phloem is marked in red. (B) Sieve tube area as a function of normalised distance from the needle tip. The dashed line is the prediction for a needle that minimises dissipation. Solid line is the prediction for a needle that optimises flow speed.

8.2 THE ARCHITECTURE OF ADAPTIVE NETWORKS

E. Katifori
J. Graewer, C. Modes (Rockefeller), M. Magnasco (Rockefeller)

Transport networks, whether engineered by man or made by nature, need to maximize efficiency and minimize cost. Man made distribution networks, such as the ones for power distribution, irrigation or information flow can be centrally designed and constructed in order to function optimally. However, in nature frequently the architecture of an efficient network is the result of gradual alterations according to local information, rather than execution of a central plan [1].

An example of such as system is the intracellular network of protoplasmic veins composing the slime mold Physarum polycephalum shown in Fig. 8.3. These veins perform cytoplasmic streaming and transport nutrients from food sources to the rest of the network. The organism redistributes the vein wall material so that little used conduits gradually disappear and heavily used ones grow.

The phsyrum network exhibits a dense array of hierarchically organized loops and has been shown to be robust and efficient [2]. Inspired by this locally adaptive network we ask a number of questions: Can such tinkering provide an efficient system? How does the system reach a steady state? What are the generic features of a network produced by self-organized adaptation processes?

To answer these questions, we adapted a mathematical model used for phsyrum in Ref. [2]. Going beyond planar graphs, we let the networks evolve on a number of prescribed underlying complex network topologies (such as regular, Erdos-Renyi, Barabasi-Albert etc.). Instead of spatially fixed sources, each pair of vertices of the network can act as a source and sink. Although the topology of the network cannot change, the conductivity of the links will grow or decrease according to the average flow through them.

Starting from a random assignment of edge conductivities, the networks gradually converge to a hierarchically organized architecture, dominated by a high conductivity backbone that spans the whole network (e.g. Fig. 8.4). In addition, the dynamical rearrangements of network links shows striking, system-spanning (i.e. global) behavior at certain key moments of the evolution that is perhaps reminiscent of glassy systems (e.g. Fig. 8.5).

The scope of this work is general and the aim is to understand the universal features of self-organized adaptation in transport networks. Besides the Hagen-Poiseulle fluid flow network, we currently examine other models such as a shortest-path model, and a capacity based model (Ford-Fulkerson maximum flow model). An understanding of the fundamental physical differences between local update rulesets and how those differences play out in the dynamics is an important first step in both describing these complex systems, and even in engineering computational or communicational analogs.


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8.3 LEAF VASCULAR NETWORK DIGITIZATION AND CHARACTERIZATION

E. Katifori
Jana Lasser, Carl Modes (Rockefeller)

Distribution networks manifest themselves in nature at multiple scales and in many forms. In biology they can be defining characteristics of the phenotype and function of an organism. A pervasive example is the vasculature of leaves: each plant species has leaves with distinctive architecture, yet they all share some common traits.

The leaf vein network is complex and typically reticulate, displaying multiple levels of nested loops. In order to properly develop a predictive model that includes the effects of vascular network architecture and topology, we must first choose a set of tools to characterize vasculature in a physically relevant and mathematically compact way.

A first step toward that goal is to collect and digitize a large number of leaf vein networks. We currently have digitized at 6400 dpi approximately 200 cleared, stained, and plasticized samples from various species (through a collaboration with the New York Botanical Gardens). To extract the topological and geometric information of the vein networks from these images, we developed a general computational framework for the processing of high resolution images of vascular networks [2]. The framework provides a fast and highly automated method to process the inherently noisy data while preserving the properties of the networks with high accuracy. With a few adaptations it can be used for images from networks in different systems, such as the vasculature of the retina. In order to characterize the nested architecture of these loopy networks we developed an algorithm that makes it possible to map loopy networks to binary trees, preserving in the connectivity of the trees the architecture of the original graph [1]. The algorithm offers a nuanced description of the loopy networks, but as originally formulated it is only applicable to planar graphs.

At this point, there is no satisfactory metric to quantify hierarchically nested loopy non-planar graphs. In order to fill this void, we have generalized our 2D algorithm [1] to a fully three dimensional setting, from whence it may be brought to bear on many problems in animal vasculature, particularly where that vasculature is extremely complex, as in the organs. The new algorithm rests on the abstraction of the physical ‘tiling’ from the two dimensional case (as in the areoles of leaf vasculature) to an effective tiling of an abstract surface that the network may be thought to sit in.

8.4 PREDICTING PHASE TRANSITIONS

J. Nagler, M. Schröder, Wei Chen (Peking University, China),
R. M. D’Souza (University of California, USA),
D. Sornette (ETH Zürich, Switzerland)

Percolation, the transition to large-scale connectedness of networks or complex environments by gradual addition of links, occurs during growth and evolutionary processes in a large variety of natural, technological, and social systems. Across all percolating systems, once the number of added links exceeds a certain critical value, \( p_c \), extensively large connected components (clusters) emerge that dominate the system [1], see Fig. 8.7. Given the breadth of experimental, numerical, and empirical studies, it is widely believed that the phase transition is entirely unanticipated - except very close to the transition point at \( p_c \), where large-scale fluctuations dominate the system and thus announce the transition [2, 3].

Figure 8.7: Illustration of the phase transition to global network connectivity by gradual addition of links.

We have found time-localized precursory fluctuations in the order parameter of different percolating systems that allow us to predict almost deterministically the transition point to global connectivity, see Fig. 8.8.

![Cascade of peaks in the relative variance of the order parameter in a percolation model.](image)

Figure 8.8: Cascade of peaks in the relative variance of the order parameter in a percolation model announces the phase transition at \( p_c \).

This demonstrates that a genuine peak in the relative variance of an order parameter, such as the total magnetization or the relative size of the largest system component, does not necessarily indicate a phase transition point. Moreover, we have established a non-trivial connection between the cut-off divergence of the order parameter of a percolation system and the scaling laws governing these micro-transition cascades [4]. This analytically demonstrates the universality of our findings. Moreover, the framework suggests the use of warning signals for anticipating tipping points in complex systems that are dominated by intrinsically stochastic fluctuations.

8.5 BURSTS, AVALANCHES, AND SELF-ORGANIZED CRITICALITY IN NEURONAL NETWORKS

A. Levina, O. Stetter, T. Geisel
M. Uhlig, J. M. Herrmann (Edinburgh)

Neuronal avalanches were predicted theoretically [1] and later discovered experimentally [2] in recordings from cortical slices. When they are critical, they are characterized by a power law distribution of sizes, which indicates that the network is in a state at the border between epileptic activity, where each perturbation leads to the response of the full network, and almost silent activity, where perturbations rapidly die out. Critical avalanches have been shown to possess various optimality properties. Cortical networks appear to self-organize towards such a critical state (i.e. without tuning a parameter), which is reminiscent of self-organized criticality (SOC) and puts them into a broader physical framework.

In previous studies [3, 4], we have demonstrated how this self-organization can be achieved by considering a neural network with biologically realistic dynamical synapses. As learning and long-term plasticity are the essence of cortical networks, an important question, on which we now focus, is how criticality is affected by long-term synaptic plasticity and learning, and whether learning in the network can profit from its critical state. In a first step we have studied, how learning by the well-established spike timing dependent plasticity (STDP) changes the state of the critical network. We found that STDP alone can already account for a broadening of the critical region of connectivity parameters. Combined with homeostatic learning, structural changes due to STDP bring the network closer to a critical state than in any random connectivity setup [5].

In a second step we investigated the interplay between criticality and memory in neural networks. We studied the effect of structural connectivity formed by Hebbian learning on the criticality of network dynamics. We found that a network endowed with Hebbian learning alone does not allow for simultaneous information storage and criticality, even if the synaptic strength is properly scaled. Adding short-term synaptic dynamics, however, stabilizes the critical regime [6]. This is

Figure 8.9: Memory retrieval quality and criticality in a neural network. Left: In a pure memory network the retrieval quality is good only outside the critical regime of coupling parameters \( \alpha \), determined by small deviations \( \Delta \gamma \) from a power law (inset). Right: The network with homeostatic regulation, however, achieves good retrieval quality also in the critical regime [6].
the first example of reconciliation of criticality and memory in neuronal networks.

Avalanches known as bursts are also a prominent feature of cultured neuronal networks \textit{in vitro}. A long-term goal is to understand the underlying self-organized wiring principles of these dissociated neurons. We therefore asked what can be learned about the structural connectivity in these networks from the observation of their network dynamics \cite{8}.

We tried to answer this question making use of a measure of directed causal influence from information theory, Transfer Entropy. By simulating fluorescence signals and computing this measure for all pairs of neurons, we extract an effective connectivity that we can overlap with the ground truth topology. It turned out, however, that this overlap is no better than chance since the effective connectivity is highly dependent on the dynamical state of the network.

Studying this dependence systematically, we were able to isolate a state in which the firing is occurring with an elevated frequency, but not yet in the synchronized manner of network bursts. In this state the effective connectivity closely resembles the structural connectivity since here the dynamics in the network are primarily driven by monosynaptic interactions.

By also accounting for the slow temporal resolution of typical calcium fluorescence recordings, we are now able to identify structural links with high accuracy even in the presence of light scattering artifacts in the recording. We call this new measure of causal effect the Generalized Transfer Entropy (GTE) \cite{7}.

Moreover, more recently we showed that GTE is able to detect both excitatory and inhibitory interactions, as long as the inter-burst firing rate is above a certain lower bound. By combining two simulations, in one of which inhibitory synapses are blocked, it is indeed possible to
label the neuronal types with high confidence [9]. Thus we are now able to analyze the complete wiring diagram of simulated circuits with a very good degree of accuracy, and are presently working on a number of verification techniques to test the performance in the experimental setting.

The dynamics of neuronal networks is fundamental to the ability of neuronal systems to perform cognitive functions such as sensory processing, working memory, and decision making. In the cerebral cortex dynamically generated activity patterns are, in general, irregular and spatiotemporally complex. The prevailing theoretical explanation for this irregular activity is that its origin lies in strong fluctuations in inputs that arise from the dynamical balance of excitation and inhibition known as the balanced state [1]. It is a long standing theme of dynamic brain theories that such complex activity patterns might serve as a rich encoding and processing space for neural computations. In particular, if the precise timing of every nerve impulse is used for information encoding, the processing capacity of neuronal circuits might be amazingly rich. We analyzed the state-space structure of spiking neural networks, namely, sparse random networks of inhibitory leaky integrate-and-fire (LIF) neurons in the balanced state [2]. Although capable of generating complex irregular spike sequences, we found that these networks actually exhibit negative-definite Lyapunov spectra. The spectra are invariant to the network size, hence this stable dynamics is extensive and preserved in the thermodynamic limit. We find that various state perturbations are predicted to decay extremely fast. In particular, in the limit of high connectivity, small perturbations to the membrane potentials of the neurons decay as quickly as in isolated cells. In addition, single-spike perturbations induce only minute responses in the population firing rates that decay on a millisecond time scale. Surprisingly, however, single-spike perturbations always lead to exponential state separation, causing complete decorrelation of the micro-states. This rapid decoherence is also established within only a few milliseconds. By examining the dynamics for arbitrary perturbation sizes, we explain this behavior by a picture of tangled exponentially separating flux tubes composing the phase space of the network. Our current work is exploring the range of single neuron dynamics and network structures that can support this exotic phase space organization.

8.7 CAUSALITY MEASURES REVISITED

J. Nagler, T. Geisel, A. Witt,
A. Gail (German Primate Center, Göttingen), D. Battaglia

In 1969 C. Granger proposed a causality measure based on time series that has become a key concept for quantifying directed causal influence and fundamentally underlies many models in biology, physics, economics, and social sciences: if the predictability of a time series $X$ is significantly enhanced when information from a time series $Y$ is included, then $Y$ is said to Granger-cause $X$ [1].

Granger causality can also be used to quantify the contribution of a certain frequency component to an oscillatory causal interaction. For this type of analysis, spectrally decomposed Granger causality (SDGC) has been proposed [2]. If a dog has been trained to a dog whistle, the whistle can be used to make the dog come back to us. Thus the tone characterized by a substantial peak at a certain frequency in our communication channel causes the dog’s action. Systems where SDGC has been successfully employed share this basic mechanism, namely frequency selective directed causal influence. In particular, a significantly elevated level of SDGC in a certain frequency range is usually interpreted as evidence for causal driving, like in inter-areal brain synchronization or in cyclic components of genetic or ecologic systems.

In contrast to textbook examples of SDGC, we have found and studied stochastic processes for which elevated values of SDGC (i.e. ‘artificial’ peaks) are obtained for frequency ranges with very low spectral power (see Fig. 8.7). The same feature occurs in experimental data like electrophysiological brain recordings or measurements of cardio-vascular dynamics. These observations are unexpected since high causality at a certain frequency necessarily requires a substantially strong spectral power at this particular frequency.

We have shown that the non-correspondence between peaks of spectral power and Granger causality is a prevalent rather than an exceptional phenomenon. Revisiting the original definition of SDGC and employing an information theoretical analysis we have unraveled the reason for this inconsistency.

Most importantly, we have proposed a new spectrally decomposed causality measure derived from first principles that accurately captures directed causal influences and overcomes the failures of SDGC. In addition, our framework is consistent with both, synthetic and real data and thus explains the seemingly paradoxical behavior that conventional SDGC generically exhibits.


Figure 8.12: Power spectrum and spectrally decomposed causality measures. Conventional SDGC (shown in red) is not well-defined as it can display artificial peaks, i.e. peaks at frequencies that correspond to negligible spectral power. In contrast, the proposed causality measure (green), derived consistently from first principles, overcomes this limitation. It correctly predicts directed causal influence, seen by the coincidence of its peaks with peaks of the power spectral density (blue).
8.8 SELF-ORGANIZED INFORMATION ROUTING IN OSCILLATING NEURAL CIRCUITS


Brain functions, from vision or motor preparation to memory or awareness, require the control of inter-areal interactions on time-scales faster than synaptic changes. In particular, the way in which information conveyed by neuronal activity is routed through the multi-scale circuits of the brain must be reconfigurable (e.g. by attention) even when the underlying structural (i.e. anatomic) connectivity is fixed. The ability to quickly reshape such “effective connectivity” is a chief requirement for performance in a changing environment. Yet it is an open problem to understand which circuit mechanisms allow for achieving this ability. How can manifold effective connectivities –corresponding to different patterns of inter-areal information flow, or brain states – result from a fixed structural connectivity? And how can effective connectivity be controlled without resorting to structural plasticity, leading to a flexible “on demand” selection of function?

We explore such general questions through computational studies of meso-scale motifs involving a few interacting cortical areas [1], each modeled as a large network of spiking neurons with random local connectivity. Profiting of the advantages of a computational framework, in which the ground-truth structure and dynamics of the analyzed systems are known with full precision, we show that “function follows dynamics”, rather than structure. Different dynamic states of a same structural network, characterized by different synchronization properties, are indeed associated to different directed functional networks, corresponding to alternative information flow patterns, as revealed by Transfer Entropy [2] and Mutual Information analyses of simulated electrophysiological recordings (LFPs and spike trains). Fully analytic derivations of information sharing patterns are provided for arbitrary network topologies of simpler phase-reduced oscillator models [3].

Switching between multiple dynamical states (either spontaneous, or induced through ad hoc local manipulations or perturbations) therefore leads to a self-reconfiguration of network-wide functional interactions without need of structural changes [1, 3]. In particular, computational exploration can be used to guide the design of closed-loop experimental protocols, in which optogenetic stimulation is applied to a given brain site conditionally to the recorded phase of ongoing oscillations [4]. Such a protocol, besides allowing the experimental testing of our predictions, might open the way to the alteration or the stabilization of brain cognitive states via tailored local perturbations.

8.9 SPATIO-TEMPORAL PATTERNS AND INFORMATION TRANSFER IN NEURAL CIRCUITS

S. Jahnke, W.-C. Chou, D. Battaglia, M. Timme
R.-M. Memmesheimer (Nijmegen), C. Kirst (Munich), S. Dipt, A. Fiala, C. Tetzlaff, F. Wörgötter (all Georg-August-Universität Göttingen)

Spatially and temporally coordinated patterns of neural activity are keys to information processing in the brain. Yet, their dynamical origin and the mechanism underlying pattern coordination is far from being understood. In three projects (one co-funded by the DFG, one by the BMBF), we study how heterogeneous network structure and non-additive coupling may induce specific activity patterns in neural circuits and how information transfer may be remotely controlled in complex network dynamical systems.

Spike patterns from non-additivities in cortical circuits

Cortical neural networks generate a ground state of highly irregular spiking activity whose dynamics is sensitive to small perturbations such as missing or additional action potentials (spikes). A robust, reliable transmission of information in the presence of such perturbations and noise is nonetheless essential for neural computation. It has been hypothesized that this might be achieved by propagation of pulses of synchronous spikes along feed-forward chains (compare for example [1]). In current models of feed-forward structures that are embedded into recurrent neural circuits, functionally relevant chains require a dense connectivity between the neuronal layers of the chain (see review by Kumar et al. [2]) or strongly enhanced synapses and specifically modified response properties of neurons within the chain [3]. Such highly distinguished large-scale structures, however, are not observed experimentally.

Can less structured networks also guide synchrony? Recent neurophysiological experiments (starting with Ariav et al. [4]) found that under certain conditions the neuronal dendrites – branch projections of the neuron that transmit inputs from other neurons to the cell body (soma) – process input spikes in a non-additive way: If the inputs arrive within a time window of a few milliseconds, the dendrite can actively generate a fast dendritic spike that propagates to the neuronal soma and leads to a nonlinearly amplified response. This response is temporally highly precise and supports the detection of synchronous inputs by a neuron.

We have now provided the first analytical studies of spiking neural circuits with non-additive dendritic interactions [5, 6]. Bifurcation analyses of mathematically tractable circuit models reveal that and how non-additive dendritic interactions enable guided synchrony propagation already in random recurrent neural circuits that exhibit only mildly enhanced, biologically plausible sub-structures. We quantify how dendritic nonlinearities compensate for dense anatomical connections and thereby promote propagation of synchrony. Using large-scale

![Figure 8.14: Neural circuits with non-additive dendritic coupling may robustly transmit signals in form of sub-network synchrony. (a) Mildly enhanced structures in random recurrent networks enable long-lasting propagation of spike synchrony (b). Too weak or too strong coupling implies no propagation or pathologic activity (insets).]
simulations of more detailed recurrent network models, we show that
feed-forward networks that occur naturally as parts of random cir-
cuits enable persistent guided synchrony propagation due to dendritic
nonlinearities (see Fig. 8.14). Our analysis explains the mechanisms
underlying robust propagation and shows in which sense non-additive
coupling – a local neuron property that dynamically changes processing
with input synchrony – may complement dense and non-local structural
connectivity that is fixed on short time scales. Our study thus adds a
novel perspective on the dynamics of networks with nonlinear interac-
tions in general and offers a viable route for the occurrence of patterns
of precisely timed spikes in recurrent networks under physiologically
plausible conditions.

Do specifically heterogeneous networks support olfaction?

The first processing circuit of olfaction (antennal lobe or olfactory bulb)
exhibits a number of surprising nonlinear features, but how these
collective features emerge remains an open challenge. We stress three
puzzling findings. First, it was long believed that the antennal lobe of
insects mainly reduces input noise and is capable of separating sensory
input representations from two different odor signals. Our joint work
with the Molecular Neurobiology group of Andre Fiala (University
of Göttingen) now suggests that the same antennal lobe may equally
join representations of other pairs of odors [9]. Second, studies on
olfactory bulb have shown that gradual mixtures of two odors generate
representations among projection neuron activities that split a large
set of mixing ratios into two distinct representational classes. Third,
first olfactory processing circuits are moreover capable of separating
inputs into classes of input concentration even for the same input odor.
Taken together, these studies suggest that the same circuit processes
information in distinctly different, nonlinear ways depending on the
inputs only. How do these nonlinear processing modes emerge in
recurrent circuits?

Our current theoretical studies (e.g., Chou et al., in preparation)
now actively use the fact that the connectivity of interneurons is highly
heterogeneous [8]. Experimental evidence suggests that whereas some
interneurons connect to only a few sensory neurons, others connect to
many and yet others to almost all sensory neurons in a given glomeru-
lus. Our main contribution is grounded in the observation that se-
lectively heterogeneous connections of interneurons may selectively
inhibit particular sets of sensory neurons, thereby reducing the high-
dimensional inputs to lower dimensional activity of a glomerulus circuit
and thus reducing the information transferred to higher level circuits
via projection neurons. Our analysis suggests that this connection
heterogeneity may indeed be key to this information channeling, trans-
lating a dense into a sparse coding scheme within the antennal lobe (or
olfactory bulb).

Intriguingly, such networks with specific heterogeneities may pro-
vide a simultaneous answer to a number of open questions in neu-
robiology. They are indeed capable of generating all three of the
above-mentioned collective phenomena. One circuit with specific heterogeneous interneuron connectivity may separate representations of some but join those of other odor pairs; split continuous mixtures of odors into discrete representation classes; and explain how even a single odor is represented as distinct inputs if at certain ranges of its concentration. Finally, our theoretical ansatz also offers an integrating view on the debated role of interneurons: Together with their heterogeneous connections, the interneurons may enable not only one of the currently discussed functions but in fact generate all of them – depending on odor inputs but in the same circuit.

Local (and remote) control of global information transfer

Finally, we revealed how complex oscillatory networks may route specific flows of information via fluctuations in their phase patterns, as may be exploited in neural, genetic, and artificial sensor networks. We developed a theory of information routing and information flows for noisy phase oscillator networks and demonstrate how effective coarse-graining may aid information routing on different network scales. Intriguingly, flow direction between two network parts can even be switched remotely by adapting local dynamic or structural properties within yet another, third part (see Fig. 8.15). Our findings highlight a co-action of interaction topology and collective dynamics for information routing in complex networked systems (see also Ch. 8.8).

8.10 EcoBus – RE-INVENTING DISTRIBUTED PUBLIC TRANSPORTATION

A. Sorge, M. Wendland, D. Manik, S. Herminghaus, M. Timme

The important aim of local public transportation (by bus, tram or similar means) is to offer an affordable mobility system to efficiently organize public travel. This should simultaneously reduce individual (car) traffic and thus free streets. Current forms of public transportation, however, are typically bound to fixed time schedules and fixed stopover points, making the usage of standard buses (or trams) often time-consuming and inconvenient. The remaining alternatives, taking a taxi or one’s own car (often with only single occupancy) are both expensive and increase total traffic. We are currently studying the fundamentals of a public transportation system called EcoBus that is simultaneously inexpensive and traffic-minimizing. The basic idea is that bus-like vehicles pick up passengers sequentially at their desired departure points and transport them to their desired destinations at or before a desired time. So far, similar problems have been studied extensively, but were restricted to specialized, and therefore often low-load problems, e.g. as school bus, rural area, or patient transport systems.

Combining coupled online route-optimization for many (spatially and temporally distributed) buses and many (also distributed) passengers with methods learned from the statistical physics of transport may in the future enable close-to-optimal passenger load per bus, therefore minimizing both street traffic and traveling costs. In the past two years, we have developed a traffic network coarse-graining, for example, the city of Göttingen (see Fig. 8.16), and complementing local insertion rules with standard route optimization techniques. We are currently investigating the scaling relations and exploring the possibility of phase transitions in homogeneous and heterogeneous on-demand transport models (see Fig. 8.17).

EcoBus shall incorporate passenger pre-registration via modern communication tools such as mobile phones or the world wide web. Thus, a functioning EcoBus system would provide an integrated complementary solution to the problem of efficient public transportation that can be economically and ecologically optimized because it uses a novel conceptual dimension between taxi and bus and simultaneously addresses the core systems level of the problem.
8.11 COLLECTIVE DYNAMICS, SELF-ORGANIZATION
AND ECONOMY OF FUTURE POWER GRIDS

M. Rohden, M. Timme, D. Witthaut
S. Klipp, A. Sorge, M. Matthiae (Aarhus, Denmark), R. Sollacher
(Siemens Corporate Research, Munich) T. Walter (Wirsol GmbH,
Waghäusel), A. Niesse (OFFIS, Oldenburg)

Switching our current energy supply to renewable sources poses one
of the greatest technological and social challenges of humankind [1, 2].
A successful transition in particular requires an intelligent upgrade of
the current electric power grid. So-called ‘smart grids’ may provide
part of the solution by enabling the transmission of demand and supply
information across the grid online, thereby adapting energy production
as well as consumption, and thus aiming to control the entire grid [3].
However, stable operation as well as failures on large scales already
today are consequences of the collective dynamics of the power grid
and are often caused by non-local mechanisms. We thus urgently
need to understand the intrinsic network dynamics on the large scale
to complement partial solutions of control engineering and to be able
to develop efficient strategies for operating the future grid.

In this project, we develop and analyze appropriate coarse-scale
models of future power grids with an emphasis on increasingly dis-
tributed demand and supply and the network topology that is getting
more intricate. First results show several intriguing features. For in-
stance, the addition of new transmission lines may destabilize power
grid operation (via Braess paradox that we identified in oscillator net-
works) [4]. In addition, replacing the few large power plants by many
small and distributed ones may stabilize grid operation, at least in the
stationary (short-time) regime [5].

We are currently working on three research projects on (1) the dy-
namics of collective failures, (2) the influence of large fluctuations by
renewable power sources and (3) the interdependence of energy mar-
kets and power grids. Preliminary findings suggest that the co-action
of electricity trading and the power grid operation may destabilize each
other even if both trading is economically and the grid is dynamically
stable (see Fig. 8.18).

In the project on collective failures we try to understand and predict
the effects of a breakdown of single elements of the network. We
analyze if and where other depending elements can be destabilized
and quantify the resilience of the grid to such breakdowns. These
fundamental results are used to identify critical infrastructures of the
network, which may have far-reaching potential applications in network
planning and real-time monitoring of grid operation.

Power generation in future grids based predominantly on wind and
solar energy, will exhibit substantial fluctuations of different types. We
analyze the influence on network stability for both stochastic and oscil-
latory fluctuations and aim to quantify the risks of large scale outages.
Intriguingly, our preliminary results (Matthiae et al., in preparation)
also suggests that certain emergency measures may control the power
generation in a way that promotes an oscillatory frequency instability of the network.

PART III

INFRASTRUCTURE
INFRASTRUCTURE

At the MPIDS an efficient infrastructure network supports both the scientists and the non-scientific staff in their work, creates an excellent research environment, and ensures smooth workflows behind the scenes. These service units are headed by the delegate manager relieving the board of directors and the managing director of many tasks.

The infrastructure is organized in three service units: administration, technical services, and information technology. Outreach activities and media relations are coordinated by a separate staff unit.

Administration

While the institute’s administration covers a wide range of responsibilities and tasks, its main focus is on the divisions human resources, financial affairs, and grant administration.

All tasks of personnel management and advisory services are at the heart of the human resources division. The team not only attends to all workflows dealing with employment contracts, stipends, and the promotion of young researchers, but also offers help and advice in questions dealing with health insurance, tax and collective bargaining law. As a first contact point for all new employees taking up their duties, the human resources division helps with all necessary formalities – both those at the institute and those at the local administration. To facilitate the first steps in the new environment, the institute has issued a visitor’s guide containing information and helpful hints for all aspects of every-day life – from opening a bank account to finding suitable day care. Visitors and new employees often spend their first weeks in one of the institute’s three guest houses. These are located at the institute’s old site in the Bunsenstraße and provide accommodation for up to thirty persons. The administration oversees the management of these houses.

The division for financial affairs oversees and manages all of the institute’s financial affairs and processes. The team takes care of bookkeeping, procurement, and travels costs. Since the MPIDS is very successful at applying for third-party funded research projects, grant administration is another important task of the administration. Experienced personnel offers the scientists advice and support when applying for third-party funds and handles all financial issues connected with the grants.

Since a few research groups are still located at the institute’s old site in the Bunsenstraße, transportation between the old and the new building is an important service organized by the administration. This helps scientists and non-scientific staff to commute between both sites in a time-saving manner. The administration also deals with the transportation of scientific goods and transportation within Göttingen and to more distant destinations.
**Technical Services**

The service unit "technical services" can be divided into facility management and maintenance on the one hand, and the workshop for precision mechanics and the scientific electronics workshop on the other.

The facility management is responsible for the upkeep and maintenance of all of the institute's technical infrastructure including heating, air condition, plumbing and ventilation, fire detection technology, telecommunication, and emergency call systems. While small and mid-sized repairs are performed by team members, larger tasks are outsourced and coordinated by the facility management. The service unit also sees to all janitorial and cleaning duties.

Many of the experimental setups and scientific apparatuses used at the MPIDS are one of a kind and need therefore to be especially developed and build. Many of these tasks are performed by the workshop for precision mechanics and the scientific electronics workshop. The staff closely collaborates with the scientists providing valuable advice and expertise in all stages of the construction process from the first idea to the finished component.

The precision mechanics workshop and the metal shop are responsible for the development and construction of mechanical apparatuses and components. Based on the request from the scientific departments, the mechanical design group develops and engineers custom tailored solutions. The group uses the most advanced software tools that allow to design complex parts in three dimensions. This includes the simulation of the components as well as their three-dimensional assembly. Once the technical design is finished, technical drawings are generated or the design is directly entered into the CAD engines that generate instruction sets understood by the CNC-machines. The workshop is equipped with conventional as well as computer controlled lathes, milling and, EDM machines. The associated metal shop manufactures frames and other large metal parts and has state of the art welding equipment for handling steel and aluminum.

From the beginning, the training of apprentices has been an important part of the work of the mechanical precision workshop. On average, the workshop educates two mechanical technicians specializing in precision toolmaking every two years. An impressive conformation of the excellent training the young technicians receive at the MPIDS is the number of all-state winners of the examinations for mechanical technicians of the State of Lower Saxony coming from the MPIDS: In the past ten years six apprentices passed these examinations as winners. In addition, several apprentices have been honored by the Commercial and Industrial Chamber and by the Max Planck Society.

The staff of the scientific electronics workshop develops and builds the electronic interfaces between computer and measurement technology for scientific apparatuses that cannot be commercially obtained. The circuits are designed with CAD engines and then build in house. The construction of conductor plates consisting of several layers is outsourced, the entire process, however, is overseen and controlled by
the workshop.

For more than two decades the electronics workshop has been training apprentices to become electronic technicians for devices and systems. All of these young people have successfully passed their exams. Many go on to university to become electrical engineers, others found jobs in renowned industrial enterprises.

**Microfabrication Facility**

The Institute is equipped with a clean-room general facility (25 m² - Class 10000). It is mainly used for microfabrication processes. Soft-lithography is performed as a standard process using SU-8 resist and UV illumination on 4 inches silicon wafers (MJB4 Suss mask aligner). A white light interferometer is used to accurately determine the thickness of the SU-8 layers deposited on silicon wafers. The microfluidic devices are then assembled outside of the cleanroom. Several other microfabrication techniques for electrode patterning, or microoptical lenses fabrication have been implemented for the production of complex functional devices. Besides the soft-lithography technique, the Institute workshop is equipped with a high-precision milling machine (DMU 50, DMG Mori Seiki) usable to pattern microchannels in hard plastic (such as PMMA). Using thermal bonding above the glass transition temperature of the PMMA, microfluidic channels are then assembled.

![Figure 8.19: SU-8 resist mold on 4 inches silicon wafers.](image)

![Figure 8.20: Microfluidic chips. PDMS obtained by replica molding (a), PMMA chips produced by micromachining (b,c).](image)

**Towards a Max Planck Microfabrication platform**

The Microfabrication facility of the Institute will become a central part of the Max Planck Network on Synthetic Biology (MaxSynBio) currently being established. MaxSynBio is a joined Max Planck - BMBF initiative for Synthetic Biology. The aim of the project as a primary goal is a bottom-up approach towards understanding biological complexity. Starting by the rational design and synthesis of functional biological systems from well-characterized modules and parts we plan to assemble biomimetic micro-compartments up to the realization of functional synthetic cellular systems. Microfluidics and microfabrication have an essential role in the control and analysis of these microcompartments. Our microfabrication facility will be used by all members of the network. We will provide training and assistance in microfabrication at all steps, from the design to the realization of the device and ultimately to the
quantitative measurements of the artificial biomimetic compartments in microfluidic environment.

**Information Technology**

**Central IT Services**

The IT service group is tasked with operating the computer network and some of the critical servers of the MPI-DS at the two sites at Bunsenstraße and on Faßberg. The IT service group also provides support for the infrastructure departments and consulting services for the scientists.

Aside from running the existing IT infrastructure there are several active projects ranging from improvement of the IT infrastructure to the development of new IT solutions.

The biggest project during the last three years was planning and implementing the IT infrastructure of the new building at the Faßberg site. This task is completed and there are now routines established for running and monitoring the network and the servers. New issues resulting from the ever increasing amount of data produced in the institute have come up and are dealt with in close cooperation with the HPC group.

**High-Performance Computing**

Ongoing advances in computer technology enable the collection of enormous amounts of experimental data, running more complex simulations and fine grained data analysis. This trend is accompanied by a higher demand for direct access to powerful computing resources in most groups at the MPI-DS. The necessary infrastructure scales well over single workstations but below traditional large computing centers, but has to allow interactive use, e.g. for developing large-scale parallel applications or directed parameter space exploration.

![Cooling cabinets with HPC clusters in the main server room of the department of Non-linear Dynamics. Open racks for infrastructure servers in the front. The cabinets have a dedicated control and monitoring unit, are built in a modular fashion so that they can easily be moved, and can be customized to cool up to 36 kW.](figure821.png)

The diverse demands for computing power of the various research groups in the MPI-DS nevertheless lead to a homogeneous landscape of HPC clusters, each with a dedicated focus. Several clusters provide an Infiniband network for fast parallel applications, have many cores in each node and large memory, or harddisk raids for the handling of...
huge amounts of data. Scientists at the MPIDS have direct access to HPC clusters with a total of 750 HPC systems with almost 10,000 CPU cores with approximately 30 TB RAM and 1.5 PB storage.

Hosting computing facilities of that scale in a single institute requires a very dense packing of servers which is provided by multicore machines and efficient designs like blade server enclosures. Power densities of 24kW per square meter cannot be cooled by traditional open air flow cooling via a double flooring. An efficient cooling system is required from an environmental perspective, but also is mandatory from a financial point of view as in traditional cooling systems electricity costs of the cooling can be as high as 30% of the electricity costs for the computers themselves. The MPIDS was among the first institutes to solve this issue by using optimized water cooled cabinets with a heat exchange and redundant fans each to cool only the necessary parts of the server rooms, as shown in Fig. 8.21.

In order to manage such a complex facility a monitoring system based on open source software was set up, which collects important health data of both the HPC hardware and the cooling facilities on a frequent basis. This data is summarized on a comprehensive overview, its history can be assessed for diagnostics and the system is able to perform emergency shutdowns autonomously in case of cooling failure to prevent machine damage by high temperatures.

GÖTTINGEN FOCUS ON COMPLEX FLUID DYNAMICS

The spring of 2014 will mark the beginning of a new phase for the MPIDS: the beginning of construction work for the new Göttingen Focus on Complex Fluid Dynamics. By the end of 2014 this Focus will be home to up to 63 scientists working together on topics such as the physically correct description of turbulent flows, the prediction of multiphase flows in complex geometries, and the behavior of active fluids in living matter. The scope of the new Focus is to significantly strengthen the research on complex fluid dynamics and to create an internationally unique and distinguished competence center in this field. Hopefully, this will lead to the deeper understanding of many basic questions necessary to tackle some of the most urgent and intriguing problems of today’s society, such as the prediction of the global climate.
as well as atmospheric and marine transport, the development of efficient wind and tidal power stations, and the use of sedimentary reservoirs for oil production or the storage of carbon dioxide.

Site of the new building will be the green area between the MPIDS and the campus’ kindergarten. The Focus will be built as a three story timber construction – the first construction of this sort within the Max Planck Society. While the two upper stories will house offices for 60 scientists and three group leaders as well as a seminar room, the lower part will make room for roofed parking spaces. The architecture of the building is simple and straightforward allowing the Focus to harmoniously complement the older building and the experimental hall. A covered walkway will connect the second floor of the existing building with the first floor of the new. The overall costs of the building are 4 million Euros, which are provided in equal parts by the Max Planck Society and the Volkswagenstiftung.

Figure 8.23: The new building will be located between the MPIDS and the campus’ kindergarten.
PART IV

PUBLIC RELATIONS, EQUAL OPPORTUNITIES, AND SUPPORT FOR YOUNG SCIENTISTS
PUBLIC RELATIONS

At the MPIDS public outreach and media relations are recognized as an important part of the institute’s work. This is can be seen not only in the increasing number of press releases, but also by the institute’s ongoing participation in public events and exhibitions. All outreach and media activities are coordinated in the institute’s press office.

Press releases

Press releases continue to be an important means of communicating with the local, national, and international media. These releases deal with scientific results from all departments and Max Planck Research Groups, inform the media about important prizes awarded to MPIDS scientists, and advertise special events the institute organizes or takes part in.

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<tr>
<td>Jul. 13, 2011</td>
<td>Low-energy pulses mean safer heart defibrillation</td>
<td>New Scientist</td>
<td>Vorhofflimmern schonend zurück in den Takt</td>
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<tr>
<td>Jul. 13, 2011</td>
<td>Kinder, gentler, defibrillator uses multiple small jolts</td>
<td>Scientific American</td>
<td>Vorhofflimmern schonend zurück in den Takt</td>
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<td>Jul. 15, 2011</td>
<td>Schwache Strom-stöße versprechen Erfolg gegen Vorhofflimmern</td>
<td>Rheinische Post</td>
<td>Vorhofflimmern – schonend zurück in den Takt</td>
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<tr>
<td>Nov. 18, 2011</td>
<td>-</td>
<td>NDR Info, NDR Kultur</td>
<td>Musik mit menschlicher Note</td>
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<tr>
<td>Aug. 23, 2012</td>
<td>Tröpfchen für Tröpfchen gezählt</td>
<td>Stuttgarter Zeitung</td>
<td>Kleine Tropfen wachsen anders</td>
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<tr>
<td>Sept. 7, 2012</td>
<td>-</td>
<td>Wissenschaftsmagazin Logo, NDR</td>
<td>Kleine Tropfen wachsen anders</td>
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<tr>
<td>Mar. 15, 2013</td>
<td>-</td>
<td>IQ Wissenschaft und Forschung, Bayern 2</td>
<td>Sonne und Windkraft können das Stromnetz stabilisieren</td>
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<tr>
<td>Aug. 18, 2013</td>
<td>Wer schleimt, der siegt</td>
<td>Frankfurter Allgemeine Sonntagszeitung</td>
<td>Amüben mit Rhythmus</td>
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</table>

Most press releases are published in German and English. In the past years, the number of issued press releases per year continued to be high and could even be increased.
In addition, time and again these press releases spark the interest of industrial partners or point other colleagues from science and research to our work.

**Institute brochure**

In 2011 a six page brochure was designed that portrays the MPIDS for a general audience. While each department is described in detail, the brochure also addresses the Max Planck Research Groups, the institute’s history and what the terms “dynamics” and “self-organization” mean. In the past years this brochure has proven to be a successful means of informing visitors, journalists, and students about the institute’s work.

**Ask the Scientist**

In the past years the series „Ask the Scientist“ was successfully continued. In this series appearing every other Sunday in the Göttingen newspaper ExtraTip, scientists from Göttingen answer questions asked by readers. These questions cover all scientific areas and often deal with topics related to the institute’s research. After five years of “Ask the scientist”, 2012 was a good time to step back and evaluate the project. While both the MPIDS and the ExtraTip agreed, that the series is a successful and popular means of fostering an interest in science, a few changes were necessary. After a pause, the series was relaunched in September 2013. “Ask the Scientist” now presents itself with shorter texts and is financially supported by the Sartorius AG.

**Homepage**

In 2013 the homepage of the MPIDS was relaunched in a new design which is in accordance with the design used by the Max Planck Society and several other Max Planck Institutes. The most important change from an outreach point of view is that now the front page offers the possibility to promote current news such as press releases, prizes or announcements.

**Open House**

The biggest outreach project in the past years was an Open House on November 5th, 2011. The event was organized together with the Max Planck Institute for biophysical Chemistry and the Gesellschaft für wissenschaftliche Datenverarbeitung mbH Göttingen. More than 3000 guests visited the Max Planck Campus on this day and took advantage of a myriad of lectures, guided tours, and activities for children all allowing for a deeper insight into the institutes’ work.

At the MPIDS the visitors found activities and information dealing with turbulence, epidemics, microfluidics, cardiac rhythms, the communication of wales, robots, chaos, and self-organization in swarms and power grids. One of the goals of the Open House was to spark an interest in the research activities of the Max Planck Campus in as wide and as diverse an audience as possible. To this end, a special
program for children was created featuring children’s lectures (all held by MPIDS-researchers) and hands-on activities.

For each activity, in which they had participated, the children received a sticker in a small booklet. In addition, the institutes had initiated a drawing contest for children: months before the Open House all elementary schools in Göttingen and the surrounding area had been invited to send in pictures showing “what a scientist does”. The lively and creative collection was displayed at the Open House and three winners were honored. The Open House was advertised with flyers and brochures throughout Göttingen and neighboring towns. In addition, the event triggered a series of articles in the local newspaper, which was published chiefly before the Open House. In 15 articles, of which most were published before the Open House, the Göttinger Tageblatt portrayed each of the scientific departments of the Max Planck Campus.

Science festivals: „Highlights der Physik“ and „Night of Science“

In 2012 Göttingen hosted two major science festivals, to which the MPIDS contributed: the festival “Highlights der Physik” (18. – 22. September 2012) organized by the German Physical Society and the German Ministry for Science and Education and the “Night of Science” (24. November 2012) organized by the University of Göttingen. At both festivals the MPIDS presented itself with lectures dealing for example with the physics of mixed beverages, turbulent flows in clouds, and nonlinear effects in musical rhythms. In addition, MPIDS scientists offered hands-on activities and information stands introducing the guests to the world of turbulent flows and complex fluids. A highlight of the “Night of Science” was a spectacular laser experiment demonstrating the turbulent flows in clouds.

Science Tunnel

The Max Planck Science Tunnel 3.0 is an exhibition devoted to basic research presenting various scientific topics with the help of impressive multimedia arrangements. The Science Tunnel premiered in the Heinz
Nixdorf MuseumsForum in Paderborn on 18. October 2012 before starting its journey around the world. The MPIDS has contributed to the exhibition topic “complexity” with information and material on turbulence and network analysis. The Research Group “Biomedical Physics” provided a special focus on the onset and control of cardiac arrhythmias.

Max Planck Science Gallery

Located in the center of Berlin, the Max Planck Science Gallery offers multimedia exhibitions highlighting various scientific topics. In 2012, the Max Planck Research Group "Network Dynamics" contributed to the exhibition "Energie - nachhaltige Optionen für die Energie der Zukunft" (engl.: Energy - sustainable options for the energy of the future) by providing material and information on stabilizing power grids. The exhibition can still be seen on demand in the Science Gallery.

Göttinger Literaturherbst

As in the years before, the MPIDS took part in the annual literary festival in Göttingen the “Göttinger Literaturherbst”. This festival features a scientific lecture series where internationally renowned scientists present their latest books in the unique atmosphere of the historic Paulinerkirche in Göttingen. These lectures are introduced and chaired by scientists from the local Max Planck Institutes thus allowing for an interesting and vivid exchange of ideas. In 2012 a highlight was the lecture presented by Prof. Dr. Brian Greene from the Columbia University. Apart from his appearance at the Literaturherbst, Prof. Green gave a public lecture at the MPIDS which was visited by more than 250 guests. The MPIDS awarded Green the Ludwig Prandtl Colloquium Lectureship 2012.

Internal Communication

For an efficient, quick, and uncomplicated internal communication an email newsletter has been initiated. It is distributed to all employees once a month and contains brief information about news items, new appointments, important dates, and publications. In addition, each month a special topic (such as new research co-operations, public events or scientific results) is highlighted in more detail. In this way, the newsletter offers both quick and in depth information.

EQUAL OPPORTUNITIES / RECONCILIATION OF WORK AND FAMILY LIFE

Creating equal opportunities for both female and male employees and reconciling work and family life is an important part of the institute’s organizational culture and identity. Every four years, an equal opportunities commissioner as well as a deputy commissioner are elected to help promote these goals and act as a contact point for employees with
questions regarding career support for female employees, work-life-
balance, day care options, legal and work-related aspects of pregnancy,
and sexual harassment or mobbing at the workplace.

For parents taking care of children the institute offers several ser-
vices to facilitate a reconciliation of work and family life. For example,
these employees may take advantage of the services of the Besser Bet-
treut GmbH, a family service specializing in finding day care solutions.
In addition, all information regarding day care is displayed in the
intranet. Since 2010 the institute offers a small playroom for children
where employees nursing babies find privacy and parents bringing
their children to work find helpful toys and a play area. Since 2006 the
quality audit “Beruf und Famile” (engl.: “Work and Family”) regularly
evaluates the measures taken at the Max Planck Society to improve
the compatibility of work and family life for women and men. In 2012 the
MPIDS was awarded the according certificate for the third time. The
MPIDS sees to a timely implementation of the objectives with regard
to the audit. For example, all employees are now regularly informed
about new and existing day care options and employees who had taken
advantage of the services of the Besser Betreut GmbH were given the
possibility to evaluate this service.

In order to promote equal opportunities for both female and male
employees the equal opportunities commissioner is involved in all
job offers and application procedures. All employees are regularly in-
formed about networking possibilities for female scientists and training
measures such as self-assertion for women. The equal opportunities
commissioner took part in compiling the operating agreement dealing
with performance-oriented payment for all employees.

Every year - excluding 2011 when the institute moved from the
Bunsenstraße to Faßberg - the MPIDS hosts the Future Day. On this
day young girls and boys throughout Germany explore different career
options. The MPIDS regularly invites approximately 20 girls and boys
to take part in different activities in the laboratories and the workshops.
The day is an excellent opportunity to interest young people (especially
young girls) for science and engineering. In order to offer positive
role models, this day is organized chiefly by the institute’s female
scientists. Both the participating children and their parents are very
enthusiastic about the activities offered by the MPIDS and give very
positive feedback.

MAX PLANCK CAMPUS

Together with the neighboring Max Planck Institute for biophysical
Chemistry (MPIbPc) and the Gesellschaft für wissenschaftliche Daten-
verarbeitung mbH Göttingen (GWDG) the MPIDS forms the Göttingen
Max Planck Campus. The GWDG is a corporate facility of the Georg-
August University of Göttingen and the Max Planck Society. It serves
the purpose of a data processing and IT competence center for the Max
Planck Institutes in Göttingen and a data processing service center for
the University of Göttingen.
Several infrastructures such as the Otto-Hahn-Library and the canteen are available to all partners of the Max Planck Campus and help cultivate an atmosphere of exchange and participation. In the past years, further efforts have been made to increase the cooperation of both Max Planck Institutes and create synergy effects.

**Board of Trustees**

Since January 2013 the MPIDS and the MPIbpc have a joint Board of Trustees. The board supports the exchange between the institutes and the general public and advises the institutes on social and scientific policy. Members of the Board of Trustees include representatives from politics, economy, science, and media. The Board of Trustees convened on April 30, 2013 for its constituent meeting, electing Gerd Litfin as chair and Gerhard Scharner as co-chair. Additional meetings take place annually.

![Figure 8.30: Joint Board of Trustees of MPIDS and MPIbpc. First row (from left to right): Stefan W. Hell, Wolfgang Meyer, Carmen Rotte, Dirk Görlich, Reinhard Jahn, Marina Rodnina, Helmut Grubmüller, Stefan Herminghaus, Ralf O. H. Kähler, Thomas Keidel, Gerd Litfin; second row (from left to right): Gopalakrishnan Balasubramanian, Heinrich Voges, Herbert Stadler, Klaus-Peter Koller, Ulrike Gerischer, Wilhelm Krull; third row (from left to right): Alec Wodtke, Thomas Oppermann, Ilse Stein, Rainer Hald, Gerhard Scharner, Bernhard Reuter; fourth row (from left to right): Theo Geisel, Jens Frahm, Eberhard Bodenschatz, Volker Stollorz, Bernd Wirsing, Reinhard Lührmann, Gregor Eichele, Herbert Jäckle, Christian Griesinger. Missing in the photo are Ulrike Beisiegel, President of the Georg August Universität Göttingen and Johanna Wanka, Federal Minister of Education and Research. Members of the Joint Board of Trustees are set in bold letters.](image)
Meetings of the Scientific Members of MPIDS and MPIbpc

The meetings of the scientific members of the MPIDS and the MPIbpc constitute the close collaboration of both institutes on a scientific level. In these meetings the directors of both institutes convene regularly to discuss not only scientific issues, but also organizational and infrastructural topics concerning the Max Planck Campus as a whole.

GWDG

The MPIDS closely collaborates with the GWDG in many aspects of IT services. The MPIDS takes advantage of the following services: mail servers and groupware (exchange server), web servers, virtual servers, storage (powerfolders), backup (data from users), archiving, internet access (DFN), W-LAN, and technical support.

Further Max Planck Campus Activities

In the past years, several tools have been established to foster the scientific exchange between researchers from both Max Planck Institutes. Most prominently this is the Campus Seminar, a regular series of lectures held two to three times per month. In these lectures, scientists from both institutes present their projects and results to their colleagues thus allowing for a first exchange of ideas and triggering scientific co-operation. A more unofficial framework for getting to know colleagues from the MPIbpc and their research is offered by mutual activities such as the summer festival. In November 2011, both institutes and the GWDG joined forces to host an Open House. Such outreach activities are an excellent way of sparking the interest of the public in the Max Planck Campus as a whole.
YOUNG SCIENTISTS

The approximately 80 PhD students at the MPIDS do not only carry out a substantial part of the scientific research, but are also active in the Max Planck Society-wide PhDnet, represent their interest in the committees of the International Max Planck Research School for Physics of Biological and Complex Systems (IMPRS PBCS) and work together with the institute administration. They organize events to support the advancement of young researchers and the interaction within the institute and between the research institutes and faculties of the Georg-August University School of Science (GAUSS). The representatives’ goal is to ensure that the best possible working conditions are provided for the students at the institute, to offer a point of contact for any issues that arise and to give students a broader perspective outside their specific field of research.

A range of events were organized by students of the institute. One notable example was the first realization of the international conference "Third Infinity" which took place from October 17 to October 19 2013 in Göttingen and attracted over one hundred participants. The conference was organized jointly by a group of five students of the IMPRS PBCS, affiliated to the University of Göttingen, the MPIbpc, and the MPIDS. Third Infinity covered a broad range of topics from the field of physics of complex systems and biophysics. Eleven excellent speakers came from literally all over the world to give talks on anomalous diffusion, single-cell microscopy, theoretical neuroscience, and robotics among many other topics. The common denominator of this large variety of topics is that they all deal in some way with the infinitely complex, which can be regarded as the third infinity of physics besides the infinitely big and infinitely small.

Another student-run event organized by graduate students of the Institute is the "Göttingen Fall Course on Computational Neuroscience". Supported by the Bernstein Center for Computational Neuroscience it has been held annually in the Institute since 2003 as a fall school of the NWG, the German Neurowissenschaftliche Gesellschaft. With lectures given by international experts it attracts students from Germany and other European countries. Also with financial and other support from the BCCN a group of female PhD-students has been organizing a series of "Seminars in Biophysics by Outstanding Female Scientists". With outstanding international invitees, frequently from the US, it is intended to promote young women’s scientific careers by lectures, tutorials, and networking.

In addition, a number of workshops were organized, for example on presentation techniques. They brought together students from different institutes and furthered their training. To provide information on career perspectives in and outside of academia, career seminars with invited speakers were offered. These provided valuable insights and very good networking opportunities.

Locally, PhD students serve as representatives on the selection panels and organization committees of the IMPRS PBCS. On the scale of the Max Planck Society, students from the institute are active in different
groups of the PhDnet, which addresses the working conditions and opportunities for the students in cooperation with the general administration. In 2012, Ghazaleh Afshar served as CPT (Chemistry, Physics and Technology) section representative in the PhDnet steering committee. During this year, they managed to realize significant progress in the long-standing discussion about the insurance situation of stipend holders in the Max Planck Society. Substantial support was offered by Daniel Herde as head of the Survey Group in 2012.

Of course the activities of the PhD students are not solely focused on scientific advancement and career perspectives. To maintain a work-life balance, social events are organized for the students, both on the level of the institute and through the IMPRS. Especially the dinners with the speakers of invited talks provide a valuable opportunity for students as they provide a very informal environment to discuss both current research and life in science in general. Also, the students attempted to convert some square meters of the greenland behind the institute into a vegetable garden.
HOW TO GET TO THE MAX PLANCK INSTITUTE FOR DYNAMICS AND SELF-ORGANIZATION

Fassberg site (new building)

Address:
Am Fassberg 17
D-37077 Göttingen

Departments:
Nonlinear Dynamics (Prof. Geisel)
Dynamics of Complex Fluids (Prof. Herminghaus)
Fluid Dynamics, Pattern Formation, and Biocomplexity (Prof. Bodenschatz)

Research Groups:
Biomedical Physics (Honorarprofessor Luther)
Theoretical Neurophysics (Honorarprofessor Wolf)

Max Planck Research Groups:
Droplets, Membranes, and Interfaces (Dr. Baret)
Emergent Complexity in Physical Systems (Dr. Schneider)

Services:
Institute Management, Administration, Facility Management, Electronics and Mechanics Workshops, IT-Services, Library, Outreach Office, Stock Rooms, Lecture Hall, Göttingen Turbulence Facility, Clean Room, and Cell Biology Laboratories

By plane
From Frankfurt am Main Airport (FRA): Use one of the railway stations at the airport. Trains to Göttingen (direct or via Frankfurt main station) leave twice an hour during daytime (travel time: 2 hours). From Hannover Airport (HAJ): Take the suburban railway (S-Bahn) to the Central Station (»Hannover Hauptbahnhof«). From here direct ICE trains to Göttingen depart every 1/2 hour.

By train
Göttingen Station is served by the following ICE routes: Hamburg-Göttingen-Munich, Hamburg-Göttingen-Frankfurt am Main, and Berlin-Göttingen-Frankfurt. From Göttingen railway station: On arrival at Göttingen station take a taxi (15 minutes) or the bus (35 minutes). At platform A take the bus No. 8 (direction: »Geismar-Süd«) or No 13 (direction: »Weende-Ost/Papenberg«). At the second stop »Groner Straße« change to bus No. 5 (direction »Nikolausberg«) and get off at the »Faßberg« stop, which is directly in front of the entrance of the Max Planck Campus (MPI DS and MPI for Biophysical Chemistry). Ask at the gate to get directions.

By car
Leave the freeway A7 (Hanover-Kassel) at the exit »Göttingen-Nord«, which is the northern of two exits. Follow the direction for Braunlage (B 27). Leave town – after about 1.5 km at the traffic light (Chinese restaurant on your right) turn left and follow the sign »Nikolausberg«. The third junction on the left is the entrance to the Max Planck Campus (MPI DS and MPI for Biophysical Chemistry). Ask at the gate to get directions.
**Bunsenstraße site (old building)**

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<td>Fluid Dynamics, Pattern Formation, and Biocomplexity (Prof. Bodenschatz)</td>
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<td></td>
<td>Network Dynamics (apl. Prof. Timme)</td>
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<td></td>
<td>Onset of Turbulence and Complexity (Dr. Hof)</td>
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<td>Physics of Biological Organization (Dr. Katifori)</td>
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<td>Emeritus Group</td>
<td>Molecular Interactions (Prof. Toennies)</td>
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<td>Services</td>
<td>Guest Houses</td>
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**By train**
Göttingen Station is served by the following ICE routes: Hamburg-Göttingen-Munich, Hamburg-Göttingen-Frankfurt, and Berlin-Göttingen-Frankfurt. From Göttingen railway station: From the Göttingen station you can take a taxi (5 minutes) or walk (20 minutes). If you walk, you need to leave the main exit of the station and turn to the right. Follow the main street, which after the traffic lights turns into Bürgerstraße. Keep walking until you come to the Bunsenstraße. Turn right – you will reach the entrance gate of the MPIDS after about 300 m.

**By car**
Leave the freeway A7 (Hanover–Kassel) at the exit »Göttingen«, which is the southern exit. Follow the direction »Göttingen Zentrum« (B3). After about 4 km you will pass through a tunnel. At the next traffic light, turn right (direction »Eschwege« B27) and follow the »Bürgerstraße« for about 600 m. The fourth junction to the right is the »Bunsenstraße«. You will reach the institute’s gate after about 300 m.