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No matter how well we understand how a single droplet of water is formed in the laboratory, we cannot predict how countless droplets form clouds that substantially affect the Earth’s climate. And although we can accurately characterize a single neuron’s impulse, we do not yet understand how billions of them form a single thought. In such systems, animate or inanimate, processes of self-organization are at work: Many interacting parts organize themselves independently, without external control, into a complex whole. At our institute we explore the mechanisms underlying these processes in order to gain a detailed understanding of complex systems. Also the major challenges of the 21st century, from climate change and economic crises to problems in energy supply and transport, are closely linked to these scientific questions. Without a deep understanding of dynamics and self-organization in complex and highly networked systems we cannot face these challenges. With our basic research not only do we want to deepen our understanding of nature, but also want to contribute to a sustainable existence on this planet.
The three directors of the MPI DS (from left): Stephan Herminghaus, Eberhard Bodenschatz and Ramin Golestanian (Göttingen, November 2021).
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INTRODUCTION

The Max Planck Institute for Dynamics and Self-Organization (MPI DS) is engaged in research activities focused on the physics of dynamics and self-organization as found in a diverse set of systems; from endeavouring to make synthetic forms of life-like organelles to understanding how the brain works; from uncovering how slime moulds evolve, sense, and decide to deciphering the inner workings of the adaptive immune system; from understanding the electro-physiology and nonlinear soft mechanics of the heart to studying turbulence and its influence on clouds and climate; from devising models and predictions on the spread of pandemics, to quantifying the fluid physics and infection risk due to human drops and aerosols. And, the list goes on. The plethora of physical problems, however, can be formally viewed within a common conceptual framework, in which the aim is to understand the collective behaviour of complex systems with many interacting degrees of freedom. This pursuit is built on solid theoretical framework within the context of nonequilibrium statistical physics, nonlinear dynamics, condensed matter physics, soft matter physics, and fluid physics. Moreover, it makes use of a broad range of theoretical, computational, and experimental tools and techniques. The commonality of the underlying principles behind the diverse research programmes naturally provides MPI DS researchers with a common language, and enables them to achieve synergistic interactions by crossing traditional disciplinary boundaries. The unique environment allows them to take ideas and techniques from one field to another and open up new horizons of research.

The 2021 Nobel Prize in Physics was a timely reminder of the strategic importance of our research area at MPI DS as underpinned by fundamental approaches that ultimately serve to find sophisticated and non-trivial solutions to the complex problems that humanity faces today. In its century-old history, our institute has always been a global leader in the physics of ħ = 0 complex systems, from turbulence to neuroscience, to nonlinear physics and complex networks, as well as various areas in soft matter and microfluidics. We note with extreme pleasure and pride that the 2021 Physics Nobel Laureate Klaus Hasselmann has completed his doctoral work on nonlinear dynamics, and in particular, on the propagation of von Schmidt head waves (elastic waves at the boundaries between two solid objects), at our institute in 1957 under the supervision of the then director Walter Tollmien.

As a good example of such an application of our expertise to address societal challenges, we would like to highlight the MPI DS Covid-
response. Immediately after the pandemic hit Germany, we took the initiative to form a Covid-19 response team that coordinated the efforts across Göttingen Campus with the active participation of all three directors, our emeritus director, and two MPRGs. These efforts immediately led to a multitude of publications and outreach activities from all directors and the other active groups, and in particular, several high-profile TV and media appearances. We helped to coordinate and lead the MPG response to Covid-19 and its interface with the public. To paraphrase the MPG president Martin Stratmann, “MPI DS became the face of the MPG in the response to the pandemic”. To name a few examples of the level of our involvements, we helped to coordinate the policy and advice papers that the MPG presented to the government, and was asked many times by the Federal Constitutional Court of Germany (Bundesverfassungsgericht), alongside the Robert Koch Institute and the National Societies of Virology and Epidemiology, to provide expert witness assessments in cases when the government of Germany was sued by one of the political parties (or others) about the decisions to impose lock-down. All of these Covid-19-response activities were carried out alongside our normal research activities, which also went from strength to strength over the pandemic.

The synergistic interactions across MPI DS have resulted in a number of major initiatives. There are many projects that aim to take ideas and techniques from physics in a research direction that can ultimately lead to novel and revolutionizing medical applications. A number of MPI DS research directions will clearly have the potential for major societal impact; these include understanding the statistical physics of epidemic spreading and how it can help us devise containment strategies, implementation of new models of shared transportation, understanding the dynamics of clouds, and the physics of wind farms. Many researchers in MPI DS are passionate about making the transition from matter to life. While the institute has been extensively involved with the Max Planck Society initiative MaxSynBio, it maintains a key role in the society-wide graduate school Matter-to-Life. These institute-wide initiatives have brought in additional opportunities for scientists across MPI DS to collaborate with each other, as well as reaching out to other institutions in the Göttingen Campus and across Germany.

We have broadly categorized the research across MPI DS during the last three years, which has been reported here in the form of 80 contributions, under the following headings: (i) dynamics in driven systems, (ii) dynamics of active matter, and (iii) dynamics, geometry, and information. These contributions highlight the strengths of individual groups and showcase the common underlying principles behind all the different projects. The report also contains information about the facilities and the infrastructure of the institute, which are widely shared and communally developed, as well as our vibrant and multifaceted outreach activities.

As our institute continues to evolve and take on new scientific challenges, it strives to preserve its current dynamic and diverse environment and help to empower its members to successfully progress through their careers at every stage.
INITIATIVES

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2.1 PHYSICS TO LIFE

Living matter, unlike its inanimate counterpart, is not naturally in equilibrium. To sustain and thrive, it must constantly convert the energy present in the environment to move, grow or reproduce, exhibiting unique properties that are impossible in thermal equilibrium. The implications of this non-equilibrium activity are already apparent at the nanoscale level of enzymes and proteins, or the complex interplay of self-organising processes within cells or complex organelles such as cilia, but can also be studied at the level of organs and complete organisms, or even at the level of populations of living organisms.

Concerning the out-of-equilibrium behavior of single biomolecules and enzymes, we have found that the presence of small-scale futile cycles (energy-consuming transitions that leave the system unchanged) in the processes that describe the conformational changes of such a biomolecular system in turn cause the emergence of large-scale conformational oscillations in these systems, which moreover are topologically-protected [1]. On the other hand, we have shown that, when two enzymes that undergo conformational changes during their catalytic action are in physical proximity, for example when they are attached to form a homomultimeric complex, they may synchronize and collectively boost their catalytic activity [2]. This occurs even if the individual catalytic events take place stochastically, as a result of a noise-activated barrier-crossing process.

While this shows that, already at the single or few-enzyme level, non-equilibrium activity results in exciting new physics, the cellular cytosol comprises a dense mixture of many different enzymes in large numbers. Combining theory and computer simulations, we have studied the behaviour of such a system, taking into account the non-equilibrium interactions that arise from the combination of catalysis and phoresis (directed motion in response to chemical gradients) [3]. We have found that particles can spontaneously cluster in a multitude of ways and even form self-propelled formations. These effects arise from a key feature of non-equilibrium interactions known as non-reciprocity, which implies that Newton’s third law of the equality of action and reaction is effectively broken. For example, one enzyme may be attracted to another whereas the second may be repelled by the first, so that one chases the other (see Fig. 2.1).

Many important functions in life are carried out not by single proteins or enzymes, but rather by complexes of several proteins or enzymes linked together, which can be dynamic and short-lived. By developing a mathematical model incorporating diffusion as well as complex assembly and disassembly, we have found that there is a sweet spot in the protein concentration which allows for a minimal reaction time of protein complexes with a distant target [4]. If assembly is space-dependent, for example in the presence of gradients of a chemical inhibitor, proteins will spontaneously accumulate in regions in which their complex form is most stable. This could act as a generic non-equilibrium mechanism that cells exploit to generate spatial gradients in the distribution of proteins.
Biomolecules also self-organise into larger dynamic aggregates, called condensates, which can be small droplets that form spontaneously in biological cells. We could show that in addition to phase separation, active processes control these condensates or drops. In particular, driven chemical reactions, such as phosphorylation of proteins, alter the interactions between proteins and thus the phase separation behaviour. Our theory demonstrates that such reactions can control the size, position and number of condensates when the enzymes controlling the reactions are localised to specific sites or droplets [5]. This exciting new class of chemically controlled droplets brings together the physical description of non-ideal solutions with the thermodynamic description of chemical reactions.

Physical theories aim to identify the minimal set of ingredients necessary to describe the larger-scale physics of interest. For example, we have shown how such minimal ingredients can help us understand the complex turbulent fluctuations characterized by new universal scaling laws in a two dimensional active nematic film composed of fueled cell extracts and coupled to three dimensional viscous fluids [6]. In a bottom-up approach, one methodically coarse-grains a microscopic theory, mathematically, zooming out further and further. Applying dynamical renormalization group theory to the equations describing chemically-interacting units, we could reveal macroscopic properties of large-scale collections of such units, uncovering signatures of their microscopic activity such as super-diffusive density fluctuations and non-Poissonian number fluctuations [7]. Such general results could, for example, shed light on how molecular regulation of chemotactic circuits can determine large-scale behaviour of cell colonies and tissues.

Other times, we may want to describe a large-scale living system, composed of many microscopic non-equilibrium components, without knowing any particular details about these components. In such a top-down approach, we use symmetries and conservation laws to formulate the most general equations that describe a system. In this way, we developed a general theory for any macroscopic system that includes non-reciprocal interactions [8], such as a collection of chemically-interacting enzymes as described above. Our theory revealed that spontaneously
broken symmetries in such systems lead to the generic appearance of oscillating and travelling states, even if the microscopic components lack a sense of direction, a result which would be impossible in an equilibrium system that lacks non-reciprocal interactions (see Fig. 2.1). The power of coarse-graining can sometimes lead to the discovery of unexpected connections between systems that are a priori entirely different from each other. As a first example, we found that magneto-tactic microswimmers, when confined in a narrow channel, exhibit a self-organized phenomenon analogous to Bose-Einstein condensation; the exotic quantum phase transition that bosons such as Helium-4 or other atomic gases undergo when cooled down to nearly zero absolute temperature (see Fig. 2.2) [9]. Another example is given by Casimir forces, the attraction between metallic plates in a vacuum that is caused by quantum fluctuations. By studying the stochastic dynamics of an electrolyte driven by a uniform external electric field we showed that, despite the presence of Debye screening in this system, its fluctuations are scale-invariant and have long-range correlations, which give rise to a Casimir-like fluctuation-induced force between neutral boundaries that confine the ions, which could be present in biological membrane ion channels [10].

As previously pointed out, living systems, whether natural or artificial, require a constant supply of energy. Building such systems from the bottom up is still in its infancy. We have experimentally demonstrated a biocompatible energy module made of light-switchable photosynthetic vesicles and demonstrated their function on the beating of demembranated flagella or axonemes. With our collaborators at the Max Planck Institute for Complex Technical Systems in Magdeburg, we have shown that light illumination controls the beating frequency of axonemes via dynamic ADP-to-ATP synthesis (Fig. 2.3). We verified the functionality of these light-driven synthetic vesicles in an in vitro assay by encapsulating microtubules with force-generating kinesin-1 motors as well as the energy module. Integrating our photosynthetic system with cytoskeletal filaments, molecular motors and other biological building blocks in microfluidically fabricated micro-compartment may allow the bottom-up synthesis of artificial cells [11].

Much of the living matter we know consists of single-celled microor-
We engineered light-switchable photosynthetic liposomes (~150 nm in diameter) as energy modules to generate ATP from ADP under illumination. To convert light into ATP, we co-reconstituted two purified transmembrane proteins, namely, bacteriorhodopsin (bR) and EF₉F₁-ATP synthase from E. coli. Upon illumination, bacteriorhodopsin pumps protons into the vesicle’s interior, establishing a proton motive force that drives ATP synthase to catalyze the conversion of ADP to ATP. Axonemal Dynein molecular motors consume ATP, converting chemical energy into oscillatory beating motion.

Figure 2.3: We engineered light-switchable photosynthetic liposomes (~150 nm in diameter) as energy modules to generate ATP from ADP under illumination. To convert light into ATP, we co-reconstituted two purified transmembrane proteins, namely, bacteriorhodopsin (bR) and EF₉F₁-ATP synthase from E. coli. Upon illumination, bacteriorhodopsin pumps protons into the vesicle’s interior, establishing a proton motive force that drives ATP synthase to catalyze the conversion of ADP to ATP. Axonemal Dynein molecular motors consume ATP, converting chemical energy into oscillatory beating motion.

Figure 2.4: (a) schematic of a floating “hovercraft” cluster of active droplets stabilised by cooperative hydrodynamic flows. (b) micrograph a non-rotating cluster, with streak lines of embedded tracer colloids (c) the same for a rotating cluster.

organisms in complex, mostly fluid environments. To experimentally explore the physics underlying their behaviour and to possibly use it for the application as smart materials, one needs well-controlled artificial model systems, from the scale of individual agents to collective dynamics and their self-organisation. A particularly versatile model system here is self-propelled microdroplets. Recently, we have shown that these droplets exhibit oscillatory rheotaxis reminiscent of the motion of parasites in blood vessels [12]. In addition, they are able to transport cargo by extracorporeal entrainment [13]. This is relevant for modelling the ingestion or dispersal of microplastics or even the exploration of the droplet’s environment by self-avoiding migration [14] and chemical signalling [15]. The latter is also found in exploratory strategies of bacterial or ant colonies. An attractive feature of such droplet systems is their tendency to self-organise into floating planar clusters that rotate through spontaneously arising collective hydrodynamic modes, reminiscent of the rotational states of sperm and Thiovulum majus. Interestingly, a nematically broken symmetry that favours helical states at the scale of individual droplets prevents rotation at the collective scale (Fig. 2.4, [16]).
similar to the non-biological counterpart discussed above, can provide insights into the complex fluid physics associated with the movement of microorganisms at low Reynolds numbers, where viscous drag dominates over inertia. We have constructed flagella-driven micro-swimmers using isolated and demembranated flagella from green algae Chlamydomonas reinhardtii (C. reinhardtii) as an ATP-fueled bio-actuator for propulsion of micron-sized beads. C. reinhardtii flagella, upon reactivation with ATP, beat with asymmetric curvature waves composed of a traveling wave component superimposed on an arc-shaped static curvature (Fig. 2.5). By combining mode decomposition of experimentally observed flagellum motion with resistive force theory, we numerically simulate and analytically calculate approximations for the mean rotational and translational velocities of a flagellum-driven bead, which agree very well with our experiments. Our analysis shows that there is a counterintuitive anomalous drive regime in which the speed of the flagellum-driven bead increases as the size of the bead increases. It also shows that in addition to static curvature and even harmonics, the asymmetric bead-flagellum attachment leads to the rotation of the microswimmer. This rotation mechanism, triggered by the sideways attachment of the cargo, has potential applications in the fabrication of bio-powered medical microrobots for targeted drug delivery and synthetic microswimmers [17].

We also applied a bottom-up coarse-graining approach to understand the emergence of metachronal waves in arrays of hydrodynamically interacting biological cilia. We proposed a theoretical framework to describe the coordination of many independently beating cilia [18]. We used a far-field approximation to analyze the dispersion relation and the stability of metachronal waves. Both the linear stability analysis and simulations show a region of stable longitudinal metachronal waves, providing an explanation for the observed metachronal waves in many microorganisms and ciliated tissues.

Besides motile cilia whose function is moving the fluid, many cilia have sensory functions and are therefore often referred to as “the cell’s antenna”. There is mounting evidence that the sensory functions are
not limited to immotile cilia and that beating cilia can also contain chemical receptors. We investigated the question whether there is a physical advantage in placing chemical receptors on a cilium in terms of sensitivity [19]. We determined the capture rates of signalling particles on immotile and motile cilia, acting alone or in bundles. We showed that the capture rates for chemical receptors located on cilia are always significantly higher than for receptors occupying the same surface area on a flat surface. The advantage of cilia becomes more pronounced if the cilia are either immersed in a shear flow or producing flow with their own beating motion. Our results show that the protruding geometry of a cilium could be one of the reasons why so many receptors are located on cilia. They also point to the advantage of combining motility with chemical reception.

Interestingly, in biological systems such as cilia the entangled molecular pathway is genetically defined and reacts to stimuli of different nature by transducing a chemical cascade reaction into mechanical responses. This cascade is a complex network and involves many information flows that determine the behaviour we observe. This made us wonder how we could re-engineer fundamental functioning principles of biological matter into a less complex form and unveil the minimal cellular components that are necessary or sufficient to sustain cilia functions. To explore this issue we developed a 2D minimal beating structure made of one microtubule clamped at one end and a few motor proteins. This structure performs sustained oscillations when the motor proteins simultaneously interact with the filament and the modified surface. Despite its extreme simplicity, the beating of the system resembles the behaviour of more complex structures such as flagella [20]. After engineering the simplest structure capable of beating, we followed up the investigation by building a structure consisting of the same components of cilia/flagella and resembling their minimal functional units, i.e. two doublet microtubules sliding under the action of axonemal dynein motors. This synthetic assembly that we name synthoneme is active and buckles its microtubules against each other as long as ATP is available. This one-of-a-kind result resembling the natural system with its beating behaviour shows that we succeeded to establish the basic functionality of a flagellar axoneme with a far smaller number of proteins [21]. Specifically, while cilia/flagella contain several hundred different proteins, our synthoneme, works with only three components. Such systems allow the investigation of the active dynamics of the ciliary beating and offer new insight into the symmetry breaking process that leads to fluid transport or self-propulsion.

In another approach to understand the fluid physics of life, we are investigating filamentous cyanobacteria. These are phototrophic prokaryotic organisms in which the individual, metabolically independent cells are stacked into linear, flexible filaments with large (≫ 100) aspect ratios that actively glide over surfaces and each other (Fig. 2.6). In natural habitats, colonies of these organisms are found in fresh and sea water, in both free-floating and sessile (benthic) lifestyles. In all forms, the colony exhibits a complex three-dimensional architecture that changes with ambient conditions. We have been unraveling the
mechanisms by which the simple behavior of individual filaments, ranging from persistent motion over random direction reversals [23] to photo- or mechanosensing, propagate across length scales, leading to self-organizing meta-materials. These individual responses are modulated by environmental conditions like temperature or salinity, which leads to an active adaptation also on a colony scale. It is this adaptive self-organization of an active, entangled, living polymer melt that led to the unrivaled evolutionary success and the ecological importance of these organisms, which belong to some of the oldest forms of life on our planet. We expect our findings to be relevant far beyond the specific self-organization as filamentous cyanobacteria played a key role in the oxygenation of our atmosphere and contributed large parts of the earth’s fossil fuels.

We also apply our expertise to the fluid physics of vascular like systems. The slime mold Physarum polycephalum is a unique physical model for living flow networks. Physarum grows into a giant cell of up to several centimeters in size, forming a fully connected network of tubes. The network tubes are filled with liquid cytoplasm, which flows throughout the network. The flows themselves affect the network architecture and also drive the organism’s remarkably intelligent decisions, which even account for simple forms of learning. Since we can experimentally control the size of the organism, we can change flow velocities across orders of magnitude and thus measure their impact. At the same time, we can quantify flows, transport, forces and network form in an unprecedented way in experiments. By combining experimental data with theoretical models of flow, we even have access to physical quantities such as pressures that cannot be measured in any other living system. With this unique approach, we found that the flows are spatially coordinated to ensure optimal transport, even over centimeters [24]. The transport ability of the flows is actively improved by a self-organizing network architecture [25] and tube’s mechanical properties [26]. Key to the self-organizing flow and network architecture is the transport of messenger substances with the flow [27, 28]. Surprisingly the transport of messengers also governs the organism’s ability to store memories in the pattern of thick and thin tubes [29].

Using model organisms such as the social amoeba Dictyostelium discoideum (D.d.) and cardiac fibroblasts, we investigate the physics
of the mechanics and dynamics of biological adhesion at the cellular and cell-cell level. *D.d.* serves as a model system for the adhesion and motility of eukaryotic cells. For example, we have uncovered the driving forces of adhesion in the unicellular state and cell-cell adhesion in the collective state of *D.d.* [30]. With the knowledge of the myosin II-based contribution to the shape, dynamics and viscoelastic properties of cardiac fibroblasts we advanced a model for the actomyosin cortex as a thin, reversibly cross-linked layer directly beneath the plasma membrane [31]. Finally, the model substrates were extended to include thermally switchable polymers for collecting cell sheets [32], paving the way for the realisation of synthetic tissue.

In summary, physics is essential for understanding the dynamics and self-organisation of life from molecular processes to whole organisms and their interaction. Only with physics in combination with biomolecular chemistry can life-like processes be created from the bottom up. To this end, we are partners in the Max Planck School Matter-to-Life, where Karen Alim, Eberhard Bodenschatz, Ramin Golestanian, Claudia Steinem and David Zwicker are part of the 50 carefully chosen fellows across Germany. As a contribution to teaching on the Göttingen campus, the study of chemotaxis with a remote-controlled experimental setup including a microscope was implemented with strong support from the MPI DS in an online course at the Max Planck School Matter-to-Life.
[31] A. Cordes et al., PRL 125, 068101 (2020)
[32] H. Kim et al., ACS Appl. Mat. & Int. 12, 33516 (2020)
2.2 PHYSICS TO MEDICINE

An important area of research at the MPI DS is the direct translation of findings from physics into applications in medicine. Research focuses on cardiac electrophysiology, contractile mechanics of the heart muscle, person-specific engineering of heart muscles to be implanted in patients, the dynamics of nerve cells and networks in the brain, their impairment and restoration from conditions of disease and trauma and COVID-19 research related to human aerosols, as well as epidemiological studies and recommendations to government agencies and the public.

In a normal heart rhythm, electrical excitation waves propagate through the heart muscle causing mechanical contraction and efficient blood pumping. This interplay of electrical and mechanical function at multiple levels, from cell to organ, is prevalent in heart disease, for which the term "dynamic disease" has been coined. Understanding the physics of the heart from the perspective of dynamics and self-organisation contributes to better medical diagnosis and therapy of cardiovascular diseases and cardiac arrhythmias. Cardiovascular disease is the leading cause of morbidity and mortality worldwide, accounting for about 30% of deaths. Sudden cardiac death due to malignant cardiac arrhythmias claims hundreds of thousands of lives every year in Germany alone. The mechanisms underlying the various forms of cardiovascular disease are still largely unknown. Two long-standing research focuses at the MPI DS have led to translation into the clinic and are currently in the clinical trial phase. Our collaboration with the University Medical Center Göttingen, the German Primate Center, and the partners in the German Centre for Cardiovascular Research (DZHK) demonstrates our strong commitment to translating basic physics research into clinical applications to improve quality of life.

In the failing heart, structural and functional changes lead to progressive, eventually fatal, loss of contractility. In collaboration with Prof. W. Zimmermann and colleagues our research focuses on patients with end-stage heart failure that would usually require mechanical assist devices or heart transplants. Engineered heart muscle (EHM) offers a very promising alternative to repair the failing heart. After successful animal experiments in macaque monkeys, the first successful human studies are being performed by our collaborators at the University Medical Center Göttingen. With our collaborators from the University Medical Center Göttingen, the German Primate Center, and Leibniz Universität Hannover, we won second place in the BMBF’s national innovation competition "Organ Replacement from the Laboratory." In "IndiHEART" we develop fiber-based 3D bioprinting of patient-specific engineered heart muscle (EHM) to be implanted on a patients heart (Fig. 2.8). To this end, we have developed a theoretical computer model of the contracting and dilating heart and devise a micro-fluidic 3D extrusion system for printing cardiac muscle fibres. In the "Alliance for Cardiac Regeneration" project funded by the German Center for Cardiovascular Research [1] we investigate the mechanical properties of the heart muscle theoretically and experimentally. The model-informed
EHM design will guide the fabrication of personalized EHM patches produced by 3D bioprinting. Understanding the transition to and recovery from heart failure is also the focus of our research within the DFG Collaborative Research Centre SFB1002 "Modulatory Units in Heart Failure".

We also have a long-standing research programme to understand the mechanisms underlying the occurrence, persistence and control of life-threatening ventricular fibrillation (VF). Cardiac arrhythmias are disturbances in the electrical excitation and mechanical function of the heart. In tachycardia, the ventricle is excited by a rotating spiral or scroll wave that can severely limit pumping function. Further breakup of spiral waves into small wavelets during VF results in complex spatiotemporal excitation (fibrillation) and subsequent termination of pump function. Sudden cardiac death is inevitable if this condition is not terminated immediately. For lack of a better strategy, high-energy electric shocks are used to terminate VF. These high power electric shocks have serious side effects, including excruciating pain, tissue damage and worsening prognosis, indicating a significant medical need. Our research has pioneered the development of algorithms for terminating low-energy arrhythmias in large animal models.

Since the first systematic observations in the mid-19th century, physicists and physicians have sought to elucidate the nature of cardiac fibrillation. Due to the complexity of the (chaotic) spatio-temporal dynamics and the experimental limitations in visualising the wave dynamics in the myocardium, however, the basic understanding remains limited. To gain a deeper insight into fibrillation dynamics we perform extensive theoretical studies and numerical simulations. To develop new and improve existing low-energy defibrillation methods, we investigate the timing and structure of external perturbations using different models of cardiac electrophysiology, including novel machine learning algorithms. Inspired by documented cases of self-termination of fibrillation, we analyse the underlying dynamics as a transient chaotic process and answer the questions of how to predict the duration of the chaotic fibrillation phase [2]. We also study the effects of small perturbations compared to sustained chaos (characterised by attractors and their basins of attraction) [3].

We advance alternative methods to control the spatial-temporal dynamics of excitable media. In recent years, we have developed optogenetic tools to explore the initiation and control of complex spatial-temporal dynamics in numerical simulations and experimentally using Langendorff-perfused transgenic mouse hearts ex vivo. In cardiac optogenetics, light pulses with an intensity above the excitation threshold result in an action potential and optical stimulation of the tissue. While subthreshold illumination does not elicit an action potential, it can be used to modulate tissue excitability and effectively perturb wave dynamics. We have shown that feedback control using subthreshold perturbation results in the highly efficient control of arrhythmias in transgenic mouse hearts in silico and ex vivo [4]. In another numerical study, we have demonstrated spiral wave control by thermal perturbation [5].

Figure 2.9: (a) Simulation of defibrillation current density in a pig heart (red - high, blue - low). The intracardiac electrode is shown in grey. (b) In vivo defibrillation experiment in pig with simulated current density based on 3D CT data. Electric field between the housing of the implantable defibrillator (gray) and the intracardiac electrode (not shown) inside the heart (red). (c) Measured current density obtained with MRT Current Density Imaging in collaboration with P. Schaten and M. Uecker (UMG/University of Graz, Austria, unpublished data)
We use data analysis and machine learning methods to reconstruct observables that are difficult to measure directly (e.g. electrical excitation in the heart) [6]. We have used them, for example, to detect spirals [7] and to predict their future evolution [8]. We aim to fuse all available measurement modalities, including multichannel ECGs, 4D ultrasound and structural information (CT, MRI). The stimulation of the cardiac muscle is by electrical currents, which so far could not be measured in the heart. We achieved a crucial milestone in collaboration with Prof. M. Uecker (University Medical Center Göttingen, now University of Graz, Austria). The novel MRT Current Density Imaging (MRT CDI) allows measuring the flow of electrical current in the heart with high spatial resolution. We also improve the MRI blood flow imaging sequence by modeling flowing spins, and refine the imaging results with physics informed deep learning.

We have achieved several milestones in collaboration with our clinical partners. Based on the development of 4D Electromechanical Imaging (4D EMI), we have demonstrated the first visualisation of mechanical scroll waves inside the fibrillating ventricles in a large animal model [9, 10]. In collaboration with our clinical partners at the University Medical Center Göttingen, Profs. I. Kutschka, H. Baraki, and G. Hasenfuss, we have started our first investigator-initiated clinical study that applies 4D EMI to VF in patients undergoing bypass surgery. Our data provide the first visualisation of mechanical rotors, the first step toward deciphering the spatial-temporal organisation of human ventricular fibrillation. Our partner Prof. W. Zimmermann and his colleagues at the University Medical Center Göttingen have made the first in man studies of implanting EHM on impaired hearts, so far with excellent outcomes.

The interaction of heart and brain is a research focus at the Göttingen Campus with high clinical relevance. A functional disorder of the heart can lead to cognitive problems and, conversely, a change in the central autonomic nervous system can lead to a functional disorder of the heart. The dynamic self-organising processes are insufficiently understood. Researchers at MPI DS in collaboration with external scientific member of MPI DS Prof. J. Frahm and Prof. M. Uecker are investigating this complex organ-organ interaction and the underlying electrophysiological and mechanical transport processes with high-resolution RT-MRI and data-driven modelling.

While in the heart excitable dynamics and mechanical action are linked in a single organ, the brain emerged in evolution by separating the dynamics of a complex network composed of expanded populations of excitable cells from the body’s effectors. This enabled the brain to perform information processing using a multitude of dynamical phases and to adjust information processing by transitioning between such phases. However, this extended dynamical repertoire also renders the brain’s excitable networks susceptible to diseases that emerge from subtle modifications of its components and collective dynamics. From its foundation, MPI DS research has made seminal contributions to understanding the dynamics of cerebral networks and over the past years we have advanced this research along several lines towards a
deeper understanding of dynamical disease mechanisms.

In the human brain, the fundamental units of dynamic information processing are not the single nerve cells but neuronal populations composed of thousands of cells, collectively transforming inputs and representing data. In prior work, we argued that the mechanisms by which nerve cells in the human brain transform analog inputs into binary action potential output was evolutionarily tailored to enhance the bandwidth and information content of such neuronal populations. In collaboration with experimental biophysicist Dr. A. Neef at the Göttingen Campus Institute for Dynamics of Biological Networks we directly confirmed this hypothesis by molecular reverting a key modification at the evolutionary origin of the mammalian spike generation mechanism [11]. Studies building on this advancement reveal that this evolutionary innovation on the one hand equips our nerve cells with mechanisms to reconfigure brain-wide networks on the fly [12] but on the other hand also renders the cerebral population code highly vulnerable to trauma and assault [13]. In conditions of stroke and hypoxia, subtle modifications of the spike generation mechanisms were demonstrated to massively degrade information capacity and network function even if the basic physiology of the nerve cells appeared completely recovered. Collaborating with Dr. M. A. Busche from University College London we developed the concept that such subtle cellular changes can generate tipping points in the progression of memory impairment in Alzheimer’s disease [14].

On the timescales of learning processes, brains dynamically reorganize their network structure by remodeling wiring patterns and the synaptic connections linking neurons into functional populations and structured networks. This type of dynamics is not only fundamental to the ability of brains to build complex circuitry by network self-organization and acquire new memories. It also provides the stage for disease processes affecting memory function. We recently advanced our understanding of the microscopic dynamics of synapses and started to uncover the impact of the molecular turnover [15] and subcellular interactions on synaptic dynamics and the persistence of synaptic memory traces [16, 17]. In collaboration with Prof. Y. Hayashi (Kyoto University), we demonstrated that a molecular mechanism associated with autism spectrum disorders induces enhanced turnover of network function inducing impaired learning capabilities [18]. Characterising synaptic dynamics under cortical neuroinflammation we demonstrated in collaboration with Prof. M. Kerschensteiner (LMU Munich) that network mechanisms can promote the recovery of lost synaptic connectivity after large-scale pathophysiological collapse and demonstrated the viability of an immunomodulatory therapy approach [19].

On the longest timescales, the process of biological evolution remolds the structure of the brain’s networks. In this process in particular, fundamental aspects of the nonlinear physics and biological evolutionary dynamics are intricately intertwined as gradual evolutionary remodeling of cellular and molecular features can lead to novel forms of emergent order at the level of networks and populations. We have previously raised the hypothesis that the structure of our visual sys-
tem resulted from a network-level phase transition at the origin of the primate order. Working with an international network of experimental groups, we critically tested this hypothesis using strategic taxon sampling, including studies of the smallest and most primitive primate species [20] and one of the largest and visually most capable rodents [21]. These studies establish beyond any reasonable doubt that the visual system’s network structure has undergone structural evolutionary transition multiple times and that an all-or-nothing transition of network structure occurred at the origin of the primate order [22]. From a biomedical perspective, these results imply that dynamical aspects of cerebral function and impairment are likely to differ qualitatively between rodent and primate brains and identify the mouse lemur as the novel model species to address these questions in future research. These and related questions are studied in the frameworks of the German Research Foundation priority program “Evolutionary optimisation of neuronal processing” coordinated by the Göttingen Campus Institute for Dynamics of Biological Networks and the transcontinental research network NeuroNex Working Memory (National Science Foundation, USA).

Given the urgency to address the issues raised by the COVID-19 pandemic, we refocused our research from cloud microphysics to human aerosols and droplets and their relationship to the physics of airborne disease transmission. To this end, we measured the size and concentration of exhaled particles in the nanometre to millimetre range of more than 200 individuals aged 5 to 80 years while they breathed, spoke, sang or shouted [23]. Our results suggest that age is the most important parameter for particle concentration, doubling in adolescence and over a 30-year period in adults, while gender, body mass index, smoking or exercise habits have no discernible influence. We found that particles <5 µm in size originate from the lower respiratory tract, 5 to 15 µm from the larynx/throat and >15 µm from the oral cavity. In addition, we have developed a novel infection risk model that fully couples infection risk to the volume of particles that may contain multiple copies of pathogens [24]. Our poly-pathogen model shows that the conventional mono-pathogen models systematically overestimate the risk of infection. Combining all these results allowed us to estimate the infection risk in the far field assuming a well-mixed room, which is presented as a freely available web application [25]. For near-field exposure, we found that for a typical SARS-CoV-2 viral load and infectious dose, the social distance alone (even at 3.0 m) between two people conversing leads to a 90% upper bound on the risk of infection after a few minutes. However, with universal masking, the very conservative upper bound remains below 30% after one hour with a surgical mask, while it is 0.4% with a properly fitted FFP2 mask [26]. In collaboration with Dr. C. Pöhler and his team at the Max Planck Institute for Chemistry, we are also investigating at BESSY II the chemical signatures of particles exhaled during various activities such as talking, singing or coughing, in order to better understand their point of origin and physicochemical properties.
[10] J. Christoph et al., In: J. Jalife and W. Stevenson (Eds.), From Bench to Bedside (in press)
2.3 PHYSICS TO SOCIETY

The arguably most important question of our time is whether (and how) humankind can devise a sustainable management of its ecological niche on planet Earth. If we do not manage to come up with satisfactory answers to this question, even science will soon become obsolete, when humans will have to care for their immediate needs for life instead of reading scientific papers. In order to mitigate the consequences of climate change, to face the challenges the current pandemic poses, and to organize a stable and sustainable Anthropocene, it is an urgent matter to better understand the earth and climate system, to lay the foundations of sustainable supply systems for energy and nutrition, and to devise viable concepts for transport and mobility systems. Central to all of these is a deep understanding of complex systems in general, and, in particular, of the collective phenomena which emerge when very many active agents are coupled to a complex whole. As this is precisely the kind of topics our institute is devoted to, there are a number of large-scale projects at the MPI DS that tackle this field of problems.

In the physics of climate systems, our still poor understanding of cloud microphysics, such as droplet size and spatial distribution as well as way they are affected by turbulence, are the main source of substantial uncertainties. They are affecting the interplay of moisture transport and air currents, the poor representation of which makes many aspects of future climate so far unpredictable. One of the many experiments in this field is conducted on the Zugspitze, the highest mountain in Germany in the Schneefernerhaus Laboratories. The
bottom right panel of Fig. 2.11 shows the interior of a Zugspitze cloud in the light of a Nd:YAG laser, making visible its pronounced structure, which inhibits pronounced ‘holes’ in the droplet distribution. Other experiments seek access to clouds more remote from the ground surface by using a combination of a kite with a buoyant balloon carrying the data acquisition setup (CloudKite).

The design of sustainable settling structures involves complex transport networks of water, food, sewage, energy, data, and the citizens themselves. The scaling properties of such systems, as well as their mutual interplay, must be deeply understood in order to guide humankind into a sustainable future sharing limited planetary resources. Projects on modelling and implementing sustainable transportation services are already very active. There is a strongly growing activity towards the development of transport systems which minimize fuel consumption at an affordable price for the customer (EcoBus). As a first step, we have investigated the statistical physics of ride pooling systems [2, 3]. Aside from important general characteristics governing the performance of such systems (Fig. 2.3, top left), it was found that they exhibit a first-order-type phase transition between a niche market (usually found if many transport systems compete with each other) and market dominance [3].

Other activities are concerned with possibilities for sustainable energy supply. Through 2017 the wind energy capacity installed worldwide has continued to grow. In Germany alone, the installed wind power capacity has meanwhile surpassed 50 gigawatts. The transition to renewable energies, however, comes with a range of challenges: for example, turbulence imposes significant structural fatigue loads on wind turbines which can lead to failure. Integrating the wind energy into a decentralized power grid, as another example, poses challenges with respect to power grid stability due to the presence of strong fluctuations. Because of its immediate potential of improving short-term energy and load forecasts as well of mitigating fluctuation-induced national-scale power outages, the understanding of turbulence and its interaction with wind energy systems has therefore become an urgent matter with an immediate societal impact.

Beyond such research focusing on individual sub-system networks, it is also of great interest to consider wider societal issues, many of which lend themselves to approaches by statistical physics methods, such as game theoretic models of society (e.g., game theory agents who play like humans do [4]).

As the climate crisis proceeds causing dramatic shifts of ecological niches for millions of species, mutation rates in bacteria and viruses are bound to increase dramatically, making outbreaks of zoonoses like COVID-19 ever more probable. It is therefore imperative to develop effective methods to forecast and mitigate epidemic spreading dynamics. This includes the estimation of the effects of mitigation interventions [5, 6, 7] as well as improved methods to derive important epidemic parameters from available data (cf. Sec. 8.5).

Complementary to understanding the spread of SARS-CoV-2 on a micro-level of interpersonal contacts (see droplet and aerosol research...
described in Sec. 2.2), it is also important to understand its spread on a macro population-scale. One basic research direction focused on the stochastic spread of the disease through a subdivided population (such as regions with high internal contact rates but low contact rates between them) and corresponding regional measures. In these theoretical studies, we were able to show that perfect isolation of small enough regions can harness small-number effects to significantly reduce the impact of an epidemic [8]. Based on the actual regional structure and infection numbers of several countries at the time, we could also show that fast and strong regional responses to increased infection numbers have the potential to stop disease spread in the overall population with substantially fewer contact restrictions than large scale lockdowns on the national or state level [6].

In an effort to quantify the effectiveness of mitigation measures (e.g., school closures) and make short-term forecasts about the disease spread, we designed a model that allowed us to estimate the change of the reproduction number \( R \), i.e. the number of offspring infections an infected individual causes on average [5]; later, we used similar approaches to quantify the infectiousness of emerging variants of SARS-CoV-2 [9]. Our work thus facilitated critical and urgent assessment of mitigation strategies. A central mitigation element is testing-trace-and-isolate (TTI), where health authorities manually break contagion chains by exploring the contacts of every new uncovered case [10]. We demonstrated that TTI enables a metastable regime at low case numbers [11] and introduces two novel tipping points between controlled and uncontrolled spread: (1) the behavior-driven spreading rate of the hidden chains becomes too large to be compensated by the TTI capabilities, and (2) the number of new infections exceeds the tracing capacity. The second tipping-point triggers a self-accelerating spread, where case numbers grow even faster than exponentially [10]. However, when case numbers are low, i.e., within the TTI capacity of health authorities, fewer restrictions are required for mitigation, offering a sweet-spot for policy planning and a great support to vaccination.

Even though the COVID-19 pandemic has brought disease modeling back to the spotlight, this is not the first global-scale health threat where the MPI DS played a central role in research. With the fast-growing connectivity between countries, new modi of disease spread emerged, enabling every local epidemic to become a potential global threat. Following the SARS-CoV-1 outbreaks in 2003, pioneering work from MPI DS pushed forward the state-of-the-art on disease modeling and has since been continued uninterruptedly. Major work involved Dirk Brockmann, a former Ph.D. student who is now a leading scientist in the field at the Robert Koch Insitute (Germany’s central agency and research institute for disease control and prevention), and described how epidemics spread in a highly connected world [13, 14, 15]. This brought to light the necessity of incorporating mobility patterns into models and also uncovered limitations of classical approaches when modeling the initial stages of an outbreak. Currently, the same group at MPI DS works on designing and assessing vaccination strategies for endemic diseases in nearly closed populations (Sec. 8.3). Their work provides helpful insights into the dynamics of infectious diseases in situations with a large influx of individuals, as is expected in the future with migrations related to the climate crisis.

Besides the research, communicating our findings to the public and decision makers was a key concern for us. Since the spring of 2020, we have regularly published our results in influential scientific journals. At the same time, we presented them in numerous international position papers published, e.g., by the National Academy Leopoldina or The Lancet [16, 17, 18], and also newspaper articles, interviews and talk shows, and regularly talked to policy makers. Based on this scientific work, one of our members, Viola Priesemann, was appointed to the COVID-19 advisory board (“Expertenrat”) of the German federal government. Thereby, the Max Planck Institute for Dynamics and Self-Organization has once again contributed to explaining and further developing the physics underlying viral spread, exponential growth and the mathematics behind mitigation measures. Our communication with the general public and politics has been met with immense interest and we very much hope that our basic scientific research continues to contribute to the containment of this pandemic during the transition to endemic COVID-19.

PART I

ORGANIZATION
DEPARTMENTS

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3.1 DEPARTMENT DYNAMICS OF COMPLEX FLUIDS

A complex fluid consists of (a large number of) equal or similar mobile entities which are complex enough by themselves to preclude a straightforward prediction of the collective behaviour of the whole. Our research aims at understanding phenomena of self-organization, such as pattern formation and self-assembly, in complex fluids as diverse as granular flows, swarming bacterial colonies, collective phenomena in human societies, or patterns in traffic flow. We employ a wide scope of methods, including analytical statistical theory, advanced simulation tools, cutting edge experimental laboratory techniques, and, wherever applicable, deployments in societal reality.

While our earlier work has largely focused on model systems, such as granular matter and active emulsions, we have increasingly embraced the innate complexity of real life systems in recent years. Based on first-principles statistical physics and state-of-the-art numerical simulations, we have studied e.g. basic scaling properties of ride-pooling systems. These theoretical studies have been complemented with real experiments, consisting in full fledged pilot project public transport systems, operational in Southern Lower Saxony. Based on these projects, which have won the Lower Saxony Environmental Award in 2019, we are now trying to establish it as intermodal demand-responsive public transport system. To this end, a startup company has been founded together with the Max Planck Society, in order to deploy the intellectual property generated at our institute on the free market.

Other research activities with direct connection to society are projects on epidemic spreading (on data from the Covid19 pandemic), on the dynamics of racial profiling, and on collective behavior in game theoretical settings. In order to perform experimental studies in this field, be it in traffic systems or on social media platforms, new software code is indispensable. To this end, a group has been established which writes such software to enable the necessary experimental infrastructure.

During the last two years, there have been substantial fluctuations among the department staff. Oliver Bäumchen and Corinna Maass left the institute for faculty positions in Bayreuth and Twente, respectively, but are still closely associated in research projects. Knut Heidemann has built a theoretical research team investigating social systems with statistical physics methods. Tariq Baig has joined the department as head of the experimental infrastructure group. Peter Keim has started to establish his independent Heisenberg Research group hosted by the department, performing experiments on topological phase transitions and spontaneous symmetry breaking beyond equilibrium. We thereby manage to keep the full scientific scope from very fundamental to very applied, and from analytical theory to simulation to experiment.
Dr. Christian Bahr received his PhD in 1988 at the TU Berlin. After Postdoctoral work at the Raman Research Institute (Bangalore, India) and the Laboratoire de Physique des Solides of the Université Paris-Sud (Orsay, France), he received his habilitation for physical chemistry at the TU Berlin in 1992 and moved to the University Marburg as a Heisenberg-Fellow in 1996. From 2001 he worked as a software developer before he joined our institute in 2004. Research topics comprise experimental studies of soft matter, mainly thermotropic liquid crystals.

Dr. Tariq Baig-Meininghaus received his PhD in Physics from the University of Göttingen in 2017. After completing a PostDoc position in the EcoBus Project at the Max Planck Institute for Dynamics and Self-Organization, he joined the Herminghaus department as leader of the working group ‘Software Infrastructure for Social Systems Research’ in 2020.

Dr. Kristian Hantke received his PhD in Physics in 2005 from the University of Marburg. After studying the optical injection of spin currents as a PostDoc he joined our institute as a scientific staff member in 2007. Being the lab coordinator for the laser and microscopy setups, his work centers around new experimental techniques based on nonlinear vibrational imaging and multi-photon laser scanning microscopy.

Dr. Knut Heidemann received a Master of Science in physics in 2012 from University of Göttingen (Germany), where he also finished his PhD in theoretical physics in 2016. After two years of applied data science research at Fraunhofer IAIS (Sankt Augustin, Germany), he returned to Göttingen in 2019 as research group leader at our institute. His group ‘Physics of Social Systems’ studies systems involving a human component, including topics like social network dynamics or sustainable mobility.

Dr. Stefan Karpitschka received his Diploma in Physics in 2007. As a PhD student he joined the MPI of Colloids and Interfaces in Potsdam, Germany, where he also completed his first PostDoc position in 2013. After other PostDoc projects at the University of Twente in Enschede, The Netherlands and the Stanford University, USA, he became a Research Group Leader in our department and in the Max Planck - University of Twente Center for Complex Fluid Dynamics in 2017. This group investigates the behavior of complex fluids at their interfaces with solids and gases.

Dr. Peter Keim studied physics at the Universities in Frankfurt and Konstanz and received his PhD in 2005. After a two-years postdoc at the University of Graz, he went back to Konstanz to lead a Junior Research group. In 2016 he was awarded the Gustav-Hertz-Prize of the German Physical Society and got the venia legendi in experimental physics. Since 2021 he leads a Heisenberg-Group hosted by the Herminghaus department, focussing on vitrification, topological phase transitions and spontaneous symmetry breaking beyond equilibrium.
Associated Scientists

**Assoc. Prof. Dr. Corinna Maaß** received her PhD in 2009 from the University of Konstanz for research on levitated granular gases. From 2010-2013, she worked as a postdoc in DNA nanotechnology at New York University, USA, from 2010-2011 as a fellow of the German Academic Exchange Service. She joined our institute in 2014 as leader of the working group ‘Active Soft Matter’. Her current research focuses on droplet swimmers in complex geometries. In 2021 she left for a faculty position at University of Twente, NL.

**Prof. Dr. Oliver Bäumchen** received his PhD in soft matter physics from Saarland University. He was a lecturer at the University of Applied Sciences (Saarbrücken) from 2007 to 2008. In 2011 he joined McMaster University, Canada, as a PostDoc (DFG research fellow). Since August 2013 he has been a group leader at our institute, studying instabilities of complex liquids and biological systems at interfaces. In 2015 he was awarded a ‘Joliot Chair’ and joined the ESPCI Paris as a visiting faculty. In 2021 he left for a chair in experimental physics at the University of Bayreuth.

**Assist. Prof. Dr. Marco G. Mazza** received his PhD in 2009 with a thesis on the 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 DS on the nonequilibrium physics of granular, soft, and biological matter. In 2018 he left for a faculty position at the University of Loughborough (UK).

**Dr. Matthias Schröter** obtained his PhD in 2003 from the University of Magdeburg. During his postdoctoral stay with Harry Swinney at the Center for Nonlinear Dynamics at the University of Austin he studied the statics and dynamics of granular media. Between 2008 and 2015 he joined the Department of Dynamics of Complex Fluids as a group leader. Since 2018 he is an associated researcher. Main research topics are the statistical mechanics of granular media, X-ray tomography of complex materials and applications of machine learning in physics.

Technical Staff

Monika Teuteberg and Barbara Kutz (top left) take care the secretary offices and administrative issues of the department and of the MPRGs. Guido Schriever (top center) is our scientific assistant, responsible for scientific reporting, web page maintenance and organizing visits and events. Diana Strüver and Markus Benderoth (top right) are responsible for our chemical and biological laboratories, which includes daily operation in all safety issues. Wolf Keiderling (bottom left) operates our mechanical workshop, and Thomas Eggers (bottom right) supports the desktop computers of the scientists, the computer clusters, the DCF network and the email accounts.
3.2 DEPARTMENT OF FLUID PHYSICS, PATTERN FORMATION AND BIOCOMPLEXITY

The department comprises the Laboratory for Fluid Physics, Pattern Formation and Biocomplexity (LFPB), headed by Eberhard Bodenschatz, and the Max Planck Research Group for Biomedical Physics (BMP), headed by Stefan Luther. Here we present the Fluid Physics, Pattern Formation and Biocomplexity Laboratory, while the BMP is presented separately.

In the LFPB we focus on the physics of dynamics and self-organisation in nature with special attention to Bottom Up Synthetic Biology, Bioengineering and Medical Physics, Physical Biodynamics, the Physics of Clouds and Atmospheres and of Turbulence. Current topics include synthetic engineering of bio-synthetic cilia, electrical turbulence and the soft mechanics of muscle contraction in the heart, cilia-based directed transport networks in the ventricles of the mammalian brain, and understanding fully developed turbulent flows (inertial/convective simple and complex fluids). Our work, while being fundamental science, also has direct implications for climate science and climate change, for mitigating the transmission of disease by respiratory aerosols, for understanding cilia-mediated transport in the ventilatary system of the brain with potential implications for ciliopathies, for curing cardiac fibrillation that can lead to sudden cardiac death, and for restoring pumping power to a weakened human heart with an engineered heart muscle.

The LFPB has established the Max Planck Turbulence Facility and the Max Planck Cloud Kite, which are part of the Max Planck University of Twente Center for Complex Fluid Dynamics. The Max Planck Turbulence Facility consists of a series of experimental systems and a pressurised gas facility that achieves the highest controlled and measurable turbulence levels on Earth. For studies of the micro-physics of clouds, we have established a field laboratory at the Schneefernerhaus Environmental Research Station on the Zugspitze at 2650m, where we are also part of the Virtual Alpine Observatory. The Max Planck Cloud Kite is a tethered 250m³ helikite facility that allows to carry atmospheric measurement equipment up to 1.5km with a payload of up to 100kg. The Max Planck Cloud Kite has been employed successfully on scientific cruises in the Atlantic. We run a microscopy facility, a cell biology laboratory and share a class 1000 clean room with the other groups and ran the micro-fluidics facility of MaxSynBio.

Research in LFPB is and will remain highly interdisciplinary, from fluid physics, statistical physics, physics of complex systems, and applied mathematics to environmental physics, synthetic biology and medicine. We link seamlessly with the other departments and research groups and are a member of the Max Planck School Matter to Life, the Center for Cardiovascular Research (DZHK) and the Max Planck University of Twente Center of Complex Fluid Dynamics.

Prof. Dr. Dr. h.c. Eberhard Bodenschatz 1989 Dr.rer.nat. U. Bayreuth; 1989-92 postdoc UCSB; 1992 - Prof. Cornell U.; 2003 - Director MPI DS; 2007 - Prof. U. Göttingen. Examples of service: 2008-11 Director of the MRS, 2008-12 member and chair SAB of KITP, 2012-17 vice chair and chair of the CPTS of MPS, 2016-20 governing board of the DPG, and 2020-24 review board DFG. He was Editor in Chief of NJP and on the editorial boards of Ann. Rev. Cond. Mat. Phys., EPJH, Physica D, Phys. Rev F. and SIAM JADS. He is member Exec. Board of the MP-School Matter to Life, Co-director of the MP-U-Twente Center on Complex Fluid Dynamics, site vice speaker German Center for Cardiovascular Research, and he heads the Software Commission of the MPS. He is member in the Göttingen Academy of Sciences, the National Academy Leopoldina, and of AAAS. He carries a Honorary Doctorate from the ENS Lyon for his scientific work, and is Fellow of the APS, IOP, EPS, and EuroMech. He is a recipient of the Stanley Corrsin Award of the APS.
Dr. Gholamhossein (Mohsen) Bagheri studied mechanical engineering at the Perisan Gulf University (BA) and the Shahid Bahonar University (MSc) (Iran), before completing his PhD at the University of Geneva (Switzerland). During his PhD, he conducted experimental and numerical studies on the dynamics of irregular particles in laminar and turbulent flows, for which he was awarded a PhD in 2015. Shortly after, he received an 18-month grant from the Swiss National Science Foundation to join the MPI DS as a visiting scientist and is now a group leader. His current research interests include the experimental study of cloud microphysics and atmospheric turbulence with the Max Planck CloudKites, the characterisation of respiratory particle emission and airborne disease transmission, and the numerical/experimental study of the dynamics of non-spherical particles.

Dr. Azam Gholami studied physics at Sharif University (Iran) where she received her bachelor in 1999. After her master in physics from the Institute for Advanced Studies in Basic Sciences (Iran) in 2001, she continued her study in theoretical physics at the LMU München and graduated in 2007. In 2008, she joined the MPI DS to work on actin-based motility and flow-driven waves in Dictyostelium discoideum. Since 2012, she is a group leader. She was coordinating the MaxSynBio project and is currently involved in the MAMI EU-project working on artificial cilia and cilia-driven motility.

Dr. Isabella Guido began her study in electrical engineering at the University of Bologna (Italy). In 2006 she joined the Fraunhofer IBMT in Potsdam and in 2010 received her PhD in physical engineering from the TU Berlin. From 2010-12 she was postdoctoral researcher at Peking University (China) and from 2012-13 at the University of Glasgow (UK) developing microsystems for single cells manipulation and characterizing cellular mechanical properties. In June 2013 she joined the MPI DS as a postdoctoral researcher working on cell electrotaxis. Since August 2014 she is a group leader within the synthetic biology initiative MaxSynBio working on synthetic active systems.

Dr. Bardia Hejazi obtained his BS in physics from Sharif University of Technology (Iran) before continuing his studies at Wesleyan University (USA) under the supervision of Prof. G. Voth. During his PhD he conducted computational and experimental work on particle-turbulence interactions, specifically on how particles can help identify fluid structures and also how deformable particles can be used to measure fluid quantities such as velocity gradient tensors. After the completion of his doctorate in January 2021 he joined the MPI DS to continue turbulence research. He is currently interested in active matter in turbulent flow, and high Reynolds number turbulence. He is also involved in human respiratory aerosol research.

Dr. Shoba Kapoor obtained her BS in biology and MS in neurobiology at the Georg-August University in Göttingen. The Master thesis project dealt with microglial cells and their binding properties to sialic acids on neurons and was carried out at the Life and Brain center in Bonn. In 2015, she joined the MPI for Biophysical Chemistry in Göttingen as a PhD student and worked on ciliated ependymal cells in the mammalian brain. Under the supervision of Prof. G. Eichele and collaborative work with Prof. E. Bodenschatz, she graduated in 2019 from the Georg-August University in Göttingen. She joined the MPI DS as a postdoctoral researcher in January 2021 to continue her research on fluid-dynamics within brain ventricles.
**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 1994-96 he studied pattern formation in liquid crystals. Starting 1999 he was a researcher at the University of Bayreuth working on pattern formation in complex fluids and soft matter theory. In 2010 he habilitated in theoretical physics at the University of Bayreuth. He joined the MPI DS in October 2013. His current research interests include nonlinear dynamics in excitable media, two phase convection and modeling of cell motility. He leads the theory group on pattern formation.

**Dr. Christian Küchler** studied Physics at the Goethe-University Frankfurt/Main (BS), in Livermore (USA), and at the University of Göttingen (MS). He prepared his MS- and PhD-theses under the supervision of Prof. E. Bodenschatz at the MPI DS. He compiled a comprehensive dataset of time series at extremely large Reynolds numbers studying the inertial range statistics of decaying turbulence in great detail. Furthermore, he designed and implemented a novel particle tracking system, which allows Lagrangian measurements in a pressurised wind tunnel. During his postdoc he improves the particle tracking system, analyses Lagrangian tracks at large Reynolds numbers and studies the flight dynamics of honeybees.

**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 (USA) in 2013 for his experimental and theoretical investigation of droplets bouncing and walking on a vibrating liquid bath. He joined the MPI DS in September 2013 as a postdoctoral researcher. He leads the experimental group on cloud microphysics investigation on Mount Zusgipitze. His research interests as a postdoctoral associate include experimental investigations of atmospheric turbulence, particles in turbulence and droplet dynamics in general.

**Dr. Freja Nordsiek** studied Physics at Michigan Technological University (USA) where she received her bachelor in 2010 and did research on the clustering of water droplets in air in the Cloud Physics Laboratory. She then received her doctorate in Physics in 2015 at the University of Maryland (USA) for research on transport in Taylor-Couette flow and granular electification. She joined the MPI DS in December 2015 as a postdoctoral researcher to investigate turbulence in the laboratory and the atmosphere. She works primarily on the CloudKite, a tethered lighter than air aerostat to measure cloud particles and turbulence in situ in clouds.

**Dr. Oliver Schlenczek** studied Meteorology in Mainz. In early 2018, he received his PhD in Meteorology from the University of Mainz where he developed a new airborne holographic system for investigating the microphysical composition of liquid, mixed-phase and ice clouds. In late 2017 he joined the institute as a postdoctoral associate. From 2017 to 2020, he was involved in development of the CloudKite instrumentation and participated in field campaigns with the CloudKite (MSM 82-2, EUREC4A) and performed cloud microphysical measurements with a holographic particle spectrometer on Zugspitze. During the course of the COVID-19 pandemic, he started to examine physical properties of human exhale particles.
PD Dr. Olga Shishkina studied mathematics at the Lomonosov Moscow State University until 1987. She received her doctorate in scientific computing from the Moscow University for Telecommunication & Informatics (1990), habilitated in fluid mechanics at the TU Ilmenau (2009) and also in mathematics at the University of Göttingen (2014). She worked at the Lomonosov Moscow State University and DLR Göttingen and finally joined the MPI DS (2014), where she leads the Theory of Turbulent Convection group. She is Heisenberg fellow (2014) and Fellow of the American Physical Society (2020).

Dr. Marco Tarantola received his diploma at the University of Würzburg in 2005 - focusing on biotechnology - and his PhD in 2010 at the physical chemistry of the University of Mainz. for the study of dynamics of epithelial monolayers. In 2010, he became coordinator of the CRC 937. He then joined the institute as a postdoctoral scientist until 2012 to work on Dictyostelium discoideum (D.d.) actin oscillations, before leaving for a stay at the UC San Diego (USA) until 2013, where he focused on adhesion and cell polarization of D.d.. Since 2014, he is a group leader and currently studies quantitative biology of D.d. and cardiac fibrosis and comparable synthetic model systems.

Dr. Yong Wang studied Process Equipment & Controlling Engineering, and Applied Mathematics at Xi’an Jiaotong University (China). In 2010, received his PhD degree (with distinction) in Engineering Thermal Physics for his development of a lattice Boltzmann method as applied to thermoacoustics and PIV measurements for oscillatory flows. From 2011–15 he was a postdoctoral researcher at UC Irvine (USA), and investigated the turbulent flow in human upper airway with DNS. He then joined the MPI DS as a group leader in March 2015. His research interests are in biofluidics, biomechanics and complex fluid dynamics, such as failing heart regeneration and cilia coordinated flow.

Dr. Christian Westendorf studied biology at the University of Rostock, finishing his Diploma thesis in microbiology in 2006. He joined the department of E. Bodenschatz as a PhD student in 2007 and graduated in physics at the University of Göttingen in 2012, with his thesis focusing on the biophysics of the actin cytoskeleton. From 2013-2015 he worked at the University of Graz (Austria) on plasmodial slime mold biology, before rejoining the MPI DS in late 2015. Since 2016 he is in charge of the department’s microscopy facility and in 2019 he started his own research group on quantitative biology of multicellular aggregates.

Dr. Xuan Zhang studied Power and Energy Engineering at the Xi’an Jiaotong University (China) from 2008 to 2012 for bachelor degree, and studied Mechanical Engineering at the University of Michigan (USA) from 2012 to 2017. She received her master in 2013 and doctorate in 2017 from the University of Michigan (USA) with focus on fluid dynamics and heat transfer. In September 2017, she joined the group Theory of Turbulent Convection at the MPI DS as research scientist to work on the numerical study of rotating turbulent convection.
Dr. Lukas Zwirner studied physics (Bachelor and Master) at the Otto-von-Guericke University in Magdeburg from 2010 to 2015. For his dissertation he joined the group of Dr. O. Shishkina at the MPI DS and in June 2020 he received his doctorate from the University of Göttingen. Currently, he works at the MPI DS as research scientist and numerically investigates turbulent thermal convection of liquid metals.

Dr. Vladimir S. Zykov studied physics at the Institute of Physics and Technology (Moscow, Russia). He graduated in 1973, received 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. S.C. Müller first at the MPI of Molecular Physiology and since 1996 at the University of Magdeburg. Since 2001 he was a research scientist at the TU Berlin and in 2010 joined the MPI DS. His research interests include pattern formation processes in nonlinear reaction-diffusion media and control methods of self-organization.

Associated Scientists

Prof. Dr. Hyejeong Kim studied mechanical engineering at Pohang University of Science and Technology (POSTECH) (South Korea) where she received her bachelor in 2012. She received her integrated PhD degree in August 2017 at POSTECH with thesis “Development of Advanced Biomimetic Technologies Inspired by Leaf Transpiration”. From August 2017 to May 2018 she was a postdoctoral researcher at POSTECH. She joined the MPI DS as a postdoctoral associated in June 2018 and worked on Living Foam project until November 2020. In 2021 she was appointed assistant professor of mechanical engineering at Korea University and stayed associated with the MPI DS. She is interested in broad range of experimental approaches to microfluidics, soft matter, and their biomedical and environmental applications.

Dr. Laura Turco received her MS in Biomedical Engineering from Politecnico di Milano (Italy) and her PhD in Biophysics at the MPI DS. She led the MPI DS microfluidic and was involved in the design and fabrication of microfluidic platforms for synthetic biology and biomedical applications within the MaxSynBio initiative and in the development of devices for cell-laden extrusion of microfibers for regenerative medicine. She currently works at Bayer AG within the International future leadership program and is an associated scientist supporting the activities for 3D printing of myocardium.

Dr. Stephan Weiß has received his diploma in physics from the University of Bayreuth in 2005 and a PhD in experimental physics from the Georg-August University of Göttingen/MPI DS in 2009. He worked as a postdoc at the University of California Santa Barbara (USA) (DFG-Fellowship) on turbulent thermal convection and at the University of Michigan (USA) on spirals in oscillating chemical reactions. From August 2015 to August 2021, he has led the experimental research on thermal convection. He works now at the German-Aerospace Centre (DLR) in Göttingen.
The vision behind the Department of Living Matter Physics (LMP) is to study living systems as self-organized active soft matter that are away from equilibrium “just the right way”. The aim is to understand the complex dynamics of living matter well enough to be able to make it from the bottom-up; i.e. from molecules to systems. The research topics cover, broadly speaking, chemical and mechanical nonequilibrium activity in Living Matter across the scales. The department is organized in such a way that allows us to study complex systems using complementary theoretical techniques that encompass multiple scales. In the first three years since its inception, the research activities in LMP has led to a number of very exciting results. Our studies of chemically active matter start from the smallest relevant unit, namely enzymes, and systematically investigate cooperativity and emergent features in systems with multiple enzymes. These range from emergent coherence in the stochastic activity of enzymes, which has resulted in a new paradigm of molecular synchronization in barrier-crossing stochastic systems, to the observation of topologically protected currents in chiral chemically active molecular systems, to the discovery of the role of cooperativity in the diffusion and reaction of enzyme clusters, to active phase separation in suspensions with enzyme mixtures. The role of non-reciprocal interactions has been further elucidated at the mesoscopic scale in the context of non-reciprocal Cahn-Hilliard (NRCH) model that we have recently introduced. We have made the surprising discovery that a theory with two scalar fields can undergo spontaneous breaking of a plethora of symmetries, including time-translation, time-reversal, and space-translation, which exist in the theory, as well as polar symmetry, which is an emergent symmetry in the system, simply by adding a single parameter that originates from non-reciprocal interactions. The systematic coarse-graining of chemically interacting systems has allowed us to discover a new polarity-induced theory of collective chemotaxis, which we studied using Renormalization Group theory, and an accompanying emergent symmetry that does not lend itself to any intuitive description in terms of the microscopic elements in the theory. In the context of a generic phenomenological scalar active matter theory, we have uncovered that the existence of a diffusivity edge gives rise to a classical analogue of the Bose-Einstein Condensation (BEC) transition, with all its thermodynamic signatures following that of the standard BEC identically. We have identified a first active matter system in which such a BEC transition can be realized experimentally; an ensemble of magnetotactic bacteria in a shear flow. We have performed a comprehensive computational study of this system, and observed that it exhibits full agreement with the corresponding BEC theory without any fitting procedure. We have continued to work on the area of active hydrodynamics, and made a number of breakthroughs. The problem of near-field effects in the non-equilibrium interaction between phoretically active particles has been solved using the elegant Lorentz reciprocal theorem. Using a systematic coarse-graining approach, we have elucidated the conditions for
the stability of emergent metachronal waves in ciliary arrays. We have investigated the interplay between the hydrodynamic activity and the sensory role of cilia. We have also formulated a minimum dissipation theorem that introduces a bound on the dissipation of low Reynolds number swimmers, augmenting the theoretical work of Lighthill after five decades. Other developments include studies of mixtures of growing active matter, as well as a number of projects in information processing such as geometric characterization of the micro-swimmer optimal navigation problem, quantifying the configuration entropy of tracer particles in a complex flow, the formulation of a first topological fluctuation theorem, and a number of publications concerning the epidemiology of Covid-19. Finally, we highlight that while LMP is still in its developing stage, it has already been successful in helping some of its more senior members to move onto faculty positions (Amir Bahrami to Assistant Professorship at Bilkent University in Turkey, Falko Ziebert to a permanent academic position in Heidelberg, Fanlong Meng to Associate Professorship at the Institute for Theoretical Physics of the Chinese Academy of Sciences in Beijing, and Evelyn Tang to Assistant Professorship at the Center for Theoretical Biological Physics at Rice University in the US).

**Group leaders**

**Dr. Andrej Vilfan** studied physics and received his doctorate from the Technical University Munich in 2000. He worked as a postdoctoral researcher at Cambridge University (UK) and as a visiting scientist at the Max Planck Institute for the Physics of Complex Systems in Dresden. Before joining the MPI DS in June 2018, he worked as a senior research fellow at the J. Stefan Institute in Ljubljana (Slovenia). As a theoretical physicist, he has worked on molecular motors, auditory receptors, hydrodynamics of biological and artificial cilia, as well as other colloidal systems.

**Dr. Jaime Agudo-Canalejo** studied physics at the Complutense University of Madrid, and received his PhD from the Technical University of Berlin in 2016. His doctoral work, on the theory of biological and biomimetic membranes, was conducted at the Max Planck Institute of Colloids and Interfaces in Potsdam. From 2017 to 2019, he was a postdoctoral fellow jointly at the University of Oxford and at Penn State University. Since 2019, he is a group leader in the Department of Living Matter Physics at the MPI DS, working on the theory of out-of-equilibrium processes induced by catalytic activity, both in biological and synthetic systems.

**Dr. Philip Bittihn** studied physics and obtained his doctorate from Göttingen University in 2013 for work on pattern formation, spatio-temporal control and structural complexity in cardiac tissue. A recipient of the Otto-Hahn medal by the Max Planck Society, he then extended his research to include synthetic and systems biology at the University of California San Diego as a scholar of the Human Frontiers Science Program, before joining the Department of Living Matter Physics in 2019. Since August 2021, he has been leader of the group Emergent Dynamics in Living Systems which focuses on multicellular self-organization and growth.
Dr. Benoît Mahault studied physics and obtained his Ph.D. from Université Paris-Saclay in 2018, working on minimal models and field theories for active matter. After a short postdoctoral position at Tokyo University, he joined the MPI DS in January 2019 as a postdoctoral researcher and became group leader in July 2021. His current research focuses on various non-equilibrium statistical physics problems, such as self-organization in living and non-living matter, optimal navigation in complex environments, and the connection between stochastic thermodynamics and topology.

Technical and administrative staff

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 a stipend from the Berliner-Ungewitter-Stiftung. He joined the institute in 2000 as an IT administrator in the former theory department. Since 2018 he has been working as an IT expert in the department of Living Matter Physics. And in 2021 he also joined the newly restructured central IT team of the institute as a Linux specialist.

Ayşe Bolik is a European Business Assistant certified in English and French and has been working at the MPI DS since 2010. Since 2018, she is assistant to Ramin Golestanian in the department of Living Matter Physics. She is also the Gender Equality Officer of the MPI DS.

Viktoryia Novak studied foreign languages at the Gomel State University (Belarus), International Economics at the University of Göttingen, and Higher Education and Research Management (MBA) at the University of Applied Sciences in Osnabrück. She joined the MPI DS in 2011. Since 2018 she has been working for the department of Living Matter Physics. She is mainly responsible for scientific visualization (conceptual implementation of graphical presentation of scientific results), coordination of grant applications and third-party funded projects, management of the guest program, and implementation of activities related to societal impact of science.

The Department of Living Matter Physics in September 2021
RESEARCH GROUPS

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4.1 MAX PLANCK RESEARCH GROUP: BIOLOGICAL PHYSICS AND MORPHOGENESIS

How can life, how can individual organisms and organs morph into desired structure? How does structure define function? Understanding morphogenesis, the collective self-organization of biological matter that gives rise to a functional structure, is at the heart of decoding life. Unveiling the physical mechanisms nature uses to control the dynamics of development also generates new concepts for bioengineering and synthetic implementations of biological processes in smart materials. We aim to identify the rules of morphogenesis by studying the physical principles underlying the formation and adaptation of biological organisms. We combine insights from biological signals with knowledge of physical processes to discover how physical forces induce, transmit and respond to biological signals and thus control development and shape morphology.

The key physical players we focus on are mechanics and fluid flows. Mechanical forces propagate quickly over large spatial scales and are therefore crucial to coordinate cell dynamics within the rapidly developing organism. Here, we develop theoretical models studying the principles of how the feedback between mechanics and cell dynamics/biochemical signalling drives collective dynamics particularly focusing on plant tissues. Fluid flows propagate resources and signals through a vascular network and thereby shape surrounding tissue and the morphology of the vasculature itself. We aim to identify the self-organising principles of the feedback between flows and network morphology. Here, the challenge is that flows are globally coupled within a network. To overcome this challenge we combine theory of fluid flows within networks with quantitative experimental observations of flow network self-organisation observing the slime mould Physarum polycephalum. This integrative strategy shows that flows are an integral part of the self-organisation machinery of life itself. We work on translating physical principles in living systems to bio-mimetic applications by developing theoretical models of active porous media.

We collaborate nationally and internationally with physicists, biologists, mathematicians and material scientists. We are members of the research unit FOR 2581 on Plant Morphodynamics. In Göttingen we enjoy collaborations with the department of Eberhard Bodenschatz and Stephan Herminghaus and fellow Max Planck Research Groups. Our group engages in service for the committee “Chances” by the Max Planck Society, the Dorothea Schlözer Mentoring program by the University of Göttingen and on the PhD student level as representatives of the International Max Planck Research School Physics and Biology of Complex Systems, the institute-wide and nation-wide PhDnet of the Max Planck Society even including the student representative on the Göttingen Graduate School for Neurosciences, Biophysics, and Molecular Biosciences Board among us.
Siyu Chen, PhD, received his bachelor degree from the Chemistry and Biology Combined Major program at Osaka University (Japan) in 2015. His undergraduate research focused on Chemical Biology, constructing model cell lines for the quantification of synthetic oligomers. Then he moved to the field of colloidal science during his D.Phil at the University of Oxford. In particular, he studied the interactions of colloidal monolayers with the ice-water interface. In the Biological Physics and Morphogenesis group at the MPI DS, his current interests include studying the behaviour of Physarum polycephalum under light stimulus and the dynamics of the thousands of nuclei within Physarum’s syncytial cell.

Dr. Agnese Codutti received her bachelor’s degree in Physics at the Università degli Studi of Trieste (Italy) in 2011, as well as her master’s degree with a specialization in the foundations of quantum mechanics. During her Ph.D. at the Max Planck Institute for Colloids and Interfaces, Potsdam (Germany), she studied magnetic microswimmers from the theoretical and computational point of view, in particular concentrating on magnetotactic bacteria and randomly-shaped synthetic propellers. In the Biological Physics and Morphogenesis group at the MPI DS, her current interests include the theory and simulation of biological fluid flow in resilient networks (such as the brain microvasculature), as well as flow in complex varying geometries such as the gut, and its effects on the microbiome.

Associated Scientists

Dr. Sophie Marbach received her PhD at École Normale Supérieure de Paris in 2018, where she worked on the transport of fluids at the nanoscale and designed innovative concepts for filtration, such as active filtration with fluctuating pores inspired by biological porins. She is now a Marie Curie Fellow at New York University in the Courant Institute of Mathematical Sciences, exploring how particles with legs (such as DNA-coated colloids or viruses) stick and move on adherent surfaces, rationalizing how detailed mechanical fluctuations of the legs feed the macroscopic behavior. Her domains of interest are fluid mechanics, biophysics, out-of-equilibrium physics, statistical mechanics, and scientific programming. She has worked with the group since 2015, investigating mechanisms leading to spontaneous pruning.

Technical Staff

Anne Weber studied biotechnology at the Ernst-Abbe-University in Jena. After her Diploma in 2007 she worked shortly in industry before joining the MPI for Biophysical Chemistry. In those years she gained experience in molecular, micro-, and cell biology and biochemistry dealing with forensic DNA analytics, single-use bioreactors, plasmid design and protein expression, purification and characterisation, among many other methods. In September 2017 she joined the group to support the laboratory work and to investigate the genetic manipulation of P. polycephalum.
Self-organized complex spatiotemporal dynamics underlie physiological and pathological states in excitable biological systems such as the heart and brain. We believe that the systematic integration of dynamics at all levels – from subcellular, cellular, tissue, and organic levels to the in vivo organism – is the key to understanding complex biological systems and, in the long term, will open new avenues for translating fundamental scientific discoveries into practical applications that can improve human health. Our research focuses on cardiac arrhythmias, a major cause of morbidity and mortality worldwide, with sudden cardiac death claiming hundreds of thousands of lives each year. The fundamental scientific questions are: What are the principles underlying spatiotemporal self-organization of cardiac arrhythmias? How can we apply this understanding to effectively and gently terminate arrhythmias? (Sec. 6.14) To answer these questions, we combine the development of advanced cardiac imaging (Sec. 6.13), data-driven modeling (Sec. 8.24), and multimodal data analysis (Sec. 6.15). Our electromechanical technology has provided the first three-dimensional electromechanical scroll waves in ventricular fibrillation and has already been successfully applied in a clinical study. This imaging technique enables for the first time a detailed characterization of the spatio-temporal organization of fibrillation in humans. Based on the data from animal experiments and clinical trials, we apply data-driven modeling and machine learning (Sec. 8.23) to develop new concepts for arrhythmia control. We have developed an innovative Open Source and FAIR research data management system that robustly maps our scientific workflow by integrating data and algorithms, from data generation to publication (Sec. 8.25). We conduct our translational research at MPI DS and the University Medical Center Göttingen within the framework of the German Centers for Cardiovascular Research. In this interdisciplinary environment, we are committed to excellence in teaching in order to attract and train the next generation of scientists and physicians.
Dr. Sayedeh Hussaini studied physics at Ferdowsi University in Mashhad, Iran. In 2015, she received her Master’s degree in Nanophysics. In September 2016, she joined the Biomedical Physics group, where she mainly focused on computational studies to control the dynamics of cardiac arrhythmias. She received her Ph.D. in February 2021 and then continued her research in numerical and experimental studies as a postdoctoral researcher. Her research interests focus on cardiac modeling, cardiac arrhythmia control, and cardiac optogenetics.

Dr. Thomas Lilienkamp studied physics at the Universität Bielefeld (Germany) and the Universitetet i Bergen (Norway). He received his Diploma degree in December 2013. Afterwards he worked as a doctoral student in the Research Group Biomedical Physics at the MPI DS, where he received the doctoral degree in 2018. His current research interests include the control, spontaneous termination and complexity measures of complex (chaotic) dynamics in spatially extended systems.

Dipl. Phys. Gisa Luther studied physics at the University of Hannover and of Oldenburg and graduated in 1996. From 1997 to 2004, she worked as project manager in software engineering and system integration (Bull GmbH, WestLB Systems GmbH). From 2004 to 2007, she was scientific staff member at the MPI DS and visiting scientist at Cornell University, Ithaca NY, USA. Since 2007, she has been scientific staff member in the research group Biomedical Physics, focusing on numerical simulations in cardiac tissue and on scientific project management.

Dr. Rupamanjari Majumder obtained her PhD degree in Physics, in 2014, from the Indian Institute of Science, Bangalore (India). She then moved to the Leiden University Medical Center (the Netherlands), to work as a postdoctoral researcher, and later as Assistant Professor. In 2018, she joined the Max Planck Institute for Dynamics and Self Organization, Göttingen. Since 2020, she has been working with the Research Group Biomedical Physics. Her current interests include cardiac modelling, optogenetics, and spatiotemporal chaos in cardiac systems.

Dr. Alexander Schlemmer studied physics at the Georg-August-Universität Göttingen, where he received his Diploma degree in 2011. He was a research assistant at the Psychology Department of the University of Hildesheim (2011-2013) and at the Research Group Biomedical Physics at the MPI DS (2012-2017). He received his doctoral degree in 2017. His research interests focus on spatio-temporal dynamics of excitable media, time series analysis and machine learning for nonlinear systems, and semantic data management in complex heterogeneous scientific environments.

Dr. Johannes Schröder-Schetelig studied physics at the Georg-August-Universität Göttingen, where he received his Diploma degree in 2012. Working for the Research Group Biomedical Physics at the MPI DS as a student assistant since 2008, he continued as a doctoral student and received his doctoral degree in 2020. His research interests focus on studying the complex spatio-temporal dynamics of the heart with simultaneous application of multiple imaging modalities including 3D panoramic optical mapping, multi-ECG, and 4D ultrasound.
4.3 MAX PLANCK RESEARCH GROUP: STATISTICAL PHYSICS OF EVOLVING SYSTEMS

Dr. Armita Nourmohammad studied Physics at Sharif University of Technology (Iran) and moved to Cologne for her graduate studies, where she developed statistical physics approaches to study evolving populations. During her PhD with Michael Lässig, she addressed evolutionary modes of gene regulation in eukaryotes and developed an out-of-equilibrium theory for evolution of molecular phenotypes. In 2012 she won a James S. McDonnell fellowship to study complex systems and joined Princeton University as an independent biophysics theory fellow to pursue her research. There, she became fascinated by the complexity of the adaptive immune system and developed a principled framework to describe non-equilibrium coevolution of immune cells and pathogens. In 2017 she won an independent Max Planck Research Group and in October 2017 started her group at MPI DS. Armita is an Assistant Professor in Physics at the University of Washington (Seattle) and an affiliate investigator at the Fred Hutchinson Cancer Research Center in Seattle. Armita is a recipient of the CAREER award from the National Science Foundation (NSF), the Early Stage Investigator R35 MIRA award from the National Institute of Health (NIH), and Early Career Award from American Physical Society (APS), Division of Biology (DBIO).

Our interest lies at the interface of statistical physics, information theory, evolutionary biology and immunology. We study the adaptive immunity in vertebrates, where a highly diverse set of molecular receptors use mechanisms associated with Darwinian evolution to collectively mount a specific response against rapidly evolving pathogens. In return, pathogens evolve to escape the immune challenge and constantly form new targets for the immune system, resulting in an out-of-equilibrium stochastic process in a high-dimensional system. Recently, it has become feasible to sequence the diverse immune receptors of a host together with infecting viruses. Additionally, protein structural data enables us to map out a functional output for immune receptors. We combine theory with such molecular data to characterize the organization and encoding of the immune system, to build predictive models of immune-pathogen convolution, and to devise control strategies that leverage immunity to curb the evolution of pathogens.

Immune strategies in light of host-pathogen coevolution. The adaptive immune system has coevolved for millions of years with bacteria and viruses. It is permissible to assume that the biochemical program encoded by the immune system may be evolved to be in tune with the statistics of the pathogenic environment, with flexibilities that can permit the anticipated evolutionary changes in pathogens during an organism’s lifetime. We have characterized consequences of such coevolutionary history for the strategies that the immune system adopts to store memory of pathogens. Furthermore, in collaboration with Prof. Luca Peliti, we have developed a general theoretical framework for optimal memory encoding strategies in biological networks that are driven out of equilibrium by evolving stimuli— an approach that brings us a high-level understanding of memory encoding in biological systems, ranging from the brain to the immune system.

Mapping out a functional immune shape space. Over the past decade, the growth of sequence data on immune receptors has advanced our understanding of the vast diversity and organization of the adaptive immune repertoires. However, a map between a receptor sequence and its function is still a challenge. In a series of studies, we have developed statistical inference approaches to characterize the statistics and dynamics of functional B- and T-cell repertoires in response to immune challenges. In collaboration with Dr. Aleksandra Walczak, we have introduced an inference framework to integrate the interpretable knowledge-based models of immune receptor generation with more flexible but powerful deep learning approaches. This framework enabled us to characterize signatures of differential functional selection on immune receptors associated with different cell types, and in immune repertoires of patients with different severities of COVID-19 infections. We are currently developing frameworks to incorporate information from the tertiary structure of immune receptors to characterize a functional shape space for the immune system.
Adaptive control of evolving populations. Controlling an evolving population is an important task in modern molecular genetics, including in directed evolution to improve the activity of molecules, and in devising public health strategies to suppress pathogens. We have developed a population genetics based optimal control formalism for stochastic and in general out of equilibrium systems to direct the evolution of multi-variate molecular phenotypes. We showed that evolutionary control is challenged by the limited predictability of evolution due to stochastic effects at the molecular or environmental level. The interplay between prediction and control is a key in devising optimal strategies against evolving pathogens. In collaboration with Prof. Florian Klein, we are developing a predictive approach for HIV escape against broadly neutralizing antibodies (BnAbs). By leveraging this predictive model, we are devising optimal therapy approaches with combinations of BnAbs to sustain viremia at low levels and suppress evolutionary escape of HIV within patients.

Our group strongly benefits from close collaborations with Cologne, Paris, and Seattle. We currently contribute to the teaching effort at the University of Washington (Seattle) and also at a number of international summer schools. In addition, we are involved in organizing international meetings on on biophysics and evolution. Recent examples include: “Out-of-equilibrium processes in evolution and ecology”, Casa Matematica Oaxaca, Mexico (2019); “From Molecular Basis to Predictability and control of evolution”, Nordita program, Stockholm (2019); “Predictability of rapid evolutionary processes”, SMBE session, Yokohama, Japan (2018). We are grateful for the support of the Max Planck Society and the DFG collaborative research center (SFB 1310).
Dr. Colin LaMont studied Physics at Reed College (Oregon) and obtained his PhD in Physics from the University of Washington (Seattle), where he developed a correspondence between statistics and thermodynamics. Since June 2018, he has joined our group as a postdoc within the DFG funded project of SFB1310. Colin’s research focuses on developing a theory of stochastic adaptive control for evolving populations and to construct control strategies applicable to HIV therapy.

Giulio Isacchini studied Physics at Trento and Oslo and obtained his Master’s degree from ETH and École Polytechnique (Paris). Since October 2018, Giulio has joined our group at MPI DS as a PhD student, in a collaborative project with the group of Aleksandra Walczak and Thierry Mora at ENS (Paris). Giulio defended his PhD thesis in September 2021 and is planning to start a postdoc position at UC Berkeley in January 2022. Giulio has used machine learning and biophysical modeling to construct a functional description of immune repertoires.

Zachary Montague studied Physics at University of Florida and at the University of Washington (Seattle) and has joined MPI DS since 2018 as a PhD student until he relocated back to the University of Washington in 2020. Zachary’s research aims to characterize the life-cycle of B-cells, as they proliferate and hyper-mutate in response to an infection, and switch to an inactivated state following an infection. To do so, Zachary is developing stochastic models of B-cell maturation that can be parameterized using B-cell repertoire data collected over a long period of time (a few years).

Michael Pun studied Physics at Bodwin College (Maine) and at the University of Washington (Seattle) and has joined MPI DS since July 2018 as a PhD student until he relocated back to the University of Washington in 2020. Michael’s research aims to construct a structure-function map for proteins in general and for immune receptors in particular. Michael is pursuing this goal by developing 3D equivariant neural networks that take protein structures as input and through transformations that respect the physical symmetries in the data, learn interpretable models of protein structures that could reflect the underlying biophysical function.

Oskar Schnaack studied Physics at Georg-August-University, Goettingen, where he earned his Master’s degree with a thesis on information theory in quantum systems. Since February 2018, he has joined our group at MPI DS as a PhD student. Oskar’s research focuses on memory strategies in out-of-equilibrium evolving systems. He has developed a formalism based on the thermodynamics of decision making to characterize the emergence of memory states in evolving populations and especially in the adaptive immune system.
4.4 MAX PLANCK RESEARCH GROUP: NEURAL SYSTEMS THEORY

Neural networks, both in the human brain as well as artificial ones, show astonishing information processing capabilities. Considering both side by side, we investigate the self-organization of neural computation with approaches from statistical physics and information theory. On this quest, our most outstanding contributions are on the problem of subsampling, on the role of second-order phase transition for the function of neural networks, and on applications of information theory to neural networks. Recently, in the context of the COVID-19 pandemic, we have studied disease spread dynamics to assess and design containment strategies. The work on these two topics—the self-organization and flow of information on neural networks, and the spread of a virus on a population network—has turned out to be complementary and highly fruitful, yielding novel insights in both domains. Below, we provide an overview of our major research foci.

I. Subsampling Theory. A classical problem when investigating complex systems is to infer their properties from measurements. In most large systems, however, it is impossible to sample the activity of all their units in parallel. For example, the mammalian brain comprises millions to billions of neurons, but current techniques allow sampling only the activity of some hundreds of neurons with millisecond precision. We showed how such spatial subsampling impedes inferences about collective properties of the full system, inducing a strong systematic bias. To overcome the bias, (A) we derived the approach of “subsampling scaling” to infer graph properties from a subsampled graph, and (B) we proved that subsampling biases the inference about collective dynamics. In particular (i) it leads to mis-estimation of measures as basic as the correlation, (ii) it leads to overestimation of system stability, and (iii) in systems close to a critical state, it leads to the underestimation of the control parameter and distorts the expected power law relations. We derived a subsampling-invariant estimator, which overcomes these problems and is unbiased, readily applicable and data efficient. In principle it can even derive the control parameter or stability from the activity of a single unit, even without knowledge about the system or sampling size.

II. Collective cortical dynamics, phase transitions and critical phenomena. A large body of experimental and theoretical work claims that the cortex operates at a critical state. Thereby, cortex could draw on maximized computational properties, including information transfer and susceptibility. By re-analyzing spiking activity using our subsampling-invariant approach, we found a novel operating regime of the cortex consistently for many species and brain areas. In this novel regime, the brain could flexibly tune its computational properties, alternating between a critical state with its computational advantages, as well as an alternative, so called “balanced state”, which instead maximizes response speed and minimizes redundancy. We analyzed how external inputs, mediated by a synaptic plasticity mechanism, can tune the neu-
ral network from one operating regime to the other, thus adapting its computational and dynamical properties depending on input strength. Based on these findings, we hypothesized that the brain tunes itself towards either the critical or the balanced state depending on task requirements. We have started to test this property as a design principle for improving artificial neural networks with our international collaborators in the domain of neuromorphic computing and experimental neuroscience.

III. Information theory, synaptic dynamics and learning in artificial neural networks. Information theory provides a natural language to quantify information processing independently of the imposed semantics. Hence, it enables us to quantify the computational capacity of living and artificial neural networks, while providing the formal framework to derive learning rules systematically. Learning –from the synapse to the network level– tunes the performance of living systems, and unlocks the power of artificial ones. However, current approaches are mainly heuristic. With our systematic approach, we can directly relate the information-theoretic fingerprint to learning and to performance on specific tasks. This enabled us to characterize how the collective dynamics (see II.) relates to performance and to derive the learning rules that enable optimal encoding of input systematically. This combined study of information theory, learning and performance in living and artificial networks promises to unravel the role of biological learning rules in shaping human information processing.

IV. Spreading and mitigation of COVID-19. With the outbreak of COVID-19, we were confronted with the challenge to contain a disease that was widely unknown. Identifying efficient strategies for disease containment was urgently needed. With our expertise on inferring spreading dynamics in the brain even under subsampling, we could quickly act and quantify the impact of non-pharmaceutical interventions on the reproduction number $R$ in Germany. We described a novel metastable regime at low case numbers, which we applied to designing general long-term control strategies without the necessity of recurrent restrictions. Extending these results, we have also tackled the problems of lifting restrictions as vaccination progresses and the challenging interplay between disease spread and information (especially when facing an infodemic). Hence, by applying our fundamental research to urgent questions of public health, and by communicating these results to the public and decision makers, this group contributed to the COVID-19 response strategies in Germany and Europe.

Dr. Johannes Zierenberg studied physics at the ETH Zürich (Switzerland) and Leipzig University, where he received his Master’s degree in 2011 and his PhD in 2016. During his PhD, he worked on equilibrium cluster formation in classical particle systems and polymer solutions, applying advanced Monte Carlo methods in generalized ensembles. In January 2017, he joined the Research Group Neural Systems Theory as a postdoc. His current research focuses on emergent collective dynamics in non-equilibrium systems covering neural networks and epidemic outbreaks.
Dr. Joao Pinheiro Neto studied physics at the State University of Campinas (Brazil), and received his PhD from the University of Göttingen in 2021. During his PhD, he worked on how sampling bias can impact our understanding of how neuronal activity spreads in the brain. His current research focus on understanding how the dynamics and topology of social networks impact opinion spreading in social media.

Sebastian Contreras studied engineering at Universidad de Chile (Chile), and received his Master’s degree in 2019. He joined the group in 2020 as a PhD student, working on disease spread and COVID-19. Using analytical and numerical tools from non-linear dynamics, he searches to uncover general principles in the dynamics of disease spread and its codependency with information (pandemic-infodemic interaction). With his work, he provided basic understanding of the pandemic, reflected in high-impact publications and communication to the general public.

Jonas Dehning studied Physics at the the University of Göttingen, where he received his Master’s degree in 2019. He joined the group of Viola Priesemann in 2015 for his Bachelor thesis to work on the inference of timescales of neural activity in macaque cortex. Currently, he is PhD student in IMPRS-PBCS doctoral program. His main research interest is to leverage the Bayesian inference methods to understand spreading dynamics, in both epidemiology and neuroscience.

Emil Nafis Iftekhar studied physics at the Friedrich-Alexander-University Erlangen-Nürnberg, receiving his Master’s degree in 2020. He did his Bachelor’s thesis at Osaka University (Japan) and his Master’s thesis at Utrecht University (The Netherlands). He started a PhD in the group in 2021, and his research focus is on the intersection between infectious disease modelling and the dynamics of opinions and behaviour. Besides his research, he engages in communicating scientific results to inform the public and politics.

Lucas Rudelt studied physics at the University of Göttingen, where he received his Master’s degree in 2018. He joined the group in 2014 for a Bachelor’s thesis and has continued his research here. In his Master’s thesis, he developed and applied a temporal embedding method for the estimation of memory in neural spiking activity. In 2019, he started his PhD in theoretical neuroscience, where he applies techniques of information theory and causal inference to understand distributed computation and biological plausible learning in neural networks.

F. Paul Spitzner studied physics at Leipzig University and received his Master’s degree in 2017. During the Master’s, he investigated equilibrium phase transitions in generalized ensembles using Monte Carlo simulations and finite-size scaling. After joining the Neural Systems Theory Group in 2018, he developed an open-source python toolbox, implementing the group’s MR-Estimator to infer intrinsic timescales from subsampled systems. In 2020, he started his PhD on modular neuronal systems. He supports the group with coding expertise, creating figures, and scientific writing.
4.5 MAX PLANCK RESEARCH GROUP: TURBULENCE, COMPLEX FLOWS & ACTIVE MATTER

From the fascinating self-organization of bacterial flows to large-scale flow patterns in the atmosphere – flowing matter gives rise to a wide range of intriguing phenomena. A common feature of these complex systems is the tight interplay of disorder, fluctuations and emergent order. The goal of our research is to gain a deeper understanding of open problems from the fields of turbulence, complex flows and active matter. Our research approach utilizes a broad spectrum of methods covering theory, simulations and, enabled through the collaborative environment at MPI DS, experiments.

Fully developed turbulence, one of our main fields of research, constitutes a paradigmatic problem of non-equilibrium statistical mechanics and, at the same time, plays a key role in many engineering applications ranging from mixing and combustion to wind energy conversion. From the viewpoint of fundamental research, we are witnessing an exciting era in which the latest experiments and state-of-the-art numerical simulations provide insights into turbulent flows at an unprecedented level of detail. In view of the recent rapid development of experimental and numerical techniques, the time is right to focus on novel theoretical concepts, which we develop in a simulation-assisted theoretical approach.

Our atmosphere and the oceans represent two prime examples where turbulence interacts with complex boundaries and additional physical phenomena. Such geometrically constrained settings give rise to entirely new dynamics, whose understanding is not only important from a fundamental point of view but also has significant implications, for example, for the field of renewable energies. The goal of our research in this area is to understand the interaction of turbulent fluctuations and large-scale dynamics in such settings. Examples for recent and ongoing work include the investigation of turbulence in the atmospheric boundary layer and in large wind farms. As part of the DFG Priority Program 1881 “Turbulent Superstructures” we are also investigating the interplay of turbulence and large-scale flows in turbulent convection and shear flows.

Particle-laden flows are another focus of our work. The particle-based, Lagrangian view of turbulence is particularly insightful as particles sample the complexity of turbulence in space and time. Furthermore, it is highly relevant e.g. for our understanding of clouds as well as the dispersion of microplastics or microorganisms in the oceans. Together with the Bodenschatz Department and collaborators from the Fraunhofer Institute for Physical Measurement Techniques (Freiburg) we are investigating cloud microphysics and atmospheric turbulence in a joint experimental, computational, and theoretical approach.

An exciting field of research that we are currently exploring is the interaction of active particles with hydrodynamic flows. Problems from this field combine aspects of the physics of fluids and active matter. Better understanding the complex distribution of motile plankton in
the oceans, for example, is one motivation for our work. In the complementary regime of high cell density, dense suspensions of motile cells constitute so-called active fluids, which exhibit a plethora of dynamical states, including meso-scale active turbulence and self-organized vortex crystals. Unraveling the origin of these phenomena is one goal of our research.

Since its founding time in early 2015, the group has expanded its scientific scope and has grown considerably. Triggered by the pandemic in 2020, we took a scientific detour and engaged in various collaborative efforts at MPI DS to model the spread of COVID-19.

The alumni of the group have been exceptionally successful in finding attractive positions ranging from application support in high performance computing to group leader and assistant professor positions. Besides central funding by the Max Planck Society, our work is supported by the DFG, the BMBF, the European Commission, and through computational grants at the LRZ Munich.

Naseem Ali, PhD is a postdoctoral researcher at MPI DS since 2020. He graduated from Anbar University (Iraq) with a degree in Mechanical Engineering. Afterward, Ali obtained two degrees in dynamic and thermal science from the University of Technology and Baghdad University. He moved to the United States and received his MSc and PhD in Mechanical Engineering from Portland State University in 2018. He spent one year of his PhD work at the University of Utah, where he developed new simulations for large wind farms under different thermal stratifications. Ali joined the Wind Energy and Turbulence Lab at the Portland State University 2019-2020 as a postdoctoral fellow. Ali’s research focuses on atmospheric flow, renewable energy, and flow control.

Dr. Maurizio Carbone studied aerospace engineering at Politecnico di Torino, from where he received his bachelor’s, master’s, and PhD with honors. For his master’s thesis, he spent a period at Los Alamos National Laboratory in 2016. In the same year, he started his PhD under Prof. Michele Iovieno, studying the dynamics of inertial particles and velocity gradients in turbulence. Within his PhD, he spent an extended period in the Theoretical and Computational Fluid Dynamics group of Dr. Andrew Bragg at Duke University. He defended his PhD thesis in May 2020. Since April 2020, he is working in the group of Dr. Michael Wilczek as a postdoctoral researcher. His interests include turbulence theory and high-performance computing for fluid dynamics.

Dr. Cristian C. Lalescu studied physics at the University of Craiova (UCv), from which he received his diploma in 2006. Between 2007 and 2011 he completed a joint doctorate program, under the supervision of Prof. Daniele Carati from the Free University of Brussels and Prof. Bucur D. Grecu from UCv, working mostly in Brussels. He was then a postdoctoral fellow with Prof. Gregory L. Eyink at the Johns Hopkins University in Baltimore, USA, mainly within the multidisciplinary Turbulence Database Group. In 2015 he joined the Wilczek group as its supercomputing expert and main developer of turbulence simulations, but also working on turbulence theory. Since December 2019 he is an associated member of the team, providing computational support from his current position within the Application Support Group of the Max Planck Computing and Data Facility.
In contrast to most man-made machines, biological organisms are largely built from soft and fluid-like material. How is this matter controlled to fulfill precise functions? To uncover the physical principles for the spatio-temporal organization of biological fluids, we analyze theoretical models of biological processes using tools from statistical physics, dynamical system theory, fluid dynamics, and information theory. For instance, we study how liquid droplets structure the interior of biological cells and how the transport of inhaled odor molecules influences the sense of smell.

The interior of biological cells consists of thousands of different kinds of proteins that all undergo chemical reactions to fulfill their function. The resulting large chemical reaction network is controlled by spatially segregating the constituents into organelles. Typical large organelles, like the nucleus and the mitochondria, are enclosed in a membrane, but there also exist numerous smaller organelles without membranes. These membrane-less organelles form spontaneously via phase separation, much like oil droplets form in water, and are now known as biomolecular condensates. However, in contrast to oil in water, these condensates exist in the complex, non-equilibrium environment of the biological cell, where fuel molecules like ATP are constantly consumed to drive chemical reactions. Moreover, the condensates themselves and their surrounding exhibit elastic properties caused by the macro-molecular composition. Finally, cells are heterogeneous and change their behavior over time, e.g., as a function of the cell cycle. A main focus in the group is to understand the influence of the complex environment on condensates. In particular, we want to unveil physical mechanisms that allow cells to control condensates. Along these lines, we have already shown that driven chemical reactions can be used to control droplet positions, sizes, and counts. We also already investigated how droplets grow inside elastic gels in synthetic systems and are now in the process of applying this knowledge to biological cells. To do this, we extend the physical frameworks that are typically used for describing phase separation to accommodate the complexity of cells and we also develop new numerical methods that are suited for describing the multi-scale dynamics. Taken together, we generally study phase separation in complex environments to better understand the organization of biological cells and also learn about fundamentally new approaches for engineering soft materials.

Our group also studies the sense of smell and the associated airflow of breathing as another example for how physical processes affect biological functions that involve fluids. Using fluid dynamics, information theory, and statistical physics, we study how molecular mixtures are encoded in neural signals by olfactory receptors, so the brain can infer the odor outside the nose. Here, we put particular focus on the influence of physical processes, like advection of odorants with the airflow and their adsorption in the nasal mucus, to understand how they affect
the sensing and how the nasal cavity might have adapted to provide optimal encoding. We aim at unraveling this mystery by using both simple physical models as well as detailed numerical simulations of the airflow in the nasal cavity.

In summary, a central aim of our group is to develop insight into biological processes using theoretical modeling. Here, we relish collaborations with experimentalists and theorists both locally at our institute as well as globally.

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**Dr. Estefania Vidal** studied physics at Universidad de Chile where she received her Bachelors and Masters degrees. She obtained her Ph.D. in Physics at the Max Planck Institute for Dynamics and Self-Organisation in 2019 where she worked on pattern formation in the amoeba D. discoideum. She then joined the MPRG Theory of Biological Fluids to study the interplay of elasticity and phase separation and how elastic networks can be used to control droplet dynamics.

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**Dr. Swati Sen** is a theoretical physicist interested in biophysics and soft matter physics. She received her bachelors from the University of Calcutta in 2010 and a masters from IIT Delhi 2012. In her PhD in soft matter physics at IISER Kolkata (2012-2019), she worked on the swelling kinetics of polyelectrolyte gels, and developed a new numerical scheme to estimate bulk modulus of gels in salt-free solvent. In 2019, she started her first postdoc position at the National University of Singapore under the supervision of Prof. Jacques Prost, where she explored nucleation and growth of lumens in living organs. In 2020, she joined MPI DS to work on the physics of olfaction. Her research now focuses on understanding the underlying principles of efficient odor detection.

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**Dr. Lucas Menou** obtained his Ph.D. in fundamental physics from the ENS de Lyon in October 2020. He is mainly interested in soft matter physics and biophysics. At the time, his work focused on the elasticity of viruses. In November 2020 he joined the group Theory of biological fluids at MPI DS. Here, he studies phase separating and non-ideal pattern formation processes beyond the Turing model. In a more general view point, he is fascinated by the way nature finds solutions to handle and organize life itself.

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**Dr. Johannes Krausser** studied physics at Ludwig-Maximilians-Universität München completing his Master’s degree in 2013 and received his PhD from the University of Cambridge in 2017. Afterwards he worked as a postdoctoral researcher at University College London focussing on coarse-grained computational modelling of the interplay between protein aggregation and cell membrane dynamics. In 2021 he joined the Research Group Theory of Biological Fluids to study the viscoelasticity of liquid-liquid phase separated droplets and the link between material properties of condensates and their potential functional implications in the cellular context.
Biological networks perform their functions as complex dynamical systems. Be it ecosystems, networks of neurons, or the paths of information and matter inside cells, their intricate design emerges through the interplay of systems-level self-organization and long-term evolutionary remodeling. The active dynamics of biological networks and the unique sense of efficiency and beauty it elicits make these systems profoundly fascinating and scientifically challenging. Currently, transformative progress is opening unprecedented research opportunities to analyze collective phenomena in biological networks and decipher the evolutionary design principles shaping them. It is the mission of the Göttingen Campus Institute for Dynamics of Biological Networks to advance theory-driven research into the dynamics of biological networks, pioneer novel research strategies integrating computational, mathematical and experimental approaches, and establish them through transdisciplinary research projects on the Göttingen Campus and beyond.

The Göttingen Campus Institute for Dynamics of Biological Networks (CIDBN) was established by the Max Planck Institute for Dynamics and Self-Organization and the University of Göttingen. The CIDBN has three departments spanning physics and biology and two central research platforms: a life science HPC unit and the Laboratory Neurophysics. To foster frontier research by young investigators, the CIDBN is designed to host up to four young investigator groups. Currently, the Max Planck Research Groups of Armita Nourmohammad and David Zwicker are associated with the CIDBN. CIDBN research contributes to three Göttingen CRCs, the Cluster of Excellence Multiscale Bioimaging and the new cognitive science research center HuCaB. Nationally, the CIDBN is the coordination site of the DFG priority program Evolutionary Optimization of Neuronal Processing. Internationally, it is the German theory hub of the transnational research network on the evolution of the primate brain, NeuroNex, funded jointly by the National Science Foundation (USA), the Canadian Institutes of Health Research and the DFG.

The frontier between complex system dynamics and evolution is a major focus of current projects at the Göttingen Campus Institute for Dynamics of Biological Networks. Emergent phenomena and system dynamics play an important role in biological evolution, in particular for complex biological networks such as those in brains, immune systems or eukaryotic cells. Understanding the role of dynamics and self-organization in complex system evolution is an emerging field at the interface of physics, biology and biotechnology. Here, our research topics range from the origins of collective computation in brain evolution, the evolutionary optimization of the biophysics of information processing and flow, to coevolution in immune systems and to the emergence of compartmentalization through phase separation in eukaryotic cells and at the origin of life.
Dr. Andreas Neef obtained his Diploma in physics in 2000 from the University of Jena, Germany. After work at the MRC Laboratory of Molecular Biology, Cambridge (UK), he joined the Research Centre Jülich, Germany, where he received his doctorate in 2004 (Cologne University). After postdoctoral research he became a Bernstein Fellow at the MPI for Dynamics and Self-Organization in 2006. From 2013 to 2019 he headed the research group Biophysics of Neuronal Computation at the Bernstein Center for Computational Neuroscience. In 2019 he became Head of the Laboratory Neurophysics at the Göttingen Campus Institute for Dynamics of Biological Networks.

Dr. Khanh P. Nguyen studied physics and mathematics at the University of Houston, Texas, USA, where she obtained her bachelor’s degrees in 2015. She was awarded the National Science Fellowship and continued her education at the University of Houston with a PhD dissertation on sequential decision-making models, obtaining her PhD in 2020. In the same year, she moved to Göttingen as a postdoc working with the DPZ Cognitive Neuroscience Lab and the Göttingen Campus Institute for Dynamics of Biological Networks. She currently works on a theory for continuous decision-making.

Dr. Matthias Häring studied physics and mathematics at the TU Braunschweig and the University of Göttingen where he obtained his M.Sc. in physics in 2016. After work at the MPI for Biophysical Chemistry, he joined the lab of Fred Wolf at the MPI for Dynamics and Self-Organization for his PhD from 2017-2021 on tissue morphogenesis, studying active dynamics and intercellular coordination in developing epithelia. Since 2021 he is a postdoc at the Göttingen Campus Institute for Dynamics of Biological Networks with research focus on data analysis, stochastic dynamics and non-equilibrium statistical physics.

Dr. Bernhard Bandow obtained his diploma in physics at the TU Berlin working on MD simulations of systems with confined geometry. In 2007 he received his PhD in physical chemistry from Kiel University for work on global geometry optimization of water clusters employing genetic algorithms. After postdoctoral research at the German Institute for Rubber Technology in Hanover, he joined the Computing Center and the North German Supercomputing Alliance (HLRN) at the Leibniz University Hannover. From 2011 to 2019 he worked at the computing center of the MPI for Solar System Research in Göttingen. In 2019 he joined the Göttingen Campus Institute for Dynamics of Biological Networks as HPC Coordinator and the group eScience of the Göttingen Computing Center GWDG.

Dr. Yvonne Reimann studied biology at the University of Göttingen and obtained her PhD with work at the MPI for Biophysical Chemistry in Göttingen. After postdoctoral research in the Department Molecular Cell Biology at the MPI for Biophysical Chemistry, she studied science management at the German University of Administrative Sciences (Speyer) from 2009 to 2010 and subsequently became scientific coordinator at the Leibniz Research Laboratories of Hannover Medical School and the Research Department of Göttingen University. Since 2012, she is Research Manager of the BCCN Göttingen and since 2018 of the Göttingen Campus Institute for Dynamics of Biological Networks.
ASSOCIATED RESEARCH GROUPS

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For many years the chemical complexity as well as the dynamics and function of biological membranes have fascinated scientists. My group aims at generating robust and stable planar multifunctional membranes in a bottom-up approach that mimic the natural situation as closely as possible to address pressing biochemical questions and to design chip-based assays.

More than 40 years ago, biological membranes were described for the first time as a fluid mosaic based on thermodynamic principles of organization of membrane lipids and proteins and available evidence of asymmetry and lateral mobility within the membrane matrix. Over the intervening years, there is mounting evidence that the chemical and spatial complexity of biological membranes is key to understand their dynamics and functions on various length scales. It is the heterogeneity of cellular membranes that can lead to specialized functional membrane domains, enriched in certain lipids and proteins, and the interaction between lipids and proteins that limits the lateral diffusion and range of motion of membrane components thus altering their function. To be able to understand the complex interplay within a membrane on a molecular level, my research group pursues a bottom-up approach. By developing and applying model membrane systems, we aim to understand membrane-confined processes such as fusion and fission, transport processes mediated by ion channels and protein pumps as well as protein-lipid and protein-protein interactions occurring at the membrane interface. On the one hand, we use planar supported lipid bilayers (PSLBs) and vesicles, such as giant unilamellar vesicles (GUVs). On the other hand, we have developed functional lipid bilayers on highly ordered pore arrays. These so-called pore-spanning membranes (PSMs) suspend nanometer- to micrometer-sized pores in an aluminum or silicon substrate (Figure 5.1). They separate two aqueous compartments and can hence be envisioned as an intermediate between supported and freestanding membranes.

**PSLBs and GUVs: Protein-membrane and protein-protein interactions**

Several proteins use specific lipid receptors to attach to the plasma membrane. We are interested in the molecular interaction between these membrane-confined receptors and proteins and how this interaction influences the overall membrane structure. In this context, we focus on phosphatidylinositol phosphate binding proteins such as ezrin and the focal adhesion kinase harboring a FERM-domain as well as collybistin binding via a PH-domain. Another major target are glycosphingolipids such as Gb₃, which serve as specific receptors for bacterial toxins such as Shiga toxin.

Ezrin links the plasma membrane to the cytoskeleton in its active state. It gets activated by binding to PtdIns(4,5)P₂ in the plasma membrane and phosphorylation of a threonine. We investigated the mode of ezrin binding and its activation by using PSLBs in combination with
surface sensitive techniques such as reflectometric interference spectroscopy, and fluorescence and atomic force microscopy. We further analyzed the coupling of actin and actomyosin networks via ezrin to these membranes thus generating a minimal actin cortex. With such a system in hand, we are able to address the question how the ezrin-PtdIns(4,5)P₂ interaction influences the architecture of actin and actomyosin networks and how this impacts the dynamics, and mechanical properties of the composite system.

Collybistin is an adaptor protein that is involved, together with the scaffold protein gephyrin, in the recruitment of GABA_A receptors to the postsynaptic density of inhibitory synapses. Our in vitro studies showed that full-length collybistin gets activated via an interaction with the C-terminal part of neuroligin-2 being prerequisite for binding of the PH-domain of collybistin to different phosphatidylinositol phosphates. To completely assemble the structures found at the postsynaptic membranes of inhibitory synapses, the question needs to be addressed how gephyrin, collybistin and neuroligin-2 act in concert, a process that can be further illuminated by using PSLBs in combination with reflectometric interference spectroscopy and high-resolution microscopy techniques.

In collaboration with the group of Prof. Dr. Daniel B. Werz (TU Braunschweig), we investigate the influence of the fatty acid of the globoside Gb₃ on the partitioning in liquid-ordered/liquid disordered coexisting membranes, which is key to understand the primary step of Shiga toxin internalization. Shiga toxin, produced by Shigella dysenteriae and Shiga toxin producing E. coli strains gets internalized into the cell after binding of the B-subunits to Gb₃ embedded in the plasma membrane of the host. We have shown that the molecular structure of Gb₃ greatly influences its membrane partition, as well as membrane (re)organisation after toxin binding.

**PSMs: Membrane fusion and transport proteins**

Membrane fusion processes, mediated by SNAREs, are a hallmark of eukaryotic life. We are especially interested in membrane fusion during neuronal exocytosis. A number of in vitro fusion assays with these proteins reconstituted in artificial membranes have been established in recent years. However, it has still been proven difficult to monitor intermediate states of the fusion process in a system that captures the essential features of the in vivo system. We develop and apply a reconstituted membrane system based on PSMs. PSMs are long-term stable and can be formed on open pore arrays as well as on cavities. These setups allow for a quantitative analysis of the different stages during fusion of a single vesicle, such as docking, intermediate states and full fusion by means of fluorescence microscopy in a time-resolved manner (Figure 5.2).

As PSMs are produced from spreading GUVs, they should also enable us to reconstitute ion channels and protein pumps with an appropriately high protein density. This is particularly important for ion channels and protein pumps that do not transport sufficient ions to

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**Figure 5.1:** Individual steps to prepare pore-spanning membranes (PSMs) on a Si/Si₃N₄ substrate by spreading a giant unilamellar vesicle (GUV) on a 6-mercaptopentanol (6-MH) self-assembled monolayer (SAM).
be detected by electrophysiological recordings on single freestanding membranes. However, classical methods to produce GUVs such as electroformation and gentle hydration do not allow for a reproducible reconstitution of transmembrane proteins in GUVs with high protein content. Thus, we search for and establish alternative methods to generate GUVs based on droplets produced in microfluidic devices. Recently, we have shown that these GUVs produced from droplet-stabilized GUVs can also be spread on porous substrates to generate PSMs. With respect to proteins, we currently focus our attention on the F₀F₁ ATP-synthase that is capable of producing ATP by using a proton gradient and which can be reversed as well as connexons that can even connect two membranes by the formation of gap junctions.
5.2 MAX PLANCK FELLOW GROUP: DATA-DRIVEN MODELING OF NATURAL DYNAMICS

The mission of the Max Planck Fellow group “Data-Driven Modeling of Natural Dynamics” is to expand machine learning in order to empower the modeling, optimization and control of complex dynamical systems in physics and biology. Machine learning (ML) has recently triggered a revolution in the fields of computer vision or natural language processing. ML has achieved remarkable progress towards solving problems previously considered exceedingly hard or even impossible with current technologies. Famous examples are playing Chess or Go. Over the coming decade, machine learning techniques are expected to transform the process of scientific discovery in the quantitative natural sciences. Our goal is to contribute at the forefront of this transformation by establishing new machine learning approaches tailored to address some of the most challenging problems in complex system research: the dynamics of clouds and atmospheric turbulence, the modeling and control of the dynamics of the heart and understanding the design and dynamics of deep neural networks in the brain.

5.2.1 Modeling of cloud microphysics and turbulence

We have recently started a collaboration with the Department of Fluid Physics, Pattern Formation, and Biocomplexity (Eberhard Bodenschatz) focusing on modeling atmospheric turbulence (Bodenschatz et al., 2010). We are exploring ways to enable 3d image reconstruction from holographic measurements in cases where existing numerical methods fail. Eberhard Bodenschatz is conducting in situ measurements in clouds. One of the instruments uses inline holography originally pioneered at the Max Planck Institute for Chemistry. In inline holography the diffraction pattern of a coherent monochromatic light beam is captured with a high-speed high-resolution video camera (in the Max Planck CloudKite project of the Bodenschatz group 25MPixel at 75hz). Based on the knowledge of the beam and a scattering model, the inverse problem needs to be calculated.

In the just completed measurement campaign EUREC4A in the trade wind region of the Atlantic, 800,000 holograms of cloud particles were taken. We expect that 200,000 contain interesting data. The analysis with the current software takes 4 core hours per hologram. Analyzing 200,000 hologram therefore requires the use of a high-performance computer (we have a 4096 core gpu cluster). Our plan is to cut this time down very significantly with appropriate deep learning algorithms. Not only will this new method be utmost useful in cloud microphysics measurements, but similarly important for methods of inline holographic microscopy.

5.2.2 Data-driven modeling cardiac dynamics

The Biomedical Physics group (Stefan Luther) and the Cardiac Dynamics Group (Eberhard Bodenschatz) perform physical modeling of
cardiac dynamics. In addition, the Luther group performs cutting edge cardiac imaging (Luther et al., 2011; Christoph et al., 2018). We plan to develop machine-learning-based predictive models of electrical turbulence in the heart during cardiac fibrillation. Modeling cardiac fibrillation is challenging, among other reasons, because every heart is different and it is constantly in motion when observing it “in action.”

We plan to build upon recent progress in self-supervised learning to learn high-level representations of both the pulsating dynamics and those of the electrical turbulence directly from imaging data without requiring sophisticated image processing to register the observations into a common frame of reference. Combining such self-supervised feature learning with transfer learning we may be able to learn an end-to-end model of low-energy stimulation. Such a differential end-to-end model allows novel ways of predicting interventions (Walker et al., 2019), which may ultimately allow us to predict therapeutic interventions such as low-energy anti-fibrillation pacing (Luther et al., 2011).

5.2.3 Self-organization and design of deep networks for vision

Figure 5.4: Neurons in primary visual cortex of the mouse.

The brain is a dynamical system operating at multiple spatial and temporal scales. We hypothesize that understanding the dynamics of information processing in local cortical circuits (Ecker et al., 2010) requires understanding their contribution to behavioral performance of the entire system. We focus on area V1 – an early stage of visual information processing and the largest cortical area in the primate brain – and study its circuitry and architecture in the context of the ventral visual stream, the multistage hierarchy that supports object recognition.

Here, deep learning has enabled exciting avenues for research. Firstly, we can capitalize on recent advances in computer vision: high-performing deep neural networks trained on object recognition provide us with working models of ventral visual stream processing. Secondly, it is now for the first time feasible to obtain data-driven models of neural function (Klindt et al., 2017; Cadena et al., 2019) that accurately represent processing at many levels of the ventral stream hierarchy.

Work at the Max Planck Institute for Dynamics and Self-Organization has predicted and uncovered universal quantitative architectural principles of primate V1 architecture and pioneered their evolutionary origins (Kaschube et al., 2010). However, it remains enigmatic what advantages these principles confer on the performance of the visual system. We plan to investigate together with the Neural Systems Theory group (Viola Priesemann) and the Theoretical Neurophysics group (Fred Wolf) at MPI DS (a) whether the same quantitative laws emerge in artificial neural networks trained to optimally perform object recognition and (b) whether obeying these quantitative principles enhances the robustness or efficiency of artificial neural networks. Thus, performance-optimized models will allow us to bridge the gap between mathematical theories of neural self-organization and the behavioral goal of the system and reveal their contribution to efficient and flexible neural processing.
5.2.4 Expected outcomes

Expanding the scope of machine learning approaches to enable data-driven and performance-optimized models of complex physical and biological systems is a major frontier of conceptual innovation in the natural sciences. Joint work with colleagues at the MPI DS on cutting-edge problems of dynamics and self-organization in physics and biology will enable us to pioneer applications ranging from fundamental problems in atmospheric and climate dynamics to translational applications such as predicting low-energy anti-fibrillation patterns. If we are successful, our joint work will achieve end-to-end prediction of the state and the dynamics of complex physical and biological systems directly from experimental data such as images, holograms or time series, obviating the need to first extract physical quantities of interest and then running costly forward simulations, and providing us with a novel avenue to generating precise phenomenological models of the collective behavior of the entire system.

5.2.5 Literature


5.3 EXTERNAL SCIENTIFIC MEMBER: BIOMEDICAL NMR

Our research is devoted to the further development and application of magnetic resonance imaging (MRI) techniques for structural and dynamic studies of biological and complex systems. Current projects focus on advanced methods that monitor human body movements and physiological functions in real time and allow for quantitative mapping of tissue parameters using model-based reconstructions. A primary aim of our Emeritus group is the translation of real-time MRI technology for scientific and medical applications.

Methodological Aspects

Our breakthrough toward real-time MRI is based on spatial encoding strategies using radial trajectories, pronounced data undersampling by factors of 20 to 40, and definition of serial image reconstruction as iterative solution to a nonlinear inverse problem with temporal regularization. In practical terms, real-time MRI allows for recordings of the functional anatomy at high spatiotemporal resolution, i.e. with image acquisition times as short as 10 to 50 milliseconds – corresponding to MRI videos at 20 to 100 frames per second.

Model-based reconstruction techniques are an extension of the basic reconstruction problem posed by undersampled multi-coil MRI data. It supports quantitative mapping of physical or physiological parameters by directly estimating the parameters of a known signal model from a suitable set of raw data. Thus, instead of computing a set of images which are then used for a pixel-wise fitting of the signal model, the parametric maps are obtained directly without intermediate image reconstruction. The procedure exploits redundancy in the raw data and – depending on the application – leads to much improved maps (e.g., almost noiseless velocity maps in phase-contrast flow MRI) or provides simultaneous access to maps from different sections (e.g., multiple maps of the T1 relaxation time).

In all cases, the computational demand is met by parallelization of the corresponding algorithm and its implementation on a computer equipped with multiple graphical processing units. This computer can be fully integrated into a commercial MRI system (by a Gigabit network connection) where it serves as a by-pass system invisible to the radiological user.

Current Work

Real-time MRI applications address a broad range of hitherto impossible scientific and clinical questions. Current collaborative studies include joint movements (wrist, temporomandibular joint), phonetic aspects of articulation (speech production, singing, whistling, stuttering), brass and oboe playing (pedagogy, dystonia), swallowing dynamics (normal physiology, dysphagia, gastroesophageal reflux disorder), cardiac function without the need for synchronization to the electrocardiogram and during free breathing, quantitative assessment of blood flow...
(aorta, carotid artery, inferior vena cava, peripheral veins), cerebrospinal fluid dynamics (normal physiology, hydrocephalus, flow disturbances), and quantitative mapping of T1 relaxation times (brain, heart, spinal cord, prostate).

![Figure 5.5: Quantitative assessment of aortic blood flow using real-time phase-contrast flow MRI. (Left) Conventional phase-difference calculation of the velocity map (28 frames per second) in comparison to (right) a model-based reconstruction with an almost noiseless floor and improved spatiotemporal resolution (40 frames per second). The selected frames refer to maximum blood flow in the ascending aorta (bright circle) and descending aorta (dark circle, opposite direction). The strength of the phase signal directly corresponds to flow velocity.](image)

Ongoing methodological work deals with extensions of the basic physical and mathematical concept underlying real-time MRI and model-based reconstructions. Examples range from velocity mapping in multiple flow directions to the separation of water and fat contributions in anatomic real-time MRI videos or dynamic mapping of the T2* relaxation time. Moreover, we recently invented a new approach for motion-robust scanning of a large volume (e.g., a whole organ) in only a few seconds. The method relies on the fact that the similarity of successive frames within a real-time image series holds true not only in time but also in space. In other words, temporal regularization of the nonlinear inverse problem is replaced by spatial regularization provided serial images represent neighboring cross-sections with sufficient overlap. In practice, similarity is ensured by cross-sectional real-time acquisitions which automatically advance the position of each frame by a fraction of the section thickness. For example, coverage of a 180 mm volume by 6 mm thick images and 1.5 mm section shift is accomplished within a total measuring time of only 6 s yielding 120 overlapping frames and a speed of 30 mm per second. Most importantly, acquisition times of tens of milliseconds per frame render individual sections robust against any patient or organ movement.

Finally, related developments exploit nonlinear inverse reconstructions with spatial regularization for other techniques such as diffusion-weighted imaging which is of high clinical relevance in a variety of disorders (e.g., stroke and tumors). In particular, reconstructions from undersampled radial encodings markedly improve diffusion-weighted single-shot stimulated echo imaging. In contrast to diffusion-weighted
Figure 5.6: (Top left to bottom right) Selected fat-suppressed T1-weighted images (every 20th) of a 6 s real-time MRI dataset covering the entire liver (180 mm volume) of a healthy subject (free breathing) by serial cross-sectional imaging (i.e., 120 frames) at 50 ms resolution (i.e., acquisition time per frame).

Echo-planar imaging, the resulting images are insensitive to magnetic field inhomogeneities. Pertinent applications therefore avoid geometric distortions and areas of signal void that commonly hamper clinical diagnostics.
5.4 EXTERNAL SCIENTIFIC MEMBER: PHYSICS OF FLUIDS

Scientific profile and characteristics of work

Lohse’s Physics of Fluids (PoF) group presently works on a variety of aspects in the fundamentals of fluid mechanics. The subjects include turbulence and multiphase flow and micro- and nanofluidics. Both experimental, theoretical, and numerical methods are used. He closely collaborates with several companies, among them Canon and ASML. Further information, including an updated list of publications, is available under http://pof.tnw.utwente.nl/.

The main characteristics of Lohse’s work is the direct interaction of experiment, theory, and numerics, all done in the PoF group. He is not method-driven, but problem-driven, and often had to acquire the required methods or knowledge from some neighboring fields to solve some particular research questions he had been obsessed with. This led to various fruitful interactions and collaborations with neighboring disciplines, such as engineering, mathematics, chemistry, acoustics, medicine, biology, or even computer science. As will be seen from the list below, various of his subjects have an “application perspective”. Lohse and his coworkers also understand to visually present the scientific questions they are addressing and their results. This led to ten winning video entries to the Gallery of Fluid Motion from the American Physical Society, Division of Fluid Dynamics, and various television reports and newspaper articles on their work. It also makes Lohse’s science very visual for laymen, with a positive effect on the outreach of science in general.

Overview on present main research subjects

Turbulence

Rayleigh-Bénard (RB) flow, the flow in a box heated from below and cooled from above, and Taylor-Couette (TC) flow, the flow between two coaxial, independently rotating cylinders, are the two paradigmatic systems of physics of fluids. They are the drosophilas of the field and various new concepts in fluid dynamics have been tested with these systems. In the last few years, in joint work between Göttingen and Twente, we succeeded to realise the transition from the so-called classical turbulence to the so-called ultimate turbulence for RB turbulence and TC turbulence, thanks to the Göttingen U-Boot facility and the Twente turbulent TC facility (T³C), with which we can achieve and precisely measure an unprecedented degree of turbulence. In the ultimate state, not only the bulk of the flow is turbulent, but also the boundary layers, which for weaker driving (in the classical regime) is mainly of laminar type. The transition from one regime to the other is so important because it dramatically changes the heat or momentum transfer properties of the system. E.g., if one used the heat transfer scaling laws of the classical regime for heat transfer estimates for large temperature differences as they occur in geophysical and astrophysical situations, one would easily be off by a factor of 10 and more! So it is...
crucial to understand the nature of the transition and the properties of the ultimate state of turbulence.

We also perform highly parallelized (10^5 cores) direct numerical simulations (DNS) on both TC and RB flow, and also on double diffusion convection and other related systems, also focusing on the understanding of the flow. These include vertical convection, horizontal convection, and penetrative convection, where the maximal density is achieved at a temperature in between that of the top and bottom plate, see Figure 5.7.

**Multiphase flow with and without phase transitions and aerosols**

The largest setup in the PoF lab is a 8m high turbulent water channel in which bubbly turbulence or turbulence with particles is studied, accompanied by numerical work. We developed new experimental and numerical techniques to follow thousands of bubbles and particles both in time and in three-dimensional space, allowing for a better understanding of the turbulent multiphase flow organization and the dynamics of particle and bubble clusters in these flows. We have also applied the numerical methods developed in this context to respiratory droplets in a turbulent vapor puff and to better understand ventilation techniques. We also shed light on the mechanism of drag reduction.

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**Figure 5.7:** Instantaneous temperature fields in penetrative convection for different density inversion parameters \( \theta_m \equiv (T_m - T_l)/(T_b - T_l) \), where \( T_{ij} \) are the temperatures of the top and bottom plate, and \( T_m \) is the temperature at which the liquid density is maximal (around 4°C for water). (a–c) 2D DNS for \( Ra = 10^{10} \) and \( \Gamma = 2 \) and (d–f) 3D DNS for \( Ra = 10^7 \) and \( \Gamma = 4 \): (a) \( \theta_m = 0.5 \), (b) \( \theta_m = 0.9 \), (c) \( \theta_m = 0.965 \), (d) \( \theta_m = 0.3 \), (e) \( \theta_m = 0.7 \), and (f) \( \theta_m = 0.87 \). One see how with increasing \( \theta_m \) the turbulent domains becomes smaller and smaller. Figure taken from Wang, Reiter, Lohse, and Shishkina, Phys. Rev. Fluids 6, 063502 (2021).

**Figure 5.8:** Snapshot of the droplet-laden cough simulation, (a) contour of the relative humidity field, and (b) droplet trajectories at time \( t = 400 \) ms. Trajectories of three different diameters are shown: 10µm (blue), 100µm (green), and 1000µm (red), respectively. Larger droplets are observed to fall out from the puff whereas smaller droplets remain protected and are carried along by the puff. For clarity, only a subset of the total number of droplets are shown. Figure taken from K. L. Chong et al., Phys. Rev. Lett. 126, 034502 (2021).
in multiphase turbulent flows, identifying the bubble or droplet deformability as a crucial condition for this phenomenon. Finally, we illuminated the mechanism at play in the nucleation and dynamics of so-called plasmonic vapor bubbles, showing that in fact their gas content is essential.

**Inkjet printing and droplet impact**

On this subject the PoF group very closely collaborates with Canon. We developed experimental methods and models to understand droplet formation and impact of various droplets (including non-Newtonian ones and multicomponent ones) on various substrates (including superheated & supercooled ones), focusing on heat exchange, splash formation, droplet spreading, and solidification.

![Figure 5.9: Liquid droplet formation in piezoacoustic inkjet printing generation visualized by an ultra-high-speed stroboscopic technique. Figure taken from D. Lohse, Annu. Rev. Fluid Mech. 54, 349 (2022).](image)

**Wetting phenomena and droplet evaporation, and the physicochemical hydrodynamics of multicomponent droplets**

We work on wetting phenomena on smooth, chemically, or geometrically structured surfaces and in particular on surface nanodroplets and nanodroplets, whose counterintuitive stability we could account for.

We try to better understand the nucleation and growth or the dissolution of nanobubbles and nanodroplets, either in another liquid or in a gas (then called condensation/evaporation). We also revealed the rich and often counterintuitive fluid dynamics of the evaporation process of binary, ternary, and colloidal droplets, including the crucial role of the so-called ouzo-effect. We firmly believe that major progress can be achieved at the interface between surface chemistry and fluid dynamics, by combining the methods from these two fields, both on the experimental, numerical, and theoretical side. This also holds for catalysis and electrolysis, where emerging nano- and microbubbles at the surface often cause a major problem.
5.5 EXTERNAL SCIENTIFIC MEMBER: TURBULENT FLUIDS AND BIOPHYSICS

Our research is devoted to various problems in nonlinear and statistical physics. Hydrodynamic turbulence provides a major source of inspiration, from fundamental questions to specific applications to various domains, in particular to geophysics. We also investigate nonlinear problems to describe the dynamics of biophysical systems. Although theoretical and numerical by nature, our work is largely inspired by experimental situations. In particular, we are working in close collaborations with experimental teams, at the MPI DS and elsewhere.

Regrettably, one of the side effects of the pandemic was to restrict the possibilities of visiting, which effectively limited the exchanges.

Small-scale in turbulent flows

The existence of motion at very small scales in very turbulent flows (at very large Reynolds numbers) is one of the main focus of our activity. Understanding the mechanisms of generation of such small scales, and providing a reliable statistical properties of the flow is the fundamental question we are studying. The study of a dynamics occurring over very small spatial scales, and very short time scales, is intrinsically challenging from an experimental and numerical point of view. This difficulty is tackled in particular by the experimental group at MPI DS. From a theoretical point of view, the analysis of the Navier-Stokes equations is hindered by the presence of nonlinear and nonlocal effects. As an outstanding difficulty, whether the amplification of velocity gradients, known to occur in a turbulent flow, can lead to the formation of infinite gradients remains an open question.

In this context, we have particularly studied the role of the nonlocality in the Navier-Stokes equation in the amplification of vorticity (the local rotation rate in the flow). Simulations of turbulent flows at a very large resolution, and at Reynolds numbers comparable to the highest values reachable in well-controlled experimental conditions, allowed us to identify a mechanism of nonlinear attenuation, which effectively provides an upper bound on the amplification of the most intense vortex structures, see Fig. 5.10 (joint work with D. Buaria and E. Bodenschatz). This suggests that the velocity gradients in turbulent flows occurring in most conditions are unlikely to become infinite. This may help in addressing the unsolved problem of establishing the regularity of solutions of the Navier-Stokes equations, a problem listed as one of the major mathematical challenges by the Clay foundation. Current studies are focusing on the role of pressure, which is known to be the main source of nonlocality in the flow.

In a different, but complementary spirit, we have studied the conceptually simple problem of interaction between vortex rings, or more generally, between vortex tubes, see Fig. 5.11. Such an interaction leads to instabilities of the interacting tubes. We have provided strong evidence that this interaction may occur through a cascade mechanism, leading from one iteration to the next, to even finer scales, following
Figure 5.10: Left: Region of intense vorticity, $\omega$ (cyan) in the flow. Right: the contribution to the production of vorticity from the local contribution of strain, $S^L$: $\Phi^L \equiv \omega \cdot S^L \cdot \omega$. The local strain, $S^L(x)$, is obtained by expressing the strain, $S_{ij} = 1/2(\partial_i u_j + \partial_j u_i)$, where $u_i$ are the components of velocity, as a Biot-Savart integral over the vorticity field, and keeping only the contribution from a ball of small radius around the point $x$. In the regions where vorticity is the most intense, $\Phi^L$ is negative, implying that the local strain actually reduces the growth of vorticity. The size of the box is $50\eta$, where $\eta$ is the Kolmogorov length in the flow. The simulation of the flow involved $(8192)^3$ grid points, at a Reynolds number of $Re_\lambda = 650$.

a mechanism predicted theoretically earlier (with M. Brenner). This cascade process can be followed for several iterations in a laboratory experiment (R. McKeown and S. Rubinstein), and also numerically (R. Ostilla-Monico). Furthermore, the numerical results clearly indicate that at the end of the cascade, the flow becomes turbulent, with a classical Kolmogorov spectrum. Whereas the existence of a cascade is often postulated in the context of turbulence, our results clearly establish the role of a cascade process in a flow at high-Reynolds numbers, ultimately leading to turbulence.

Figure 5.11: Destabilization of a pair of interacting vortex tubes. Iso-surfaces of the vorticity field, $\omega$, are shown at two different times. As the tubes are coming together, at $t = 16$ (left panel), the cores are only slightly distorted. Later, at $t = 25.5$ (right panel), the instability of the cores have led to a destruction of the cores, via a very fast break-up process. This ultimately leads to turbulence.

Further theoretical efforts on turbulence have been devoted to the analysis of the motion of several points, forming a tetrahedron. This
simple configuration allows us to define the ‘perceived velocity gradient tensor’, and provide insight on the interaction between strain and vorticity as a function of scale (collaboration with H. Xu and P. Yang, Tsinghua University).

Turbulence and transport in a geophysical context

Stratified turbulence. Atmospheric and oceanographic flows involve not only very large Reynolds numbers (a consequence of the very large scale of the flows) but also oftentimes a density stratification. Our interest has focused on stably stratified flows. From a fundamental point of view, the stable stratification leads to (inertial) waves in the flow, and waves and eddies can influence the dynamics, depending on the Reynolds number of the flow, but also on the intensity of stratification. Our study has revealed a transition between a wave-dominated regime (when the stratification is important) towards an eddy-dominated regime (closer to fluid turbulence), induced by a wave instabilities, and leading to strong up- and down-drafts in the fluid. This mechanism strongly affects the transport of tracer particles, and leads to a strong increase of the energy dissipation in the fluid (collaboration with R. Marino, Ecole Centrale de Lyon).

Transport of ice crystals in clouds. In clouds, turbulent fluid transports small particles, droplets or small ice crystals. Collisions between these particles is an important process leading to the growth of the particles size, and therefore, to precipitation. Over the past few years, we have been particularly interested in the settling of ice crystals in mixed-phase clouds and their collisions. The description of ice crystals settling through a turbulent fluid turns out to require particular attention. Our earlier attempts to model the problem led us to consider simplified equations of motions, using the Stokes approximation to describe the relative motion between the crystals and the fluid. This simplified description, however, leads to qualitatively incorrect results, in terms of the orientation of anisotropic crystals in the flow. A thorough analysis reveals that the torque induced by fluid-inertial effects plays a crucial role, and in fact, greatly affects the orientation of settling crystals. Using a more correct description, we have in particular obtained a complete parametrization of the orientation distribution as a function of the intensity of turbulence and of their shapes. This could be particularly useful to interpret satellite (LIDAR) observations. The study of the collision between crystals, and between ice crystals and droplets (riming) is ongoing (joint work with A. Naso, E. Lévêque, Ecole Centrale de Lyon, and K. Gustavsson and B. Mehlig, University of Gothenburg).
5.6 MAX PLANCK EMERITUS GROUP NONLINEAR DYNAMICS

Dynamical phenomena are diverse and widespread in nature; some are easy to dissect for a human observer, others have challenged theoreticians for decades. A formidable example is the complexity of brain function, which is achieved by a multitude of dynamical states of the networks of neurons in our brains. The field of nonlinear dynamics has established mathematical tools for the analysis and characterization of such nontrivial dynamics in complex systems. Developing and applying specific methods the former Department of Nonlinear Dynamics was devoted to clarifying the relation between the dynamics and function of neural networks, classical and quantum mechanical transport in nanostructures, and the spatiotemporal dynamics of epidemics, activities which are carried on by the Max Planck Emeritus Group of Nonlinear Dynamics on a smaller scale.

This broad scope of topics has often led to cross-fertilization in the former department which helped to meet new challenges and led to new developments such as uncovering human travel statistics through dollar bill tracking, modeling the spread of epidemics with Levy flight approaches, and discovering random focusing effects of rogue waves and tsunamis. In the past three years the focus of the group was on the dynamics of endemic diseases in partially open populations and on the analysis of musical sequences. These projects are described in more detail in Sections 8.3, 8.26, and 8.27.

Time series analysis of musical sequences is a fascinating application of the tools developed in nonlinear dynamics. It allows us to elucidate the relation between stochastic properties of musical compositions or performances and the way we perceive music. In particular, our group has studied temporal fluctuations in musical rhythms and resolved the long-standing controversy on the role of microtiming deviations as a component of the swing feel, a salient feature of jazz.

The former 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 initiated and hosted the federally (BMBF) funded Bernstein Center for Computational Neuroscience Göttingen, in which it cooperated with experimental neuroscience labs and established a high performance computing facility. Today Theo Geisel is heading a small emeritus group on nonlinear dynamics, which interacts with other research groups in the Institute. Among his community services are the organization of annual French-German Heraeus Seminars for the DPG and scouting for new directors of the MPG.
The brain is a compact mass of neurons forming networks that define who we are and direct what we do. Inside this brain machine is a branched system of ventricles – cavities - through which flows cerebrospinal fluid (CSF), a substance-rich liquor. Greek and medieval physicians regarded the CSF filled ventricles as the seat of thinking, memory, consciousness and feelings. Medical science later degraded ventricles to a drainage system filled with compounds that the brain needs to dispose of. Research during the past decades found that CSF contains neuroactive signaling molecules and not just waste. It's safe to say that the interconnected ventricles are canals that transport and deliver signaling factors to specific brain regions.

To execute this transport function, the walls of the ventricle carry precisely positioned motile cilia that set in motion and guide CSF flows over distances of millimeters and even centimeters. The cilium is eyelash-shaped and protrudes from the cell surface. Inside the cell, the cilium is attached to a basal body. In the cells of the brain ventricles, cilia form bundles made of 30-60 units and each cilium is equipped with motility proteins that make cilia beat in a whip-like fashion. In effect, this cilia whipping pushes CSF along the ventricular wall in diverse but precisely defined directions.

In recent years, we have studied cilia-driven transport in the brain ventricles (doi.org/10.1126/science.aae0450). We focus on the third ventricle that resides in the hypothalamus, a brain region that regulates many endocrine functions in the body. We investigate when and how during brain development directional CSF flows are established. A key process of directional flow development is imposing asymmetry to the cells that form the ventricular wall. Therefore, we study when cell asymmetry first appears, and how the spatiotemporal expression pattern of plasma membrane-associated cell polarity proteins confer cell polarity and cilia beating direction.

We investigate the geometry of transport routes within the third ventricle by locally applying fluorescent liposomes and video-recording vesicle transport. This led to the discovery of cilia-driven micro-flows, only a few cells wide, “crawling” along the walls of the ventricle and thereby delivering vesicle content - cargo - to target regions. The micro-flows obey a set of traffic rules that allow a well-ordered distribution of cargo. More recently, our studies include the transport of extracellular vesicles (EVs) that naturally occur in CSF.

We also investigate which signaling factors are contained in extracellular vesicles. EVs are produced within the ventricular cavities by a secretory epithelium termed the choroid plexus. We isolate the vesicles from choroid plexus cells and study how purified vesicles regulate the physiology and behavior of stem cells that reside in a particular sub region of the third ventricle. Methods of study include functional analysis of stem cells that differentiate upon contact with our purified EVs. We carry out protein mass spectrometric analyses of both, the EVs and
the recipient stem cells. The aim is to identify molecules that the micro-flows transport and eventually deliver to the stem cells. The broader significance of this work is that it investigates a cilia-driven, directional transport system that delivers signaling factors within ventricles and to brain tissue underneath the ventricular wall. The transport is powerful enough to directionally move nanoscopic particles within seconds and do so in a low Reynolds number environment.

Figure 5.12: Top: The third ventricle (speech balloon in the middle) was thought to accommodate the ability of the brain to think (from Reisch, Margarita Philosophica, 1503) (left). Thousands of cilia bundles cover the walls of ventricles and generate diverse flows whose direction is color-coded (right). E.g. green flows go down, blue ones to the right. Center: Nanoparticles applied to the ventricular wall (arrow) form micro-flows that fan out (left). Cilia form bundles; each ventricular wall cell carries one bundle. Cilia dock on basal bodies (red and green structures) that form a grid-like array that gets its geometry from polarity-conferring transmembrane proteins (right). Bottom: For the circadian clock to keep ticking, BRD4 and BMAL1 proteins must bind - in a 24-h-rhythm - near the transcription start site (TSS) of clock-controlled genes such as Dbp (left). To track circadian clock-controlled locomotion as is occurring in DVM - over days - this Arcatia tonsa copepod was fed with fluorescent algae that form a trackable, fluorescent dot in the intestine (right). Image credits: S. Kapoor, A.-K. Günther, C. Westendorf, N. Petkau

A long-term interest of Eichele is the molecular clockwork that drives many physiological and behavioral processes (doi.org/10.7554/eLife.43235) including dial vertical migration (DVM) of plankton. DVM is colossal, daily translocation of biomass and profoundly influences the food chain in the world’s oceans. In collaboration with Dr. J. Söding (MPIBPC) and Prof. em. O. Larink (University of Braunschweig) we determine the transcriptome sequence of a variety of zooplankton species with the focus on their circadian clock system and the role of this clock in regulating the oceanic DVM. This research encompasses laboratory cultured plankton and fresh plankton collected at the AWI Helgoland and in the Atlantic Ocean on board of S/Y Eugen Seibold (MPIC, Mainz).
5.8 MAX PLANCK EMERITUS GROUP MOLECULAR INTERACTIONS

Together with the late Hans Pauly (1928 - 2004) our group came to Göttingen in 1969 from the University of Bonn to establish the new research direction of molecular beam investigations of elementary collision processes between atoms and molecules. According to the Eigen-plan the idea behind our being called to the Max Planck Institute for Flow Research (Strömungsforschung) was to investigate the elementary processes behind the macroscopic fluid dynamic process and thereby achieve a better understanding. In the following years the Institute became one of the leading international centers for experimental and theoretical molecular beam research in determining with unprecedented precision the van der Waals forces and the collision dynamics between atoms and molecules. The intermolecular forces are of fundamental importance for understanding both the static and dynamic properties of gases, liquids and solids as well as their phase transitions. One of the important developments from our Institute was the development of a new analytic model for the van der Waals interaction in place of the well-known Lennard-Jones potential. The Tang-Toennies potential, which is presently widely used for accurate simulations, has been cited 1600 times since 1984.

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 \[ \frac{\delta v}{v} \approx 10\% \] the helium atom beams had very sharp velocity distributions and were nearly monoenergetic with \[ \Delta v/v \lesssim 1\% \]. 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 \( \approx 10^{-3} K \) in the expanding gas rises to \( 259,000 \, \textrm{Å}^2 \), more than 4 orders of magnitude larger than the cross section at room temperature. These nearly monoenergetic helium atom beams have found widespread application. In seeded beam 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 sharp velocity helium atom beams for exploring the structures and the phonon-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 inelastic helium atom scattering (HAS) and the complimentary method of inelastic electron scattering (EELS) have led 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 many surface phenomenon such as corrosion, friction and 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 flow without resistance. Thus it was natural to ask if small finite-sized clusters and droplets of helium might also exhibit superfluidity. In molecular beam experiments we observed that atoms and molecules could be inserted and trapped in the droplet’s interior. This opened up the possibility of employing spectroscopy to interrogate the physical properties of the trapped molecules and also the state of the helium droplets. Surprisingly the sharp spectral features of the embedded molecules indicated that the molecules were unaffected by the helium environment and could rotate freely as if they were in a vacuum and not at all strongly hindered as expected for an ordinary liquid. From the highly resolved rotational spectrum the temperature of the droplets was found to be 0.37 K. Subsequent experiments revealed that the free rotations were related to the superfluidity of these droplets. This is the first evidence that superfluidity occurs in a finite-sized system and is now called microscopic 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 photo-excitation. 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. Experiments were also directed at exploring the nature of small pure clusters consisting of a few helium and hydrogen molecules, which show large quantum effects. 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 very weakly bound dimer and the precise measurement of its size. Unexpected magic numbers were found in larger clusters (\( N \approx 50 \)), which have led to the first insight into the elementary excitations of these nano-sized superfluids.

At present we are working in three main areas of research. (1) At the end of 2018 we finally completed our 600 page Springer monograph with Prof. Giorgio Benedek (University of Milan) entitled “Atomic Scale Dynamics at Surfaces: Theory and Experimental Studies with Helium Atom Scattering”. This monograph provides the only up-to-date survey of the theoretical and experimental methods for studying the vibrations at the surface of single crystals and the surface vibrations of adsorbed atoms and molecules. The appendices provide a complete overview of the literature for all the systems studied and the corresponding theoretical investigations. Since then we have continued our investigations of electron-phonon coupling at the surfaces of metals and superconductors and surface plasmons. (2) In collaboration with several bachelor
students we have investigated a new modified Tang-Toennies model for
describing the van der Waals potentials of the alkali diatomic molecules
made up of the atoms Li, Na, K, Rb, and Cs in the weakly bound triplet
state. These potentials are of great current interest for understanding
the collisions in laser trapped ultra-cold gases and their Bose-Einstein
Condensation. We have recently demonstrated that our model with
only three parameters provides an equal or better description of all
the spectroscopic data than numerical fits with up to 50 parameters.
Recently in collaboration with K. T. Tang (Pacific Lutheran Univer-
sity, Tacoma USA) and Xiaowei Sheng (Anhui University, Anhui, China)
we have demonstrated that with an analytic extended Tang-Toennies
model potential it was possible to describe the van der Waals potentials
between all the homonuclear and heteronuclear rare gas dimers in
excellent agreement with ab initio potentials where available. (Phys.
Rev. Lett. 125, 253402 (2020)). (3) Presently we are editing a 10 chapter
open access Springer Nature book entitled “Molecules in Superfluid
Helium Nanodroplets: Spectroscopy, Structures and Dynamics” All the
chapters have been quite recently submitted and the book will shortly
be sent to the printers. This will be the first edited volume in this
emerging field of research.
PART II

RESEARCH
DYNAMICS IN DRIVEN SYSTEMS

The dynamics in driven systems represents an active interdisciplinary research field at the interface of physics, biology, medicine, ecology and engineering. Most of physical phenomena that are significant in nature occur in systems that are driven - in other words - in systems that are kept out of thermal equilibrium. The drive can be either external or internal. Typically, these systems possess spontaneous symmetry breaking in space and/or time and develop spatio-temporal complexity and order.

Such self-organisation processes greatly reduce the number of degrees of freedom in the system dynamics. Moreover, although it may sound contradictory, spatio-temporal complex driven systems demonstrate well-defined universal properties that generally describe an entire class of systems that exhibit very different physical phenomena. Thus, spatio-temporal complex driven systems exhibit an order within their complexity that can be captured at a universal level using the physical tools of non-equilibrium physics, nonlinear dynamics and statistical physics.

In this chapter, we present our recent results on a number of systems and phenomena that are of great physical, biological, societal, and ecological importance. They include purely physical phenomena such as the behavior of droplets and turbulence in flows of gases and liquids, biological systems such as interactions in networks or of cilia, and medical systems such as the heart or the brain.

The MPI DS remains a key driver in these rapidly evolving fields. Our goal is not only to achieve a better understanding of physics through a strong interaction between novel experimental approaches and the use of analytical and numerical tools, but also to contribute to some of the most pressing challenges of our time, such as enabling longer and healthier lives.

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6.1 TESTING KINETIC THEORY WITH A COOLING GRANULAR GAS

M. Schröter, P. Yu (DLR Cologne), M. Sperl (DLR Cologne)

In contrast to molecular gases, granular gases are characterized by inelastic collisions and require therefore permanent driving to maintain a constant kinetic energy. If classical kinetic theory is expanded to take the dissipative collisions into account [1], it makes two predictions for the cooling of a granular gas after the driving is switched off: a) the decrease of the average particle velocity $\langle v(t) \rangle$ as function of time $t$ will follow the so-called Haff’s law: $\langle v(t) \rangle = v_0 / (1 + t/\tau)$ where $\tau$ is a material and density dependent characteristic time scale. And b) if the individual particle velocities are rescaled using the square root of the kinetic energy of the system, the probability distribution of the rescaled velocities $c$ has an exponential tail: $P(c) \sim \exp(-kc)$. Which means the high-speed part of the distribution will be overpopulated compared to a Maxwell-Boltzmann distribution.

Of these two results, only a) had been previously experimentally confirmed in a qualitative way [2, 3]. Experimental studies need to overcome two problems: First, heating a granular gas requires constant energy injection. But doing so via moving boundaries, e.g. by shaking the sample container, results in strong spatio-temporal gradients. Secondly, on earth the gravitational field will always collapse the granular gas into a granular solid where collisions are replaced by enduring contacts. We did overcome these obstacles by doing a microgravity experiment in a sounding rocket and creating a spatially homogeneously excited granular gas using changing magnetic fields and ferro-magnetic particles, cf. fig. 6.1.

Using particle tracking velocimetry, we first confirmed Haff’s law qualitatively, as shown in fig. 6.2. However, we find that kinetic theory predicts a time constant $\tau$ which is a factor of 2.6 times larger than the fitted value of 0.507 s. This discrepancy might originate from the fact that the theory only includes the inelastic aspect of the collisions, not the also dissipative frictional interactions. We expect this quantitative deviation to stimulate further theoretical work.

The main result of our experiment [4] is shown in fig. 6.3: we confirmed for the first time that the high energy tail of $P(c)$ decays exponentially, as predicted by the kinetic theory of granular gases. A nonlinear fit of the experimental data using $P(c) \sim \exp(-kc^a)$ results in $a = 0.96 \pm 0.19$, which is again in good agreement with the theory.

In summary, granular gases deviate significantly from molecular gases. However, these differences also signify the chance to “reinvent statistical mechanics in a new context” [5].

6.2 EVAPORATION, WETTING & PHASE SEPARATION

O. Ramirez-Soto, Y. Chao, C. Bahr, S. Karpitschka
M. Prakash (Stanford), N. Cira (Harvard), A. Marin (Twente)

Evaporating sessile droplets of volatile liquid mixtures are abundant in natural phenomena and technological applications [1]. Many examples are found in everyday life, like blood and tears, inks for printing, and paints for artistic techniques. Contact line motion and drop evaporation are multi-scale processes that involve both macroscopic transport and molecular interactions [1]. Compositional gradients near the edge of the droplet give rise to Marangoni flows which readily impact shape and composition of the droplet. This, in turn, again alters wetting and evaporation. Given the strong coupling of several multi-scale processes, predicting the drying behavior of such droplets is challenging.

Particle-laden salt water droplets are a rather simple example of such a system, yet their drying behavior turns out to be quite complex (Fig. 6.4). In our work [2], we discovered that the usual coffee-stain flow is reversed by the salt: Enrichment of salt near the edge of the droplet increases surface tension, leading to an outward, Marangoni-driven surface flow that is compensated by an inward bulk flow. This changes the aggregation mechanism of particles near the contact line, which now proceeds along the free surface, not the substrate.

The opposite flow direction is observed when the residual component decreases surface tension which, on high-energy substrates, leads to Marangoni contraction (Fig. 6.5): Although the surface is fully wetted by the mixture and its components, a non-vanishing contact angle is observed. This mechanism is widely used for drying and cleaning in semiconductor or printing industries, but its physical explanation remains debated in literature. One may postulate that Marangoni contraction can be enhanced by using more surface active residuals. However, we could show that surface activity also promotes autophobic, a phenomenon by which a droplet dewets from its own wetting precursor [3]. Breaking with precedent, we demonstrated that Taylor dispersion can consistently be included in a long wave expansion for the evolution of thin films, and that the compositional evolution of contracted droplets is governed by it [4].

Since Marangoni contraction relies on diffusion-limited evaporation, neighboring droplets interact with each other, mediated by the vapor field they generate. In a pair of neighboring drops, evaporation is reduced on the proximal hemisphere of each drop, which breaks the axisymmetry of the internal flow and leads to an attractive interaction. Using substrates with hydrophobic barriers (Fig. 6.6), this phenomenon can be exploited to study many-body interactions. The simplicity of the system allows for a rapid exploration of various geometries and the degeneracy of the associated energy landscape [5].

Currently, we study droplets of non-ideal, partially miscible liquids: Evaporation of the volatile component or heating will drive this system into the two-phase region (Fig. 6.7 A,B). Phase separation in pinned droplets has been extensively studied [1], in contrast to the case of
dynamic wetting, where drop motion is coupled to physico-chemical processes in the drop and at its boundaries [6]. Remarkably, we observe an abrupt spreading motion (Fig. 6.7 D,E) when the two-phase region is entered, well before the nucleation of microdroplets (Fig. 6.7 F). Thus wetting dynamics are highly sensitive to phase separation at interfaces, with important implications in cell biology where membrane-less organelles are currently studied intensely.

Figure 6.6: A. Marangoni-contracted droplets interact by their vapor fields. Hydrophobic barriers prevent coalescence, establishing a discrete manybody system. B. Shape and placement of elementary cells can be tuned to mimic various models. C. In a hexagonal tiling, each vertex can be occupied by zero to three droplets, representing different energy levels. D. Finite honeycomb lattice of 61 cells, trapped in a local energy minimum. E. Random initial configuration of an experiment. F. Typical final state.

Figure 6.7: A,B. Non-ideal mixtures phase-separate when they are driven into their two-phase region, leading to microdrop nucleation in sessile drops. We study the interplay of wetting dynamics and phase separation. C. Surface tension and contact angles in the one-phase regime. D,E. Droplets with freely moving contact lines abruptly spread when driven into the two-phase regime. F. The spreading occurs well before microdrop nucleation and is a sensitive indicator for processes at the interface.

6.3 DROPLET DYNAMICS IN ELASTIC MEDIA

E. Vidal-Henriquez, D. Zwicker

In recent years it has been shown that liquid-liquid phase separation plays a fundamental role in the formation of many intracellular structures such as stress granules, nucleoli, and P granules, among others [1]. These structures, known as biomolecular condensates, are droplets of protein and RNA molecules that phase separate from the cytoplasm. Classical phase separation is characterized by the growth of large droplets at the expense of smaller ones in a process known as Ostwald ripening. However, many cellular processes require precise control over condensates in terms of their position, size, and number. Cell must thus possess mechanisms that arrest Ostwald ripening. Since the cytoskeleton spans the entire cell volume, its elastic properties could provide such control by moving droplets to desired locations or preventing the uncontrolled growth of big condensates.

To understand the effects of an elastic environment on phase separation, we studied a synthetic system, which allowed us to rule out active processes, such as cross-linker decay and network rearrangement. Recent experiments [2] produced monodisperse droplet size distributions by combining two oils in a polymer matrix and then decreasing the temperature until the oils become immiscible and form droplets. Surprisingly, the mean droplet radius depended on the cooling rate and changing the cooling rate during the process resulted in a bimodal size distribution [3]. We studied this out-of-equilibrium system theoretically to understand how the surrounding elastic material and the cooling process affects the droplet size distribution.

We have shown that droplets need to break the surrounding elastic mesh in this system to grow up to macroscopic sizes [4]. When a droplet breaks the surrounding polymer matrix, the pressure exerted on it decreases, see Fig. 6.8, resulting in a cavitation event and a rapid expansion of the droplet. During this expansion, the droplet absorbs the surrounding excess material and effectively prevents cavitation of the neighboring droplets, arresting them at a microscopic size comparable to the mesh size. This interplay between material diffusion towards the fast-growing droplets and the creation of excess material due to the temperature decrease defines the number and size of observable macroscopic droplets, producing more and smaller droplets at faster cooling rates. The cavitation events occur almost simultaneously throughout the system and the cavitated droplets grow in a similar manner, so the random effects of droplet nucleation are buffered, which results in a monodisperse size distribution. If the cooling rate is increased during the process, new cavitation events can occur, leading to a bimodal size distribution of the macroscopic droplets.

The cavitation of some droplets while others remain constrained by the mesh relies on small material heterogeneities, which provide the different critical pressures for the droplets. Examples for such heterogeneities are different cross-linker strengths and mesh sizes. So far, we assumed that these heterogeneities are local, while the large-
scale material properties of the mesh are homogeneous. However, if the critical pressures vary over a larger length scale throughout the system, additional dynamics can occur. In particular, such pressure differences can drive material diffusion in a similar manner to Ostwald ripening. In Ostwald ripening, the dissolution of smaller droplets of radius $R$ is driven by their surface tension $\gamma$, which leads to a Laplace pressure $\gamma / (2R)$. Consequently, smaller droplets exhibit a larger pressure and dissolve. A similar effect can be observed when the pressure exerted by the elastic material is inhomogenous: droplets will dissolve in regions of higher pressure, i.e. stiffer parts of the material, and grow in regions of lower pressure [6]. We termed this phenomenon Elastic ripening to distinguish the external origin of the pressure from the Laplace pressure in classic Ostwald ripening.

Experimentally, Elastic ripening has been observed by bringing two polymer gel samples of different stiffness into contact [3]. In this case, droplets start dissolving close to the interface between the two materials, see Fig. 6.10. The dissolving droplets form a front, which invades the stiffer side of the system until droplets remain only on the soft side. The direction of the front is independent of the original droplet size and can even oppose Ostwald ripening [5]. Using mean field theory and numerical simulations (see Sec. 6.4) we were able to show that the dissolution front appears at the point of the highest curvature of the stiffness gradient and that it travels inside the stiff material in both directions initially [6]. We also showed that this front has a diffusive movement with a travelling speed that increases with higher stiffness differences.

By studying a synthetic system we have neglected many effects present in the biological setup, where the elastic network is active and can rearrange in the presence of condensates. Furthermore, the individual interactions between droplets and fibers, such as wetting, cannot be neglected, given the comparable sizes between condensates and the network size. These elements, along with the viscoelastic properties of the cytoskeleton, need to be considered when analysing the original biological setup. Nevertheless, our results show some of the complex phenomena appearing when phase separation occurs in an elastic medium and provide an initial framework to understand the effect of the cytoskeleton in biomolecular condensates. More generally, studying phase separation inside an elastic material opens many possibilities for material engineering with precise droplet size and distributions.

6.4 EFFECTIVE SIMULATION OF INTERACTING DROPLETS

A. Kulkarni, D. Zwicker

Phase separated condensates play an important role in the spatio-temporal organization of molecules in biological cells. It is fascinating that cells can precisely control many droplet-like condensates, despite their complex environments. To understand this process, we develop novel simulation techniques to describe emulsions without solving the computationally expensive Cahn-Hilliard equation that describes phase separation. The main idea is to use insights from analytical results based on a thin-interface approximation [1]. In such an effective droplet model, we characterize each droplet by its position $\bar{x}_i$ and its radius $R_i$, since droplets are typically round due to surface tension effects. The droplets coexist with a dilute phase, which is described by a discretized volume fraction field $\phi(\bar{x}, t)$. In the typical situation where droplets are far away from each other, we can study their interaction with the dilute field by discretizing their surrounding:

![Figure 6.11: Coarsening behaviour of $10^4$ passive droplets using the effective droplet model. The mean radius $\langle R \rangle$ follows the Lifshitz-Slyozov-Wagner scaling law.](image)

![Figure 6.12: Schematic of an isolated droplet. The dilute phase $\phi(\bar{x}, t)$ is discretized on a grid, while the vicinity of the droplet is cut into $n$ annular sectors. Boundary conditions for the reaction-diffusion equation inside each sector follow from an interpolation of $\phi(\bar{x}, t)$ (black dots) and the Gibbs-Thompson relations (red dots) [1].](image)

The growth dynamics of droplets follow from the material fluxes between the droplet and the dilute phase, which are obtained from solving a steady-state reaction-diffusion equation inside all sectors discretizing their surrounding. These fluxes also affect the dynamics of the dilute phase itself, together with an ordinary reaction-diffusion equation describing the bulk dynamics. Taken together, we developed an efficient numerical simulation that can handle many droplets (see Fig. 6.11), capture chemical reactions (see Fig. 6.13), and has been used to describe the interaction of droplets with elastic matrices in other work of our group (see Sec. 6.3).

6.5 TURBULENT FLOWS


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Turbulent flows are omnipresent. Their role in geophysical and astrophysical systems and many engineering applications can hardly be overestimated. We investigate turbulence experimentally, theoretically, and numerically and focus in our studies on large-Reynolds-number flows and turbulent thermal convection.

6.5.1 Turbulent Flows at High Reynolds Numbers

(C. Küchler) Turbulent flows at large Reynolds numbers $R_\lambda$, where viscosity $\nu$ plays only a minor role over a wide range of spatial and temporal scales, exhibit a remarkable level of self-organisation, which largely remains to be understood at a fundamental level with wide ranging applications, among others, to atmospheric dynamics. Of particular importance are scales $r$ much smaller than the turbulence excitation scale $L$, but larger than the viscous length scale $\eta$. The statistical properties of motion are expected to be dominated by inertia and to be universal for small $\nu$. Using the MPI DS Variable Density Turbulence Tunnel (VDTT), we have shown that the statistics of these inertial scales approach an asymptotic shape when increasing $R_\lambda$. This shape is different from the classical predictions [1], which postulates simple power laws as a function of scale. This is illustrated in Fig. 6.14 for the local scaling exponent of the second-order velocity increment statistics, i.e. $\xi_2 = \partial \log \langle u(x+r) - u(x) \rangle / \partial \log r$. We have collected evidence that the time-dependence of the decaying flow causes this $R_\lambda$-independent breaking of scale invariance. In the past, such effects were attributed to finite $R_\lambda$ and predicted to fade when $R_\lambda$ is large enough. Our results indicate that this may only be true under the highly idealised conditions of homogeneous, isotropic and statistically stationary turbulence, which do not apply in real flows even in the conceptually simple configuration of a wind tunnel, where (time-dependent) large-scale effects appear to influence small-scale statistics even when $R_\lambda$ is extremely large.

In Fig. 6.14 a small knee is visible in the experimental data around $r/\eta = 100$. In this region the statistics are dominated by the bottleneck effect leading to a small excess of energy at the scales small enough that viscosity begins to matter [2]. This excess energy has been shown to diminish with increasing $R_\lambda$ in numerical simulations [3]. Using the flexible parameter space of the VDTT, we have corrected the non-
constant frequency response of our flow sensors to measure this subtle effect. We find good agreement between the numerical simulations and the experiment at low $R_{\lambda}$ and show that the reduction of the effect continues up to at least $R_{\lambda} = 3500$, beyond what can be explored numerically. A defining feature of turbulent flows is their efficiency to mix and transport within a fluid. This is most intuitively described by following a fluid element, e.g. by seeding the flow with light particles and tracking their position at high frequencies. This extremely demanding technique has been recently implemented in the VDTT. Using this setup we have measured the highly intermittent accelerations in turbulence at unprecedented Reynolds numbers. Fig. 6.15 shows the acceleration statistics and velocity increment statistics up to $5.6\tau_{\eta}$ at $R_{\lambda} \approx 5500$ - more than two times higher than all previous measurements. The heavy-tail nature of the PDFs is clearly visible and we find consistency with earlier experiments at lower Reynolds number (e.g. Refs. [4, 5, 6]). Future studies will investigate the normalised acceleration variance $a_0$ testing a long-standing scaling prediction [7, 8] at unprecedented Reynolds numbers.

6.5.2 Turbulent and multiphase convection

(A. Krekhov, O. Shishkina, S. Weiss) Thermal convection is one of the most important heat transport mechanism and drives large scale turbulent flows, for instance in many geo- and astrophysical systems. We study convection experimentally and theoretically using the Rayleigh–Bénard (RB) setup [9], where a fluid layer of height $L$, is confined by a warm plate from below and a cold one from above. The dimensionless Rayleigh number ($Ra$) represents the strength of the thermal driving in this system, and is directly proportional to $L^3$ and the maximal temperature difference in the system. Our research focuses on different aspects of convection, such as convection at very large thermal driving (large Ra) [10, 11, 12, 13]. We also consider the effect of rotation [14, 15, 16, 17], or of the roughness of the heated and cooled surfaces [18, 19], or of a phase transition in the fluid [20], and other aspects.

The largest convection cells are used in the “U-Boot of Göttingen”, which is a 4 m long pressure vessel filled with Sulfur hexafluoride (SF$_6$) and pressurized up to 19 bar. Using compressed gases allows to change fluid properties and thus the relevant dimensionless control parameters over a very large range. Furthermore, SF$_6$ is a very dense gas, and thus well suited to achieve very large $Ra$ ($Ra \propto \rho^2$). With this apparatus $Ra$ of up to $2 \times 10^{15}$ can be reached and the transition to the “ultimate state” has been probed in the past [12, 13]. We currently investigate the large scale flow structure in thermal convection using a 3.50 m long and 70 cm large aspect ratio convection cell inside the U-Boot.

In turbulent RB convection, the flow in boundary layers exhibits strong fluctuations. Furthermore, the time-averaged large-scale circulating velocity vanishes far away from the top and bottom plates, and the motion arises from buoyancy. We have derived the full set of boundary layer equations for a RB flow, taking into account all the above effects. The solutions of these boundary layer equations give the RB flow field
profiles [21, 22]. We further study the global structure of RB flow, in particular the role of the thermal plume impacting and ejecting zones [23]. The influence on the temperature- and pressure-dependence of the fluid properties, i.e. the so-called non-Oberbeck–Boussinesq effects, have been investigated as well [24, 25]. In particular, we have studied convection in cold water and derived the way to accurately predict the bulk temperature [25].

One of our main focus is to investigate the effect of rotation on the flow field and the heat transport, a topic particularly relevant for geo- and astrophysics. For this we conduct experiments using our $L = 2.20$ m high convection cell inside the U-Boot, in order to achieve very large thermal driving. One of our main finding [14] was the existence of the boundary zonal flow – BZF close to the sidewall of the cylindrical cell under rotation. This flow is characterised by a positive averaged azimuthal velocity, in contrast to a negative velocity close to the radial center, as well as periodically alternating warm (upflow) and cold (downflow) regions. These regions furthermore drift in retrograde direction. The region close to the sidewall, where these flow features are observed, shrinks with increasing rotation rate, but still remains to be very important in heat transport in the system, see [14, 15, 16, 17].

The large-scale circulation (LSC) of fluid is one of the main concepts in turbulent thermal convection as it is known to be important in global heat and mass transport in the system. In turbulent RB convection in slender containers, the LSC is formed of several dynamically changing convective rolls that are stacked on top of each other. We have revealed that the mechanism which causes the twisting and breaking of a single-roll LSC into multiple rolls is the elliptical instability [26], see Fig. 6.18.

In contrast to the situation in slender RB containers [26], the heat and momentum transport in RB convection in wide cells, represented by the Nusselt and Reynolds numbers, is always weaker (stronger) for larger (smaller) number of the rolls in the LSC structure [27]. For exactly the same values of the control parameters, RB flow can take different statistically stationary turbulent states, with different transport properties. What state the system takes depends on the initial conditions. In the case of wide containers, the state in determined by the aspect ratios of particular rolls of elliptical shape, for which we have derived the bounds [27].

Many natural and industrial turbulent flows are subjected to time-dependent boundary conditions. We have studied how the time periodic modulation in the temperature boundary condition [28] or imposed travelling thermal waves [29] can influence heat transport (Nusselt number) and formation of zonal flows. In another ongoing project we investigate the heat transport across a sheared thermally unstable boundary layer. There, the hot plate is located in a wind tunnel, so that advection close to the plate surface is caused both by buoyancy and a shear instability. We measure velocities above the plate and the heat flux from the plate as a function of the flow speed and the buoyancy. With this we probe the transition from the regime of natural convection, where buoyancy dominates over the shear forces to the regime of forced convection, where buoyancy can be neglected (see Fig. 6.19).
Apart from the classical RB flow configuration we also studied horizontal convection \cite{30, 31}, where the heating and cooling are applied to the same horizontal surface of the fluid layer, vertical convection \cite{32}, where the fluid is confined between two vertical surfaces of different temperatures, and inclined convection \cite{33, 34}, i.e., a mixture of RB and vertical convection.

Finally we should also mention our studies of another omnipresent phenomenon in many geo- and astrophysical convective flows, i.e. internally heated convection, which is a convective fluid motion driven by the internal heat generation. An important question in these studies is how the mean temperature and the global flow strength depend on the internal heating rate and the operating fluid. Recently we have offered a theory to address this question \cite{35}; the results of the theory agree well with direct numerical simulations.

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Figure 6.19: (a): Snapshot of the smoke-seeded shear flow over a flat plate heated. (b): Heat transport as a function of the Reynolds number of the incoming flow (x-axis) and the thermal driving (Grashof number \(Gr\), color code).
6.6 LAGRANGIAN MODELS FOR THE VELOCITY GRADIENT DYNAMICS IN ISOTROPIC TURBULENCE

M. Carbone, M. Wilczek
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Intense vortices and strain sheets are hallmark features of small-scale turbulence, whose rich dynamics can be comprehensively characterized through the velocity gradient tensor $\mathbf{A} = \nabla \mathbf{u}$. The velocity gradient tensor contains information about a range of important quantities such as the local energy dissipation, enstrophy, and, more generally, the topology of small-scale turbulent structures. It has also immediate implications for the orientational dynamics of small particles immersed in a fluid, which sample the history of velocity gradients along their paths. In statistical models for the velocity gradient dynamics, the non-local effects of turbulence give rise to unclosed conditional averages, namely the average pressure Hessian and viscous Laplacian, both conditional on a local velocity gradient configuration [1, 2].

In recent work, we explored the general structure of these terms using tensor function representation theory [3]. The key idea in this approach is to treat the unclosed conditional averages as tensor functions of the local gradients, which can be expressed as a combination of only a few tensors $\mathbf{B}_i$ constructed from the symmetric part, $\mathbf{S}$, and the anti-symmetric part, $\mathbf{W}$, of the velocity gradient. For example, the conditional anisotropic pressure Hessian takes the form $\langle \mathbf{H} | \mathbf{A} \rangle = \sum_{i=1}^{5} \phi_i (\mathbf{A}) \mathbf{B}_i (\mathbf{A})$. As a simple starting point, we explored a class of closure models, in which the components $\phi_i$ were kept constant [4]. The resulting reduced-order stochastic model for the velocity gradient enabled far-reaching insights into the small-scale dynamics of turbulence, including the emergence of non-Gaussian statistics as well as temporal correlations of vorticity and strain. Importantly, this enabled us to predict the orientational statistics of anisotropic tracer particles in turbulence (Fig. 6.20). Currently, we are exploring generalizations of this model. In particular, we are investigating how the components $\phi_i$ depend on velocity gradient tensor invariants. To this end, we use tools from information theory to identify the most important invariants. Specifically, we analyze the mutual information between the gradient invariants and the local pressure Hessian components (Fig. 6.21), and we find that the enstrophy (that is $I_2$ in Fig. 6.21) is among the most important invariants to include. By using data from direct numerical simulation we explore the trend of the components as functions of those invariants (Fig. 6.22). Remarkably, the sharpest variations of the components $\phi_i$ occur in the phase space region where current models [4] are not very accurate. We therefore expect that the outcomes of this work will allow developing models for the velocity gradient that are accurate across the whole phase space.

6.7 CHARACTERIZATION OF THE SLING EFFECT IN TURBULENCE

T. Bätge, M. Wilczek
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In understanding clouds, the formation of rain droplets and the related size gap constitute a major open problem. The size gap denotes those particle sizes where neither condensation nor gravitational settling can explain droplet growth. Here, collisions, which are significantly enhanced by turbulence, are likely to drive the growth of droplets [1]. The encounter of droplets with highly intermittent small-scale turbulent structures can, despite their rarity, dominate the overall collision rate [2]. Intuitively, strong vortices may act as slings for inertial particles, leading to large collision velocities. This so-called sling effect leads to intersections of trajectories [3] (in the following referred to as sling events), which corresponds to caustics, see Fig. 6.23.

We developed a quantitative criterion for sling events based on the velocity gradient history along such particle paths. Combining theory and direct numerical simulations (DNS) of Navier-Stokes turbulence, we demonstrated that the problem reduces to a one-dimensional localization problem. This problem is known most prominently from condensed matter physics. From our theory, we could identify a threshold for the occurrence of sling events for the most negative eigenvalue of the velocity gradient tensor. Depending on the duration and depth of excursions below this threshold, we established a quantitative criterion that separates velocity gradient excursions leading to sling events from those that do not. We use fully resolved turbulence simulations to confirm this criterion, see Fig. 6.24.

Using phenomenological arguments and large-deviation theory, we characterize the statistics of excursions below the threshold for a range of Stokes (St = 0.1 – 1.0) and Reynolds (Re_l = 100 – 500) numbers at Froude numbers Fr ≫ 1. Based on their frequency and joint statistics of depth and duration, we can apply our criterion and predict the rate of sling events.

Fully resolved simulations confirm in good approximation our predictions for small Stokes numbers and the considered range of Reynolds numbers. While the covered Reynolds numbers are significantly smaller than expected in cloud conditions, the prediction can be straightforwardly extrapolated, enabling estimates of rate of sling events at higher Reynolds numbers previously inaccessible to theory.

To capture a broader parameter range and, therefore, make our prediction applicable to a broader spectrum of cloud conditions, we plan to rigorously include the effects of gravity in future work.

6.8 MULTI-LEVEL STOCHASTIC REFINEMENT FOR COMPLEX TIME SERIES AND FIELDS

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Many high-dimensional nonlinear systems display a remarkable degree of complexity in space and time. As a consequence, spatio-temporal records of such systems often exhibit non-trivial statistical features, including multi-scale correlations and scale-dependent deviations from Gaussianity. A comprehensive statistical characterization of such systems requires knowledge of the full multi-time–multi-point statistics – a prohibitive task given the high dimensionality of typical systems. Significant simplifications arise if a hierarchy of scales in space and/or time can be identified, as it is the case for hydrodynamic turbulence [1] and many other scale-Markovian systems [2]. In these systems, the transition probabilities contain the full statistical information of the system, leading to a significant reduction of complexity. In many situations, however, a purely statistical characterization is insufficient. Rather, a complete spatio-temporal record is needed, yet, in practice, it is challenging or even impossible to obtain.

In [3], we introduce a data-driven method, which allows generating statistically well-defined time series or fields with non-trivial features in a hierarchical fashion. To do this, we use a hierarchy of three-point conditional PDFs, $p(u_c|u_l, u_r)$ at levels of increasingly smaller scales $L$, containing the information about the distribution of the velocity $u_c$ at a center point, given the left-bound velocity $u_l$ and the right-bound velocity $u_r$, each separated by the scale $L$. By iteratively generating center velocities by drawing velocities from these conditional PDFs, we can generate a synthetic field with a desired resolution from coarsely sampled initial conditions corresponding to the lowest level 0.

To illustrate the capabilities of this method for turbulent flows, we use experimental turbulence data from the Variable Density Turbulence Tunnel VDTT at the MPI DS [4, 5] to directly extract the transition PDFs and to generate synthetic time series. The original time series and the synthetic data show a virtually indistinguishable behavior (see figure 6.25) and share key statistical features such as an increasingly intermittent behavior towards the smaller scales, as seen in the scale-dependent PDFs of the velocity increments, $v$, in figure 6.26. Due to the low requirements of the method, as well as due to the fast and efficient generation of surrogate data, the multi-level stochastic refinement appears to be a promising method for a broad range of applications.

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**References**

Water droplets, ice crystals, and aerosols (dust, volcanic ash, pollen, soot, pollutants, etc.), which we collectively refer as particles, are ubiquitous in Earth’s atmosphere. Aerosols are the seeds (condensation nuclei), which are essential for the formation of water droplets and ice crystals. These particles affect precipitation and radiative transfer due to their light-scattering and absorbing properties, which has impacts on both local weather and global climate.

Yet, much remains to be understood about the dynamics of cloud particles, in large part due to the large range of scales involved, from the size of the particles themselves (nanometres to millimetres) to thousands of kilometres. One of the problems concerns the transport and settling of non-spherical and irregular particles such as aerosols and ice crystals, which determines how far particles can be transported and how long they stay in the atmosphere before settling to the ground (or in the case of ice crystals, possibly sublimating before they reach the ground).

In clouds, how particles grow is yet another open question. It starts with the activation of cloud aerosols where water vapour condenses onto them to form droplets and ice crystals. The growth dynamics of water droplets across the so called “size gap” between the diffusive growth regime dominated regime ($d < 20 \, \mu m$) and differential gravitationally settling induced collision dominated regime ($d > 100 \, \mu m$) remains unclear. These problems make accurate aerosol transport, rain, and snow prediction difficult and a detailed understanding is necessary for reliable climate prediction and weather forecasting. To better understand these processes, the LFPB investigates many aspects of these problems by carefully controlled laboratory experiments, numerical simulations and field measurements in atmospheric clouds. These range from experiments with small settling ellipsoidal particles and activation in the cloud aerosols in hydrometeor wakes all the way to direct measurement of water droplets at small scales in atmospheric clouds in the field.

### 6.9.1 Clustering of cloud droplets

(G. Bagheri, J. Moláček) The life-cycle of clouds strongly depends on the poorly understood collision rate between cloud particles in the “size gap”. Quantifying the collision rate in a laboratory setting or numerical simulations is complicated by the potential influence of hydrodynamic interaction or electrostatic forces between the droplets, and by the low dissipation rate and large Reynolds number typical for atmospheric
flows. To investigate the cloud droplet collision rate, we have built a particle tracking setup (see Fig. 6.27 and [1]) at the environmental research station Schneefernerhaus, dubbed the "Seesaw" for its ability to tilt. With this device, we can not only obtain the three-dimensional droplet positions to within a few micrometers, but also deduce the individual droplet diameters from the amount of light scattered onto each camera aperture.

From the position information, we can derive the droplet velocities and accelerations, and thus quantify both the droplet spatial distribution and the statistics of their relative velocities, the two main components yielding the collision rate. Knowing the droplet sizes on the other hand allows us to compute the Stokes number, the dimensionless parameter capturing the droplets’ inertia, and thus compare our measurements with results of existing numerical simulations and theory. The clustering and velocity statistics that are most interesting from the point of view of droplet collisions are naturally those for droplets at smallest, nearly touching separations. Although such separations are inaccessible to us due to the fundamental limits of the optical method used, we were nevertheless able to resolve sufficiently close separations (see Fig. 6.28) to essentially confirm the validity of certain numerical simulations [2] and rule out observable hydrodynamic interaction effects reported in some laboratory experiments [3]. More work is needed to put our data on droplet relative velocity statistics into the context of existing literature, due to their higher dimensionality.

6.9.2 The Max Planck CloudKites (MPCKs): Airborne characterisation of cloud microphysics and atmospheric turbulence

(G. Bagheri, F. Nordsiek) In order to investigate the dynamics of cloud droplets relevant to better understanding their growth processes, the MPCKs were flown to measure clouds in situ and their surrounding environment. The LFPB’s MPCKs are 35–250 m$^3$ helium-filled aerostats carrying atmospheric instrument packages to size and image cloud droplets and measure turbulent and thermodynamic quantities. Helium-filled aerostats were chosen because their low flight speed compared to airplanes and helicopters, which must fly at medium speed to keep instruments out of the prop wake. Using the MPCKs allows higher spatial resolution measurements, higher cargo capacity than UAVs/drones, longer flight times (limited only by the instrument battery) compared to powered aircraft including UAVs/drones, and greater travel distance from topographic effects than surface stations.

The MPCKs have flown on two ocean based field campaigns to investigate marine boundary layer clouds: a campaign in the Atlantic Ocean on the RV Maria S. Merian (MSM82-2, 2019), and the EUREC4A campaign (2020) in the vicinity of Barbados on the RV Maria S. Merian (MSM89) and RV Meteor (M161) together with CIMH (Caribbean Institute for Meteorology and Hydrology) as part of the EUREC4A collaboration [4]. The MPCK is also part of the TWISTER collaboration.
to investigate the dynamics of atmospheric boundary layer through numerical and experimental approaches, see 6.10.

One MPCK from EUREC4A is shown in Fig. 6.29. During EUREC4A, 28 flights with recoverable data were flown (there were 4 additional flights: 2 test flights with no instruments, 1 test flight with just a radiosonde, and 1 flight lost to the sea) for a total of approximately 250 flight hours with data being successfully acquired for approximately 210 of those hours. This includes 144 hr of CDP (Cloud Droplet Probe) data, 900879 holograms (about 200 min worth), and 447737 images from the 2-frame PTV/PIV system (about 250 min worth).

Fig. 6.30 shows hologram reconstructions of several large droplets from a cloud and a vertical profile of the virtual potential temperature during an ascent in stable conditions ($\partial q_v / \partial z > 0$). The long endurance of the MPCKs allowed long flights up to 19.5 data hours (nearly double the endurance of the other long endurance aircraft). The MPCKs, along with the P-3, were also the only aircraft to fly at night which was, coupled with the long flight endurance and many flight hours, very important for capturing the full diurnal cycle.

6.9.3 Dynamics of non-spherical particles

(G. Bagheri, Y. Wang) The settling of small non-spherical and irregular particles (includes most aerosols and ice crystals) is poorly understood. In particular, it is not quantitatively understood how particles of different shapes orient themselves in turbulent flows and how fast their orientation responds to flow fluctuations. Experiments on single particles in a quiescent medium are the first step to characterise this.

Our work was initially focused on freely falling ellipsoidal particles in the "intermediate" regime of particle Reynolds number 1–10 using shadowgraphy in an air-filled column setup. The particles are well-defined ellipsoids with the same volume (equal to that of a 140 $\mu$m diameter sphere), but different ratios of their axes. This only became possible thanks to 2-Photon-Polymerisation, a recent commercially available 3D-printing technique with unmatched accuracy (down to 200 nm). The density ratio between the particles and the medium (air) is approximately 1000, which is representative of atmospheric particles. The experiments are performed using four high-speed cameras to capture both the transient and the terminal state. Fig. 6.31 shows several printed particles in free fall as recorded with the described setup. In addition, Lattice-Boltzmann simulations are being performed as a base for comparison and to widen the parameter space. This allows us to look into terminal velocities, drag, and the transient dynamics to answer the following questions. Do stable fixed points in the orientation or oscillatory motions exist and is there a stable orientation that the particle will take? For particles with unstable transient orientation, what is the steady-state orientation? Further shapes are currently under research, covering non-homogeneous particles and complex shapes, such as irregular ice crystals and aggregates.
6.9.4  Cloud aerosol activation by precipitating hydrometeors

(G. Bagheri, Y. Wang) One of the many mysteries in clouds is that we still do not understand how and why the number of ice particles inside clouds exceed the number of ice nucleating particles that could be activated based on the bulk temperature and super-saturation. What are the major sources behind this excess (secondary) production of particles? We have found and investigated a possible mechanism – how large precipitating raindrops and ice particles can cause surrounding cloud aerosols to activate, thereby resulting in new water droplets and ice crystals [5]. As the large hydrometeors fall under gravity, they can activate in their wake aerosols that would not be activated otherwise. Warm droplets with a diameter of \( \sim 2 \) mm were able to induce activation of the ambient sodium chloride and silver iodide aerosols as water droplets and ice crystals in their wake when precipitating through a sub-saturated colder environment (Fig. 6.32). Extending the experiments, the numerical work [6] studied the flow pattern around hydrometeors (e.g., droplets, sleet, or hail) and presented a detailed analysis of various physical factors that lead to an excess of water vapour condition behind the hydrometeors and investigated the effectiveness of this process on activation of aerosols to create new cloud particles [7]. It is found that not all aerosols, but only some ‘lucky aerosols’ are entrained in the wake behind such precipitating hydrometeors, where they can reside in a highly humid environment for a sufficiently long time (Fig. 6.33). This fulfills the necessary conditions for the aerosols to be activated as new cloud condensation nuclei or ice nucleating particles by deposition of water vapour.

![Figure 6.32: Nucleation of water droplets and ice particles in the wake of a falling drop (diameter \( \sim 2 \) mm) that is warm relative to the ambient cold conditions. Ambient temperature \( \sim -18 \) °C, relative humidity \( \sim 60 \) %. The initial drop temperatures are (a) 10 °C, (b) 10 °C, and (c) 20 °C. The number concentration of the Snomax aerosol particles in the chamber was \( \sim 10^4 \) cm\(^{-3}\) in all cases except in (a), where it was \( \sim 10^3 \) cm\(^{-3}\).

![Figure 6.33: Tracks of the excess water vapour (S>0) that two aerosols experience when they entered the water vapour rich environment behind a precipitating frozen hydrometeor at 0 °C temperature falling through an ambient at -15 °C and 95% relative humidity condition.](image)

6.10 INVESTIGATION OF ATMOSPHERIC TURBULENCE AND CLOUD MICROPHYSICS IN THE TWISTER PROJECT

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A major challenge in understanding, modeling and consequently predicting atmospheric flows on our planet arises from the enormous range of scales involved. While weather patterns can extend over hundreds of kilometers, local processes that govern the generation and sustainment of clouds range from sub-km down to µm scales. Even the most advanced simulations of our Earth’s climate cannot resolve the complex physics of local atmospheric flows. On these scales, turbulence plays a crucial role, having a significant impact on cloud mixing, the growth of water droplets, and ultimately the initiation of rain. Our current understanding of these processes remains very limited. The Max-Planck-Fraunhofer Collaboration Project TWISTER investigates turbulence in the atmospheric boundary layer in a combined experimental, computational and theoretical approach. In particular, we focus on the interaction of turbulence in the atmospheric boundary layer with cloud microphysics.

The Max Planck CloudKites (MPCKs), each composed of an instrument box and a tethered hybrid of kite and helium-filled balloon commercially known as Helikite, are the main experimental platform in our work for in-situ measurement of fine-scale atmospheric turbulence and cloud microphysics (see also Sec. 6.9). The MPCKs have proven to be very reliable for field measurements during the EUREC4A field campaign [3]. The MPCK+ instrument box shown in Fig. 6.34, equipped with state-of-the-art holography and particle image velocimetry modules, in combination with a variety of meteorological sensors, can provide a detailed picture of the atmospheric boundary layer and the clouds within it. In addition, within TWISTER and in collaboration with Fraunhofer IPM, a compact Light Detection and Ranging (LiDAR) system is being developed specifically for the MPCK to measure the much needed undisturbed three-dimensional wind speeds in the vicinity of the MPCK. These detailed in-situ measurements, together with computational investigations, form the core of the TWISTER project aimed at characterizing the dynamics and evolution of the atmospheric boundary layer and clouds.

A major focus of our current work is the characterization of small-scale turbulence properties. This comprises the accurate determination of the dissipation of kinetic energy as well as a characterization of the local instationarity, inhomogeneity and anisotropy (Fig. 6.35). In addition to field data, numerical simulations provide ground-truth data to develop calibration techniques and software for data analysis.

Collisional droplet growth, a key process in rain formation, is an-
other major focus of our work. To study droplet growth in controlled conditions, we explore in a combined computational and theoretical study how individual droplets grow in a turbulent flow with a statistically stationary background droplet distribution (Fig. 6.36). This enables a precise assessment of the collision kernel and the statistical details of the collision process. For example, we have found significant correlations between subsequent droplet collisions which are commonly neglected in simple models for collisional growth. This theoretical work will guide future analysis of droplet measurements with the MPCK.

We also aim at connecting the microphysical processes in clouds with larger-scale phenomena in the atmosphere. To this end, we perform computational investigations of convective boundary layers (CBLs) in which turbulence is driven by shear and convection. We specifically aim for a statistical description of the relevant atmospheric variables like wind velocity and temperature [1]. To this end, we have derived the evolution equations for the corresponding probability density functions. The equations feature unclosed terms which we investigate using simulations [2] (see Fig. 6.37). The results will help to statistically characterize various atmospheric conditions and to derive accurate statistical models. We plan to compare our results to field measurements obtained within the TWISTER project as described below.

High-resolution wind velocity measurements have been identified as the most important quantity for characterizing atmospheric turbulence. To address this need, a compact Frequency-Modulation Continuous Wave (FMCW) LiDAR is currently being developed by the Fraunhofer IPM to be installed on the MPCK. The unique feature of the design is that the LiDAR will be equipped with three independent telescopes. This creates a flexible system that can measure three line-of-sight wind speeds while keeping weight and power consumption low. The LiDAR can provide three-dimensional wind velocity at a distance of \( \sim 15 \text{ m} \) from the MPCK, which is far enough from the MPCK so that none of the velocity components are affected by the MPCK itself. With 1 m\(^3\) and 10 Hz spatial and temporal resolutions, respectively, and flexible telescope-head arrangements, which allows it to be used for forward or lateral probing with minor modifications, the LiDAR will significantly enhance the capabilities of the MPCK. While the Continuous Wave (CW) feature allows for high spatial resolutions, the Frequency-Modulation (FM) feature enables it to significantly suppress background from clouds or hard targets (e.g. the ground if facing downwards) as well as a verification of the distance where the wind is measured, yielding a higher measurement accuracy. First tests with the new system are planned for early 2022 in preparation of forthcoming measurement campaigns.

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6.11 INTERACTIONS BETWEEN BIOLOGICAL CILI A AND BETWEEN CILI A AND PARTICLES

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Motile cilia are hair-like organelles beating with a whip-like stroke that breaks time-reversal symmetry to transport fluid or propel microorganisms in environments at low Reynolds numbers. On surfaces with many motile cilia, the cilia can coordinate their cycles such that their phases form metachronal waves. The flows generated collectively by beating cilia are involved in a number of physiological functions including mucus clearance in airways, L/R symmetry breaking in embryonic development and establishment of complex and dynamic flow patterns of the cerebrospinal fluid in brain ventricles (Sec. 8.16). Natural cilia have inspired various designs of artificial biomimetic cilia (Sec. 7.17).

How can we predict the collective behaviour of arrays of many cilia coordinated by hydrodynamic interactions, and in particular, the properties of the emerging metachronal waves, from the single-cilium characteristics? We addressed this question using a bottom-up coarse-graining approach and obtained results that contribute to understanding how the dynamical self-organization of ciliary arrays can be controlled, which can have significant biological, medical, and engineering implications.

Figure 6.38: (a) Spontaneous emergence of metachronal waves in numerical simulations on an array of $10 \times 10$ model cilia. The phase $\phi$ across the array is shown at 6 points in time, measured in units of the beating period $t_0$. (b) Dispersion relation of metachronal waves. Blue shaded regions indicate the stable wave zones as determined by linear stability analysis.

We proposed a theoretical framework for understanding the coordination of many independently beating cilia through hydrodynamic interactions [1]. We use a simple model of a cilium, which is represented by a small sphere moving along a tilted circular trajectory above a substrate. Each cilium is driven independently by a tangential force acting on the bead. In a 2D array of cilia, the hydrodynamic interactions also influence the beat cycle, because a single cilium creates a flow that affects the speed at which other cilia move along their trajectories. We used a far-field approximation (assuming the distance between cilia is large in relation to their size) to analyze the dispersion relation and the stability of metachronal waves in an array of cilia on a lattice with periodic boundary conditions. A wave with a wave vector $k$ is stable if the growth rate of perturbations with all possible wave vectors $q$ is negative. The results show a stable region for longitudinal waves (Fig. 6.38b), in agreement with numerical simulations (Fig. 6.38a).
Primary cilia, which are usually immotile, have primarily sensory functions as receptors for chemical or mechanical signals. However, there is mounting evidence that the sensory functions are not limited to immotile cilia and that beating cilia can also contain chemical receptors. This raises the question whether there is a physical advantage in placing chemical receptors on a cilium in terms of sensitivity. To answer this question, we studied the capture rates of signalling particles on a model cilium embedded in a flat surface [2]. The particles were subject to diffusion and advection, and were considered as absorbed upon the first contact with the surface of the cilium. We derived approximate analytical solutions for some limiting cases (immotile cilium in a quiescent fluid or in a shear flow at high Péclet number). In general, we solved the Stokes equation for the flow around the cilium by representing the latter as a chain of beads using the Rotne-Prager approximation and subsequently simulated particle trajectories using Brownian dynamics with advection.

Figure 6.39: The particle capture rate per cilium (length of red bars) for: (a) an isolated immotile cilium, (b) a group of 7 immotile cilia, (c) an isolated beating cilium and (d) a group of 7 beating cilia. While the capture rate in a group of immotile cilia is reduced due to depletion, motile cilia benefit from mutual enhancement by the generated flow.

To quantify the advantage of receptors located on cilia, we calculated the surface area of a flat circular absorbing region and compared it to the surface area of the cilium. We showed that, even in a quiescent fluid with no advection, the cilium already achieves the same capture rate as a surface patch with $4 \times$ the surface area. When the cilium is placed in an external shear flow, the equivalent surface ratio rises to $6 \times$. A motile cilium can achieve a significant enhancement of the capture rate at high Péclet numbers, but only if it beats in a non-reciprocal way and thus induces a long-range net flow in the surrounding fluid, which provides an influx of signalling particles. When many immotile cilia are placed in proximity, the capture rate per cilium is reduced because of depletion of the concentration field. However, when the same cilia beat asymmetrically, their capture rate can exceed that of a single beating cilium (Fig. 6.39). The reason is that the capture rate on each cilium is enhanced by the flow generated by the surrounding cilia.

A quantitative analysis shows that the sensitivity enhancement is particularly relevant either in viscous fluids or for large particles, for example small vesicles that have been hypothesized to establish the left-right asymmetry in embryonic development [3].

Simple equilibrium models of electrolyte solutions, which incorporate Coulomb interactions and the thermal fluctuations of the ions, conventionally rely on the screening phenomenology of the Debye–Hückel theory [1]. Out-of-equilibrium descriptions of an electrolyte in the presence of external electric fields, on the other hand, commonly utilize mean-field assumptions and thus neglect the statistical correlations among the ionic dynamics [2].

We theoretically investigate the nonequilibrium ionic fluctuations in a simple setup – which comprises of a strong binary electrolyte that is driven by a constant electric field – through systematic coarse graining of microscopic Langevin description [3]. In sharp contrast to the screened correlation functions of equilibrium electrolytes, our results show that ionic correlations beyond the Debye screening length are generally long ranged (\( \sim r^{-d} \) in \( d \) dimensions) in the presence of an external field; the novel dipole-like power-law correlations are a manifestation of the so-called generic scale invariance in anisotropic diffusive dynamics that break the detailed balance condition.

Having established the existence of long-ranged correlations in the driven electrolyte, we analyze its immediate implication in terms of the stress exerted on confining boundaries, in the context of nonequilibrium fluctuation-induced forces (FIFs). We analytically show that in the Casimir geometry with the electric field parallel to the boundaries (see Fig. 6.40), the steady-state perpendicular FIF per unit area of boundaries at separation \( H \) is given by \( F_S = \frac{k_B T H}{d E^4 A(\mathcal{E}, \lambda)} \), where \( \mathcal{E} \) is the dimensionless electric field, \( A \) is a (nondimensional) amplitude, and \( \lambda \) is the dielectric contrast between the electrolyte and the boundary material. Numerical and analytical examination reveal that the steady-state FIF can change sign, indicating that both its magnitude and direction may be controlled by changing the external field.

Furthermore, we examine the dynamics of the FIF when an electrolyte solution is quenched from its equilibrium state by a constant external electric field [4]. Over time, the force develops toward its steady-state value diffusively, and therefore the transient forces decay algebraically slowly (\( \sim t^{-d/2} \) and \( \sim t^{-(d-1)/2} \), depending on the value of \( \lambda \)). The transient and steady fluctuation forces in driven electrolytes that are uncovered by our analysis are important to correctly understand the force generation mechanisms in nonequilibrium electrolytes and might be useful, e.g., in manipulating colloidal particles immersed in charged solutions.

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6.13 OPTOGENETIC CONTROL OF THE HEART

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Lethal cardiac arrhythmias are associated with sustained spiral and scroll waves of electrical activity in cardiac tissue. The development of new treatment strategies requires a deep understanding of the underlying mechanisms. Optogenetics provides an excellent research tool for detailed investigations. From the identification of new nonlinear mechanisms of arrhythmia termination, such as the dissolution of the spiral organising centre or "core" (see Fig. 6.42 A-E), to the implementation of established mechanisms, such as directional drift [1, 2] of the associated spiral wave, in favour of termination, we have applied cardiac optogenetics in a wide range of studies to better-understand the spatiotemporal evolution and control of complex arrhythmias in the heart [3, 4]. Currently, we are exploring the possibility to terminate arrhythmias using a method called feedback-controlled drift [2] (see Fig. 6.43), whereby a measuring electrode guides the drift of a spiral wave towards a region of inexcitability. Finally, we are trying to expand the scope of cardiac optogenetics to provide physiological "upgrades" to the heart as and when needed. To this end, we are testing the implementation of anti-tachycardia pacing (ATP) (a clinically approved method for terminating cardiac arrhythmias) in optogenetically modified hearts, by using the heart's own pacemaker to eliminate abnormal electrical activity [5] (see Fig. 6.44).1

Figure 6.42: (A) A single spiral in simulated optogenetically-modified mouse ventricular tissue in the absence of illumination. (B-D) Progressive termination of a single spiral wave in the presence of low-intensity global illumination. (E) Voltage time series from a representative point in the simulation domain (indicated with a cross marker in (A)), showing the transient termination time (red-dashed rectangle). See also Sections 8.22, 8.24 and our website.

Figure 6.43: (A) ECG signal from a mouse heart showing feedback-based control of an arrhythmia using a sequence of global optical pulses (shown with a blue trace). (B) Schematic diagram of the experimental setup for global periodic illumination using three LEDs around a hexagonal bath that contains the mouse heart (red dot). (C) Numerical demonstration of drift and termination of a single spiral wave during feedback pacing with a measuring electrode located at the right bottom corner of the domain (red dot). See Sec. 6.14.

Figure 6.44: (A) (Top) Experimental evidence of increased sinus rhythm frequency under illumination in the mouse heart. (Bottom) Numerical reproduction of top panel in human SA node model. (B - E) Removal of a spiral wave from 2D human atria with pulsed illumination of the SA node (left bottom corner of the square simulation domain) and surrounding atrial tissue. For detailed demonstration of spiral wave termination via opto-ATP, see our website.1

1https://bmp.ds.mpg.de/research/optogenetics/

The control of the spatiotemporal dynamics of excitable media is a fundamental research problem in the physics of complex systems that has important applications in clinical cardiology. In the heart, ventricular fibrillation (VF) is associated with vortex-like rotating waves of excitation that can prevent the heart from pumping and lead to sudden cardiac death. For a lack of a better strategy, terminating VF requires high-energy electrical shocks that have significant side effects, including excruciating pain, tissue damage and worsening prognosis. Research at MPI DS has contributed to the development of low-energy termination of atrial and ventricular fibrillation \cite{1}, paving the way for painless and non-damaging arrhythmia control. Figure 6.45 (a,b) shows an example of low-energy control of VF compared to the conventional defibrillation in a Langendorff-perfused pig heart (ex vivo). The translation to clinical application, however, requires additional optimization. Therefore, we have further improved the efficacy and robustness of low-energy defibrillation by developing 4D cardiac imaging \cite{2}, elucidating the dynamic mechanisms underlying fibrillation using simulations \cite{3,4,5,6}, optimizing control algorithms using machine learning (see Sec. 8.23) and optogenetic tools (see Sec. 6.13). We have conducted numerical and experimental studies to investigate the effect of electric field geometry on defibrillation efficacy \cite{7}. In collaboration with the Uecker lab (Graz), we have developed an MRI-based measurement technique and numerical simulations to determine the three-dimensional current distribution in tissue to further optimize low-energy defibrillation towards clinical application (Fig. 6.46).\cite{2}

**Figure 6.45:** (a) Experimental setup for arrhythmia control in a Langendorff-perfused pig heart (ex vivo) using mesh electrodes. (b) Success rate of termination of VF in a pig heart (ex vivo) using single shock (blue) and pulsed electric currents (orange) as a function of electrical current normalized by heart mass. (c) Simulation of current density in pig using 3D-CT data (ICD housing - gray, heart with catheter electrode - red).

**Figure 6.46:** MRT Current Density Imaging in an excised pig heart.

\[1\] S. Luther et al., Nature 475, 235 (2011)
\[2\] J. Christoph et al., Nature 555, 667 (2018)
\[6\] T. Lilienkamp, U. Parlitz, Chaos 30, 051108 (2020)

\[2\]https://bmp.ds.mpg.de/research/cardiac_control/
6.15 ELECTRO-MECHANICAL DYNAMICS OF THE HUMAN HEART

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Understanding the spatio-temporal organization of cardiac fibrillation has challenged the scientific and medical community since the first reported observations in the 19th century. In their seminal work, J. Jalife and coworkers demonstrated vortex-like rotating waves during cardiac fibrillation in rabbit hearts using fluorescence imaging (optical mapping) [1]. The development of this technique has revolutionized the ability to characterize the electrical excitation of the heart, but it has two major limitations: First, fluorescence imaging can only visualize the surface of the heart, and second, it is very sensitive to mechanical motion. Our research has contributed to overcome these limitations and created a new approach to simultaneously measure electrical and mechanical waves in the heart. We have performed several studies to further develop and validate electro-mechanical imaging of the heart [4], to model contractile cells and their interaction [5, 6], and developed machine learning techniques to reconstruct spatio-temporal dynamics of the heart from sparse measurements. Based on first measurement of 4D mechanical vortices in the myocardium in preclinical experiments (Fig. 6.47), [2, 3] we are currently conducting a first in human study with patients undergoing bypass surgery. We have obtained the first measurement of 4D mechanical vortex during human fibrillation (Fig. 6.48), which enables the first comprehensive characterization of human ventricular fibrillation.3


3https://bmp.ds.mpg.de/research/cardiac_dynamics/
6.16 VEIN LOCATION DETERMINES VEIN FATE DURING NETWORK ADAPTATION

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Vascular networks continuously adapt their morphology by growing new or shrinking existing veins to accommodate for changing demands and to mitigate vein lesion or blockage. For nearly a century, local feedback from flow shear force on vein walls has been set forth as the driver for this continuous adaptation [1]. Yet, shear feedback alone cannot account for the observed diversity of network dynamics—a puzzle made harder by scarce spatio-temporal data. We quantify network-wide vein dynamics as well as associated shear forces in the prototypical vascular networks of *Physarum polycephalum*. Our experiments reveal a plethora of vein dynamics including stable as well as growing, shrinking or even vanishing veins as depicted in Fig. 6.49 [2].

Figure 6.49: Time series of network reorganization. Color scale indicates the ratio between the resistance of an individual vein $R$ and the rest of the network. Red arrows highlight unstable veins, black crosses indicate veins that disappeared within the previous time frame. The last frame highlights that an entire region vanished even though just a few veins are initially predicted to be unstable. Blue arrow highlights a vein that stabilized in the course of veins vanishing nearby.

We find quantitative agreement of data with our model—derived from a force balance on the tube wall—where shear feedback occurs with a time delay. The model reveals that local network properties are key to predict vein fate [2]. In particular, vein location relative to the rest of the network determines vein fate. As network reorganization changes the relative vein location of individual veins, a cascade of reorganization events unfolds which can cause clusters of veins to vanish. Our quantitative study predicts not only local vein adaptation but also cascading of vein dynamics leading to entire network reorganization (see Fig. 6.49). The physical foundation provided here allows to transfer findings across the different forms of life and to hijack life’s mechanisms for autonomous artificial designs of adaptive networks.

6.17 SAMPLING OF NEURONAL NETWORKS BIASES
ESTIMATES OF DYNAMIC STATES

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When inferring collective properties of complex systems experimentally, most often only a fraction of the system can be recorded — or, when recording the entire system, it can only be done in a coarse manner. We showed that such spatial sub-sampling or coarse-sampling (Fig. 6.51) can strongly bias inference about the collective properties of the full system [1, 3, 4]. To overcome that systematic bias, it is essential to understand how the sampling procedure affects the inference, and to derive analytical approaches to overcome the spatial sampling bias.

Sampling constraints are particularly severe for neuronal recordings: To date, only a few thousand of the million or billion of neurons of a mammalian brain can be sampled with high precision. Whereas subsampling does not pose a problem when inferring single neuron properties, the inference of collective properties, such as the population activity, can be severely biased. To enable reliable inference nonetheless, we have developed a subsampling framework for neuronal spiking activity and now provide tools to infer its collective properties (e.g. the spreading parameter c.f. Sec. 8.32, [2, 3] and cluster or avalanche size distributions [4]). Thereby, we could infer the spreading of activity reliably in experiments, investigate how it differs among brain areas, and shed light on spreading activity in epilepsy [5].

A typical sampling ansatz is to record spatially coarsened measures of neural activity (such as LFP or EEG). In this case, every electrode samples a spatial average of the activity of many neurons. While this enables sampling of larger parts of the system, the exact spatial reach of each electrode is hard to know (and may even depend on the dynamic state that is being recorded). This leads to two problems: First, the unique contribution of each neuron is hard to identify, which makes single-unit properties inaccessible. Second, multiple electrodes may record partly from the same neurons. Due to such measurement overlap, the recorded signals are spuriously correlated, and hence population-level observables may be biased. We showed that such coarse-sampling may cloud the difference between collective dynamics across brain areas or tasks [1]. In contrast, for subsampling we derived closed-form solutions that overcome the sampling problem.

6.18 PUNCTUATED EQUILIBRIUM NEURAL CIRCUIT EVOLUTION

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Brain evolution encompasses both extended periods of gradual refinement as well as major transitions in network architecture. Our previous studies \[1, 2\] raised the hypothesis that during visual cortex evolution, neural circuits must have switched between discrete but otherwise invariant architectural types. Testing this hypothesis in primates, we discovered a striking confirmation for such a punctuated-equilibrium mode of neural circuit evolution \[3\].

![Figure 6.52](image)

**Figure 6.52:** We examined V1 of one of the smallest living primates, the 60-g prosimian mouse lemur (Microcebus murinus). Mouse lemur V1 contains robust orientation domains and pinwheel singularities. Surprisingly, domain size was found to be only marginally smaller compared to much larger primates, suggesting that these circuit elements are nearly incompressible. The spatial arrangement of pinwheel singularities is well described by a common mathematical design of primate V1 circuit organization.

In rodents, we established the invariance of the alternative disordered architecture \[4\]. Together, our results demonstrate beyond any reasonable doubt that V1 architecture exhibits quantitative universality. We conjecture that the disruptive transition to this invariant architecture at the origin of the primate brain points to a fundamental switch in processing strategy \[5\].

We recently reported strong evidence for all-or-nothing transitions in network architecture during the evolution of visual cortical circuits [1, 2, 3]. This circuit remodeling presumably proceeded through intermediate stages that might be preserved in missing-link brains and which need to be understood to reconstruct the selective drivers of the transition.

To explore such transition states, we developed a synthetic biology approach to resurrect hypothetical transition architectures. Specifically, we use neuronal interface technology to connect a computational model of the retino-thalamic pathway to a ChR2 expressing in-vitro model of a cortical processing layer [4]. Using this system, we demonstrate a self-organized transition between a disordered rodent-like processing architecture and the domains and pinwheel singularity architecture universal in primate V1. Our synthetic hybrid circuit approach lays a foundation to experimentally probe the computational capabilities of transition state architectures and directly test the benefits associated with the V1 transition at the origin of the primate brain.

6.20 A DIRECT SPIN LIQUID TO QUASICRYSTAL
TRANSITION

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The primary visual cortex (V1) of all mammals contains orientation-
tuned nerve cells, selectively activated by visual stimuli of a particular
orientation. The underlying cortical circuits have been remodeled
during the evolutionary divergence of rodents, primates and carnivores
leading to two distinct designs: the rodent-typical salt-and-pepper
architecture, in which different preferred orientations are randomly
intermingled, and the pinwheel architecture of primates and carnivores,
in which preferred orientations are spatially clustered into orientation
domains around pinwheels. Accumulating evidence suggests that the
salt-and-pepper architecture is the likely ancestral state. It is, however,
unknown which mechanisms could have mediated an evolutionary
transformation between the two architectures [1, 2, 3, 4]. Here we show
mathematically that a gradual modification of the rules for dynamical
self-organization of visual cortical circuits can induce a direct transition
between a spin-liquid and a quasicrystalline state.

Figure 6.54: Direct transition from a disordered spin-liquid state to quasicrystalline
order in a model for the self-organization of large-scale neuronal circuits in visual
cortex. The model demonstrates that reducing unspecific recurrent inhibition and
enhancing specific and local recurrent excitation can induce a direct transition between
the architectures observed in rodent and primate V1 respectively.

This theory predicts that the salt-and-pepper architecture does
not emerge from random wiring but emerges from the capacity of
rodent cortical circuits to actively generate maximal response diversity.
We propose experiments to directly test this prediction using neural
interface technology.

DYNAMICS OF ACTIVE MATTER

As a young and rapidly evolving field in physics, active matter research focuses on systems in which individual units use energy from the environment or an internal energy source to drive themselves away from thermodynamic equilibrium. This activity can manifest in a variety of ways, most prominently self-propulsion, but also including chemical activity, momentum transfer to a surrounding fluid, growth and a variety of particle-environment interactions. The study of these systems relies on their characteristic features such as non-reciprocity, fluctuations, (possibly turbulent) flows, instabilities, phase transitions, symmetries and symmetry breaks. An understanding of the individual and collective behavior of active particles is one of the grand challenges of non-equilibrium statistical physics and may hold the key to a fundamental understanding of the emergence and self-organization of living matter.

Work on active matter at MPI DS bridges the scales of biological living matter, from enzymes, cellular organelles and cilia to cells, unicellular organisms and tissues, which possess fascinating emergent properties. Another research focus is on artificial, life-like active matter such as phoretic colloids and active droplets – physical systems which can often be described within the same theoretical framework – and systems that use components known from biology in a new context to create living matter. Success in dissecting the fundamental mechanisms that drive the complex behavior of these systems crucially depends on well-controlled experimental techniques, advanced theoretical tools and high-performance simulation techniques.

This chapter showcases the broad spectrum of active matter research at MPI DS, including both the study of concrete experimental systems, as well as theory-driven approaches that identify entire classes of active matter and characterize them based on their unique non-equilibrium properties.

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7.1 LATTICE BOLTZMANN AND JONES MATRIX STUDIES OF SELF-PROPELLING NEMATIC DROPLETS


Mesogenic oil droplets, self-propelling within an aqueous surfactant solution, are driven by a Marangoni flow in their surface [1] (see also Sections 7.2, 7.3, 7.4, 7.5). The surface flow induces within the droplet a convective flow which, if the droplets are in the nematic state, considerably influences the director field of the droplet. We report numerical simulations aiming at the determination of the nematic director field [2].

Figure 7.1(a) shows the internal flow field, resulting from a lattice Boltzmann (LB) model [3], of a droplet moving in the downward direction driven by a symmetric surface flow velocity \( v \propto \sin \theta \) which is taken as a prescribed boundary condition for the LB simulation. The symmetric flow field corresponds to a neutral squirmer moving on a straight trajectory. Experimentally, nematic droplets move on a straight trajectory only if they are confined to a capillary or a straight channel. In a 2D or 3D environment, the droplets self-propel on a curved trajectory and the inner (and outer) flow field is asymmetric [4], as is exemplified in Fig. 7.2(a) which shows an LB simulation for an asymmetric surface flow.

Both the symmetric and asymmetric flow field change considerably the nematic structure in the droplet. The \(+1\) point defect, which is in a resting (not self-propelling) droplet located at the center, is shifted in the symmetric case to the leading pole of the droplet. In the asymmetric case, the defect is deflected away from the leading pole to the side of maximum surface flow. Figures 7.1(b) and 7.2(b) show the director field structures predicted by the LB simulation. Polarizing micrographs, obtained numerically from a Jones matrix framework, show good agreement with experimental polarizing micrographs (Fig. 7.3), thereby confirming the reliability of the simulated structures and flow fields. Future studies will concern self-propelling nematic shells [5].

Figure 7.1: Symmetric convective flow field (a) and resulting director field (b) with advected point defect (red dot).

Figure 7.2: Asymmetric convective flow field (a) and resulting director field (b) with advected point defect (red dot).

Figure 7.3: Experimental polarizing micrographs (crossed polarizers with diagonal wave plate) of nematic droplets self-propelling in a capillary (a) and in a quasi 2D environment (c). Panels (b) and (d) show calculated micrographs based on the director fields shown in Fig. 7.1(b) and 7.2(b).

7.2 STOP-AND-GO DROPLET SWIMMERS

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In this project, we document multi-gait, bimodal motility in self-propelled artificial swimmers, consisting of oil droplets gradually dissolving in a micellar surfactant solution [2]. Self-propulsion is mediated by an unstable dipolar mode \( n = 1 \) in the distribution of oil-filled micelles around a droplet, which translates into propulsive Marangoni flows caused by a solute concentration gradient at the interface [1] - the oil-filled micelles act as a self-generated chemorepellent (Fig. 7.4a). We find a dynamical transition from quasi-ballistic to bimodal chaotic propulsion with increasing Péclet number \( Pe \) by controlling the viscosity of the environment, which we were able to quantify by simultaneously visualizing hydrodynamic (via tracer colloids) and chemical filled micelle fields (via fluorescent dyes). For increasing \( Pe \) we find a quadrupolar, non-propulsive \( (n = 2) \) mode that increasingly dominates the droplet dynamics. We interpret these observations by quantitative comparison to established advection-diffusion models via a linear stability analysis for dipolar and quadrupolar modes. Particularly, we derive an expression for \( Pe \) based on experimental parameters like viscosity and solubilization rate and match our experiments to the stability and growth rates for the respective modes within this framework (Fig. 7.4b).

We show that, with increasing viscosity, the non-propulsive \( n = 2 \) mode is preferably excited from the quiescent state, and the droplet is forced out of this mode by a local buildup of a self-generated chemorepellent gradient: the droplet recurrently switches between the two states, leading to a unique ‘stop-and-go’ motion (Fig. 7.5). This type of self-interaction promotes self-avoiding walks mimicking examples of efficient spatial exploration strategies observed in nature.

7.3 OSCILLATORY RHEOTAXIS OF SELF PROPELLING DROPLETS IN MICROCHANNELS

C.C. Maaß, R. Dey, C.M. Buness, B. Vajdi Hokmabad

Both artificial and biological microswimmers need to navigate in confinement and under external flow - examples are parasites in blood vessels, bacteria in pipes, navigating sperm or active sensors in lab-on-a-chip channels. Here, one typical feature is oscillatory upstream motion in microchannels, tubes and vessels. While the swimming strategies of biomicroswimmers are in many cases characterised by their complex shape and dynamics of moving parts like flagella, hydrodynamic theory suggests that oscillatory rheotaxis can already result from the pure hydrodynamic interaction of active swimmers – even spherically symmetric ones or point particles – with the parabolic shear flow inside a channel [2]. Active droplets are such spherically symmetric swimmers, and can be hydrodynamically modelled as weak pusher type squirmers. In this project, we placed them in quasi-2D microchannels and imposed varying degrees of imposed flow ([1], Fig. 7.6). Indeed, we observed an extremely regular oscillatory motion between the channel walls, which we were able to tune from upstream rheotaxis over trapping in place to downstream drift by controlling the imposed flow. The corresponding theory model comprises force and source dipoles and a source quadrupole placed in a plane Poiseuille flow. Interactions with the channel side walls, as well as top and bottom, which constitute no-slip boundaries, are implemented by the method of images. An advantage of this extended set of singularities over similar approaches, which e.g. do not account for the finite size of the swimmer by adding source terms, is that it correctly predicts the orientational and speed evolution of the squirmer during its interaction with the side walls: instead of crashing into the wall, the swimmer slows down, gradually reorients, and accelerates away from the wall (Fig. 7.7), leading to characteristic trajectories in real and phase space. We further established that the interaction of the droplet’s chemical footprint (see Sec. 7.2) with the Poiseuille flow has no measurable effect on the oscillation dynamics.

Figure 7.6: (a) Oscillatory upstream rheotaxis for weak flow, experiment (b) Oscillatory downstream drift for stronger flow. (c) Theory model for upstream rheotaxis. Colour coding: rheotactic velocity \( v_r \).

Figure 7.7: (a) Setup schematic of an active droplet in a microchannel. (b) Micrograph of rheotactic droplet with measured Poiseuille flow.

Microorganisms do not need to incorporate matter to transport it—they can also carry it along by entrainment. The exact manner of this mechanism matters, e.g. to determine feeding efficiency or to model the mixing and transport of small particulate matter like microplastics by microorganisms. To model transport in schools of swimmers, it is important to take a closer look at the single agent scale, especially the Darwin drift volume, i.e. the amount of fluid permanently displaced by a swimmer. It can be shown analytically that this volume depends both on the hydrodynamic characteristics, e.g. whether the swimmer is a pusher or puller type squirmer, and on the degree of confinement in the bulk fluid. In nature, this corresponds to transport in a porous medium, where the Stokes equations appropriate for unconfined bulk at low Reynolds numbers should be replaced by a Brinkman model. Interestingly, the idealized hydrodynamic model squirmer, a sphere with a prescribed interfacial velocity $v_q$, is experimentally realized by self-propelled droplets (see Sec. 7.2), in our case weak pushers. Droplet speed, $v_q$ and the drift volume can be determined quantitatively using tracer particles, and compared to analytical predictions.

In this study, we investigate the transport of fluid by a self-propelled droplet in quasi-2D confinement using tracer colloids ([1], Fig. 7.8). We then quantify the amount of liquid entrained, and derive the corresponding Darwin drift volume analytically for a Brinkman squirmer model. We find that the Brinkman model provides an excellent fit of the experimental hydrodynamics as compared to the unconfined Stokes squirmer. Numerically, we then extend our findings to cover collectives: To reveal how fast a school of droplets can push cargo particles through a microfluidic channel, the transport velocity was computed by integrating over successive entrainment events. We find that the total cargo capacity can be enhanced significantly compared to transport inside the micro-carriers alone by this type of ‘collective entrainment’ when the swimmers align with one another in a school (Fig. 7.9).

7.5 HISTORY CAGING IN ACTIVE EMULSIONS

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The constituent elements of active matter in nature often communicate with their counterparts or the environment via chemical signaling which is central to many biological processes. Such communications affect individual motility strategies as well as collective migration patterns: self generated chemical gradients aid fungal or bacterial colonies in effectively exploring space.

Here, in a purely physicochemical system, we use self-propelling oil droplets as a model for chemically active particles that modify their environment by leaving behind chemical footprints of oil-filled micelles [1]. These long-lived trails then act as chemorepulsive signals to other droplets. We first explore this communication mechanism quantitatively on the scale of individual agent-trail collisions. We start from the observation, by videomicrography, of droplets being repelled by the trails of other droplets (Fig. 7.10). We have confirmed by fluorescence measurements in the wake of dye-doped swimmers that the distribution of oil-filled micelles in the trail can be well approximated by a diffusing moving point source: we can therefore estimate the local chemorepulsive gradient from the Gaussian cross-section of the trail. We then match the trajectories for recorded trail interactions to an active polar particle model [2] incorporating both chemorepulsive force and torque coupling. We find in both experiment and theory that this interaction is primarily torque dominated and that the probability to cross a trail increases with the time lapse between passages and decreases with the incidence angle (Fig. 7.11 a).

Collectively, droplets actively remodel their environment while adapting their dynamics to that evolving chemical landscape - local density fluctuations are enhanced by frequent reorientations that lead to a transient trapping, where swimmers are caged between each other’s trails of secreted chemicals, until the droplet is pushed out by its own chemical buildup (Fig. 7.11 b). Dynamically, this is evident in the evolution of a plateau in the mean squared displacement for increasing number densities (Fig. 7.11 c).

7.6 MECHANISMS OF CHLAMYDOMONAS ADHESION TO SURFACES

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From a physiological perspective surfaces are highly relevant habitats of bacteria and also eukaryotic cells. Motile microorganisms may attach to surfaces from their planktonic, i.e. free-swimming state, thrive and form vital communities. We study the adhesion forces and kinetics associated to the early stages of surface colonization of ciliated microbes using contrast-enhancing microscopy and novel in vivo micropipette force measurements techniques [1]. The latter approach allows for quasi-static (adhesion) force [2, 3] and dynamic (propulsion) in vivo force measurements [4] on motile microbes, illustrated in Fig. 7.12. We discovered that the flagella-mediated adhesion of Chlamydomonas is reversibly switchable by light within a few seconds [2] and independent of the surface properties, e.g., its hydrophobicity [3].

More recently, we started exploring the underlying biophysical mechanisms of Chlamydomonas adhesion to surfaces from different angles. Complementing single-cell measurements with modern gene editing tools allows for dissecting specific biological functionalities and, thereby, unraveling their potential evolutionary advantages. More specifically, we teamed up with experts from the life sciences and study strains with targeted deletions related to a) sensory photoreceptors and b) glycosylation of the flagellar membrane proteins that mediate surface adhesion. We also explore the effect of chemical agents targeting the activity of the molecular motors to control microbial adhesion to surfaces. So far, the sensory photoreceptor triggering light-switchable adhesions yet remains to be identified, since deletions of the most prominent candidates can be excluded, see Fig. 7.13. The glycosylation of the flagellar membrane glycoproteins indeed directly affects the adhesion force of the flagella, see Fig. 7.14. In addition, we found that the presence of ciliobrevin-D, an inhibitor of the molecular transport machinery inside the flagella, may enhance the adhesion, both for the wild type and the glycosylation mutant [5].

Future studies will address further photoreceptor knockouts and combinations thereof to unambiguously identify the photoreceptor controlling light-switchable adhesion. These insights may inspire applications in bioengineering related to drug development and renewable energy, where control of biofilm formation is an outstanding challenge.

7.7 SELF-GENERATED OXYGEN GRADIENTS CONTROL
AGGREGATION OF PHOTOSYNTHETIC MICROBES

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Photosynthetic microbes have evolved under the periodic exposure
to sunlight and can be found in essentially all ecosystems of our planet.
These cells may dynamically respond to alterations of the luminous
intensity in their microhabitats, e.g., by performing phototaxis and
light-switchable surface association and maintain diurnal cell cycles.
However, in the absence of light, the microbes can sustain metabolic
functionalities and motility by switching their energy production to
aerobic respiration. Since aerobic respiration dominates in low-light
conditions, the microbial motility sensitively depends on the local
availability of oxygen if the light intensity is reduced.

Using microfluidic experiments (shown in Fig. 7.15) together with
continuum theory based on a reaction-diffusion mechanism, we show
that oxygen-regulated motility in self-generated oxygen gradients en-
ables a suspension of photoactive microbes to form highly localized
regions of high and low cell densities [1]. This aggregation is completely
reversible and directly depends on the light-regulated photosynthetic
activity, see Fig. 7.16. If the cell density is high and oxygen is not
replenished externally (oxygen may diffusive in from the sides) at a
sufficiently high rate, oxygen is locally deprived resulting in a decrease
of the microbial swimming velocity. As a result of a generic power-
law coupling between cell density and swimming velocity $\rho \propto v^{-2}$,
swimming microbes will aggregate in regions of reduced motility.

The continuum model starts from homogeneous initial conditions.
Due to aerobic respiration, we then observe a reduction of the oxygen
concentration at the center of the chamber, leading to a local slow-
down of the microbes and a subsequent accumulation of cells. In
particular, for low cell densities, oxygen is not sufficiently depleted and
all cells exhibit high velocities yielding a homogeneous distribution.
At a critical density of cells, a separation into regions of low and high
densities becomes noticeable, see Fig. 7.17. The minimal continuum
model suggests that the accumulation is driven by the collective oxygen
consumption and accurately predicts the critical cell density.

In conclusion, this light-regulated microbial aggregation is a direct
consequence of the ability of planktonic photosynthetic microbes to re-
versibly switch their energy production from photosynthesis to oxygen
respiration in unfavorable light conditions. The aggregates of motile
microbes form in the complete absence of light gradients (phototaxis),
nutrient sources (chemotaxis), aerotaxis and quorum sensing and thus
represent manifestations of a remarkable collective behavior of motile
living cells.

7.8 EMERGENT PROBABILITY FLUXES IN CONFINED MICROBIAL NAVIGATION

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When observing motile microorganisms under a microscope, their motion appears erratic and unpredictable. In confined environments, however, microbes are found to self-organize and produce striking examples of coherent mesoscale motion and patterns. Unraveling the nature of the underlying physical mechanisms requires an advancement of our understanding of the non-equilibrium forces that act on the single-cell level and also how the interactions between motile cells and solid boundaries are linked to emergent patterns.

Here, we study the swimming motility of a single bi-flagellated microalga *Chlamydomonas reinhardtii* in quasi-2D confinement. We revealed that the motion of the cell is guided by the curvature of the compartment, and that the microbe is likely to be detected in the vicinity of highly curved interfaces as a result of their steric flagella-wall interactions [1]. In this work, we theoretically predict a universal relation between the probability fluxes and global geometric properties of the microhabitat that is directly confirmed by single-cell experiments [2]. Employing active Brownian dynamics simulations, analytical theory and microfluidic experiments we find that the boundaries of the compartment induce flux loops in the interior of the compartment. Figure 7.18 displays a representative section of the cell’s trajectory in an elliptical compartment (a) as well as the underlying probability fluxes obtained from the experiment (b) and the simulations (c). We find quantitative agreement between experiments and simulations (Fig. 7.19). These insights enable us to decipher the most probable trajectories of motile cells in complex geometries (Fig. 7.20) and may inspire topological design principles for guiding their time-averaged motion.

Figure 7.18: Representative trajectory of a motile *C. reinhardtii* cell in quasi-2D confinement (a). The experimental data reveals emergent probability fluxes (b) that are in excellent agreement with results from active Brownian dynamics simulations of a puller-type microswimmer (c).

Figure 7.19: Mean flux in the vicinity of the boundary in tangential (red) and normal direction (blue) versus the boundary curvature. Experiments (circles) and simulation results (rectangles) exhibit quantitative agreement.

Figure 7.20: Active Brownian dynamics simulations reveal the topology of probability flux loops for a puller-type microswimmer exploring different types of compartment geometries. Flux strengths: color code; flux directionality: grey arrows.


7.9 MOTILITY & SELF-ORGANIZATION OF GLIDING CHLAMYDOMonas POPulations

S. Till, F. Ebmeier, A. Fragkopoulos, O. Bäumchen
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The model microbe *Chlamydomonas reinhardtii* exhibits the unique ability to reversibly switch between swimming motility and surface-based gliding motility in response to light [1]. In both modes of motility, the flagella play a key role for the force transduction. Once the cells have attached to a surface, an intraflagellar transport (IFT) machinery translocates the cell body along the flagella, which are oriented in a 180° configuration (see inset of Fig. 7.21a). While the swimming motility has been widely studied and is known to provide phototaxis as an important functionality, the evolutionary advantage of the gliding motility remains elusive so far.

We demonstrate that the gliding motility enables surface-associated *Chlamydomonas* cells to cluster and form compact, interconnected microbial communities [2]. We detect and analyze cell positions and trajectories at different times after the cells have adsorbed at the flat surface in response to a light switch, see Fig. 7.21, and calculate the Euler characteristics, shown in Fig. 7.22, as one of the two-dimensional Minkowski functionals to characterize the spatiotemporal evolution of the cell positions within the population. We find that simulations based on a purely mechanistic approach cannot capture the non-random cell positions, as shown in the inset of Fig. 7.22 (top). For sufficiently high cell densities, we find that the Euler characteristics evolves with time.

As shown in Fig. 7.22, quantitative agreement with experimental data is achieved when considering flagellar mechanosensing, which is implemented through a minimal cognitive model representing the flagellar exploration of available space. Extending a recent theoretical approach [3], we postulate a cognitive force associated to the cell’s mechanosensing and exploration of its surrounding. We also find that simulations that incorporate cognitive forces reproduce the experimentally observed percolation threshold, i.e. the surface coverage of cells for which an interconnected network emerges from isolated clusters.

In summary, gliding motility appears to be a key mechanism for the formation of dense clusters of *Chlamydomonas* cells on a surface, which enables the population of photosynthetic cells to form compact surface-bound monolayers for highly efficient light harvesting. Swimming motility and phototaxis are essential for *Chlamydomonas* in their natural habitats to map their environment for light sources. Once the cells have found optimal light conditions for photosynthesis, the cells may use their flagella to cling onto any surface and, subsequently, employ their gliding motility to cluster and form dense networks.

7.10 FUNCTION OF MORPHODYNAMICS IN FORAGING PLASMODIA

L. Schick, M. Kramar, K. Alim

Foraging for nutrients and shelter in an heterogeneous environment is key for the survival of living organisms. Foraging behaviour of animals is generally viewed as optimised for maximal energy uptake per search time by balancing time spent for environmental exploration and food exploitation [1]. Yet, it is unclear which foraging behaviour can be adopted by spatially extended organisms like the unicellular slime mould *Physarum polycephalum*. What foraging strategy does the large and adaptive network-like morphology allow for?

![Figure 7.24: Energy density distribution for elastic energy of tube contractions by viscous energy from the fluid scaled by number of tubes in a network for different morphological states.](image)

![Figure 7.23: P. polycephalum changes its morphology during the time course of foraging. It varies between three states (stationary (A), network (B), lightning (C), scale bar 10mm). Morphodynamics are described by the velocity of the plasmodium and the normalized radius of gyration. A trained neural network detects the state diagram in (D).](image)

Here, we follow the plasmodial network of *P. polycephalum* as it adapts its morphology, gradually moving its body mass as it is foraging for food. We evaluate the morphodynamics of the foraging plasmodia by calculating the normalized radius of gyration as well as the velocity of the moving front according to [2]. We identify three different morphological states by network compactness and the density of moving fronts. We distinguish between a low mobility stationary state, a network state and a potentially fast lightning state. This allows for the training of a neuronal network (Fig. 7.23). In order to understand the purpose of the continuous morphological changes, we investigate the energy distribution within the different morphologies (Fig. 7.24). We find that while the lightning state is minimising elastic energy spent during migration, denser and more heterogenous networks are minimising dissipation loss [3]. The morphological variability therefore allows the organism to adjust its energetic costs during foraging.

7.11 SELF-ORGANIZED ADAPTATION OF LIVING SYSTEM VIA PUMPING CONTROL

F.K. Bäuerle, S. Chen, S. Karpitschka, K. Alim

Wavelike patterns are ubiquitous in biological systems - from the undulatory locomotion of cells and animals, the cardiac cycle to myosin contractions. The patterns’ functions vary, but all are governed by a wave’s key parameters: amplitude, wavelength, frequency, and phase. When the environmental settings change these systems have to adapt their parameters - yet parameter choice is limited by physical or biological constraints. Which strategies does a living system use to fulfill the wave’s function given its constraints?

We, here, investigate how *Physarum polycephalum* controls its waves’ performance by stimulating it with light. We find that *Physarum*’s wave train consists of a dominant wave and its second harmonic introducing the phase difference $\Delta \theta$ between them as an additional adjustable parameter. We turn to theoretically study influence of the phase difference between harmonics on the pumping efficiency, see Fig. 7.25. We analytically show that the flow rate can be controlled by adjusting the phase difference while optimizing the required elastic energy for deformation. At the optimal phase difference the resulting wave shape occludes the tube most tightly, which optimizes pumping performance by over 25% under physiological conditions [1]. Investigating the peristaltic waves in Physarum, we initially find that unforced specimen favour minimal occlusion. Only when forced to transport mass by the light stimulus, specimens adjust their phase differences toward maximal occlusion optimal for pumping performance. The phase difference serves as a subtle, but powerful parameter, in line with our theoretical predictions.

Further, stimulating *Physarum* specimen of minimal topological complexity reveals that junctions such as in a Y-shaped topology also allow for more efficient pumping upon phototactic stimulus than topologically simpler I-shaped specimen. Given the abundance of wave phenomena, the strong impact of the seemingly subtle phase difference between harmonics and topology is likely important in a broad class of biological systems. Further, the discovered mechanism can be implemented in smart materials allowing for self-organisation of pumping rates.

![Figure 7.25: (A) Scheme of an axis symmetric tube undergoing peristaltic pumping driven by traveling wave. (B) Flow rate of a peristaltic pump as a function of the phase difference $\Delta \theta$ between dominant wave and second harmonic. (C) Scheme of dominant wave (yellow) and second harmonic (red) and their superposition (green dashed). Occlusion is maximal for $\Delta \theta = \pi$, where the minima of dominant wave and second harmonic align (right panel, compare arrows)](image)

![Figure 7.26: *Physarum* adapts its phase difference $\Delta \theta$ when forced to increase mass transport. *Physarum* with illuminated area (blue) at the onset of stimulus (A) and after (B). Bar 1mm. (C-E) Histograms of phase difference in three consecutive time windows after onset of stimulus.](image)

Droplets form by liquid liquid phase separation in an equilibrium process driven by weak interactions between the droplet material and the solvent. One important example in biology are droplets inside cells, which consist of biomolecules like proteins and RNA. In this case, the weak interactions can be tuned by chemical reactions like conformational changes, (de-)phosphorylation, or other posttranslational modifications [1]. This suggests that cells use chemical reactions to tune protein interactions and thereby control how droplets form.

In this project, we extend a model for phase separation [2] to include chemical reactions based on thermodynamic arguments. This is important, because the law of mass action and Fick’s law of diffusion break down for phase separating systems because they are neither ideal nor dilute. The aim is to identify how biochemical reactions can be used to control droplets in cells.

In our model, a protein is either in a state where it is soluble or it can phase separate from the solvent. A reaction can switch between the two states [3]; see fig. 7.27. At equilibrium, the ratio of the two states is given by the equilibrium ratio \( K \) of the reaction, while the total amount of protein is conserved. Therefore, the concentration of the phase separating state, which determines if droplets form, depends on the total amount of protein and the ratio \( K \). Because the equilibrium ratio \( K \) depends on the internal energies of the two states, it can be tuned independently of the protein interactions. Thus, \( K \) can be used as a control parameter to stabilize or dissolve droplets. This corresponds to tuning protein composition or global parameters like temperature or pH. Furthermore, we find that \( K \) differs in droplet and solvent phase [3]; see fig. 7.28. This implies that droplets are chemically different from the solvent, which can be used to control other reactions spatially.

Many biochemical reactions are driven away from equilibrium by consuming fuel molecules, like ATP. We model this by introducing a second reaction that uses the fuel to bias the transition towards the soluble state. We show that the driven reaction alone can be mapped to a quasi equilibrium reaction and the energy \( \Delta \mu \) that is liberated by the fuel determines the effective equilibrium ratio \( K \). If the reaction can happen with and without the use of fuel, a non-equilibrium reaction cycle between the two pathways arises which depends on the ratio \( \eta \) of the two reaction rates. If the driven reaction is faster (\( \eta \gg 1 \)) droplets shrink, because the soluble state is favored, while droplets are stable if the driven reaction is slow (\( \eta \ll 1 \)); see fig. 7.29. Taken together, a driven reaction cycle can control droplet formation and dissolution either via varying the driving strength or the reaction rates. This process is faster than changing protein amounts or interactions, but has an energy cost proportional to the amount of fuel consumed. Reaction rates can be controlled by enzymes that speed up the reaction,
e.g., kinases for phosphorylation reactions of proteins. Enzymes do not influence the reaction equilibrium and thus the equilibrium and the rate of a reaction can be tuned individually by changing $\Delta \mu$ and $\eta$, respectively.

Under the conditions discussed above the steady state will be a single large droplet due to Ostwald ripening. However, for the cell it could be advantageous to stabilize multiple droplet and control individual droplet size. In several biological examples, enzymes that catalyze reactions of key droplet components co-phase separate with the protein, which could allow individual size control of droplets [1]. In our model the enzyme speeds up the driven reaction and is enriched in the droplet by a factor $\exp(\chi_E)$. Here, $\chi_E$ describes the enzyme interaction with the droplet material. As a result, the driven reaction is faster in droplets, which leads to a chemical potential gradient between both phases, inducing diffusive fluxes, see fig. 7.30(a). While the reaction removes phase separating proteins proportional to the droplet volume $S \propto R^3$, diffusive fluxes lead to an influx that scales with the droplet area $J \propto R^2$. The balance between both fluxes leads to a stable droplet radius $R_\star$, see fig. 7.30(b), and the droplet size can be controlled by the enzyme segregation; see fig. 7.30(c). To conclude, we identify three conditions for size control of droplets: First, a reaction switches between a separating and a soluble state of the dominant droplet component. Second, a reaction cycle with external driving creates a non-equilibrium steady state determined by the reaction rates. Third, the reaction rates differ in droplet and solvent phase, e.g. by enriching an enzyme in the droplet. This drives diffusive fluxes between the phases that counteract ripening. The mechanism we unveil in our work allows biological cells to control the size of their droplets using non-equilibrium chemical reactions that also regulate virtually all other cellular processes.

Figure 7.30: Segregating enzymes can stabilize multiple droplets and control droplet size. (a): Chemical potential as a function of distance from droplet center. The different reactions in droplet (orange) and solvent (blue) lead to a chemical potential gradient which leads to diffusive fluxes between both phases. (b): Droplet growth rate (black line) is given by the sum of diffusive influx $J$ (blue) and reactions in the droplet $S$ (orange). The competition between both leads to a stable droplet radius $R_\star$ (black dot). (c): Stable radius $R_\star$ as a function of enzyme segregation strength $\chi_E$. Stronger enzyme segregation leads to smaller droplets.

Phase separation explains how biological cells can organize a plethora of intracellular compartments without membranes. These biomolecular condensates are involved in many cellular processes on all scales. Unique to the cellular context, these condensates can consist of only a few hundred molecules and are affected by non-equilibrium processes. In particular, active chemical conversion between condensate material and proteins in the surrounding cytoplasm can control their size; see Sec. 7.12. Moreover, the fluctuations due to the small molecule number imply that spontaneous nucleation and dissolution are likely. Yet, it is unclear how the driven reactions affect these stochastic processes.

We study the influence of chemical reactions on the nucleation of active droplets using a stochastic field theory. Here, we combine Cahn-Hilliard dynamics with chemical reactions converting a soluble precursor \( P \) into the droplet material \( B \) that can phase separate. We then study numerically the nucleation times for different reaction strengths using forward flux sampling to sample the probability distribution. We find an increase in the nucleation time with the increased strength of the chemical reactions; see Fig. 7.31. To investigate this effect further, we also analyze the transition from a homogeneous state to a state with a single droplet in detail. In particular, we use a mapping onto an equivalent equilibrium system, which allows us to evaluate the concentration profiles of the tiny nucleus and the associated energies along the nucleation paths; see Fig. 7.32. We find an energy barrier, which is caused by surface tension, similar to the passive case. However, we also identified that stronger reactions lead to higher barriers and classical nucleation theory correctly predicts the observed increase in nucleation time. For high reaction rates, the nucleation of droplets can be suppressed completely. Driven chemical reactions thus provide a mechanism that can suppress the formation of droplets, which might be relevant for biological cells.

In suspensions of microscopic active agents, complex dynamics emerge due to the collective driving of the fluid flow by individual agents. For agents with nematic interactions, the chaotic motion has been termed active nematic turbulence due to its qualitative similarity to classical turbulence. Continuum theories for active nematic turbulence have deliberately excluded inertial effects because the Reynolds number of microscopic flows is very small on the scale of individual agents. Yet, it is currently unclear whether the collective driving of microscopic agents can excite inertial effects. To address this question, we investigate a two-dimensional continuum theory for active nematic turbulence [1]. In essence, the theory couples the flow field and the orientation of the nematic agents. The coupling leads to distortions in the orientation field (defects), which in turn stir the flow (Fig. 7.33). We compare active nematic turbulence with and without the effects of advective inertia by systematically turning on and off individual terms in the non-dimensionalized equations of motion. Most strikingly, inertial effects give rise to large-scale fluid motion and an increase in the total kinetic energy for sufficiently strong driving (Fig. 7.34). A detailed analysis of the spectral energy budget reveals an energy transfer to large scales mediated by inertial advection. While this transfer is small in comparison to energy injection and dissipation, its effects accumulate over time. Adding friction, which is typically present in experiments, can compensate for these effects. By scanning a broad range of parameters, we found a large variation in the turbulent Reynolds number, a typical measure for the importance of inertial effects. Excluding inertial effects a priori in terms of a low-Reynolds number approximation is, therefore, only valid for parts of the parameter range. Our findings suggest that the inclusion of inertia and friction may be necessary for dynamically consistent theories of active nematic turbulence.

Figure 7.33: Streamlines and vorticity of the flow field (top), and orientational order of the active agents (bottom) in active nematic turbulence. Distortions in the orientation (green) give rise to strong local vorticity (dark red, blue).

Figure 7.34: Comparison of active nematic turbulence without inertia (O), with inertia (I), and with inertia and friction (IF). Top: time evolution of the kinetic energy. Bottom: snapshots of the flow field in each regime.

7.15 EMERGENCE AND MELTING OF ACTIVE VORTEX CRYSTALS

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Dense suspensions of swimming cells, such as bacteria or sperm, exhibit complex multicellular behaviors spanning from mesoscale turbulence to highly ordered coherent flow patterns. A major discovery was the spontaneous formation of regular vortex arrays in high-density suspensions of sperm cells [1] and microtubules [2]. Despite major efforts, such coherent flow patterns, and active vortex lattices in particular, remain poorly understood theoretically.

We conducted fully resolved active-fluid simulations on macroscopic domains to investigate the emergence and melting of active vortex crystals (see Fig. 7.35) in a generic, experimentally validated active fluids theory framework [3]. Through massive numerical computations at an unprecedented scale, we were able to compute the complete non-equilibrium phase diagram and identify melting pathways [4].

We revealed a complex transition scenario between active vortex crystal and active fluid phases. Depending on the precise path through parameter space, we find either a hysteretic phase transition or a two-step melting transition. In the latter case, the crystal first loses long-range orientational order and then melts into a liquid phase, see Fig. 7.36. The melting transition through this so-called hexatic phase is well known from the melting of equilibrium crystals, but so far has not been observed in an active matter system featuring self-organized vortex arrays. Our study therefore establishes analogies to phase transitions in equilibrium condensed matter systems, which will help to further explore and classify emergent phenomena in active matter.

Plankton in the ocean is an example of microscopic organisms in a fluid flow. These organisms form an integral part of the global carbon and nitrogen cycles. Understanding their interaction with the turbulent flow is therefore ecologically relevant. Self-motility, which allows organisms to consume internal chemical energy to self-propel in a fluid, and buoyancy regulation, by which organisms can move vertically in the water column, are two main strategies that enable cell migration.

As a model for microorganisms in the ocean, we study collision rates of ellipsoidal sedimenting or self-motile particles in turbulence to shed light on the dependence on their shape, turbulence intensity, and density offset or motility. We use direct numerical simulations (DNS) of the incompressible Navier-Stokes equations to obtain a statistically stationary turbulent flow that resembles the conditions of the upper ocean layer and that advects the ellipsoidal particles. The small-scale features of the flow induce tumbling and spinning of the particles, which reorient following Jeffery’s equations [1]. We include the above-mentioned mechanisms in particle dynamics: the particles are either self-motile or sediment due to negative buoyancy. We then measure particle collision rates of these particles as a function of their relevant parameters.

Shape plays a crucial role in determining the collision rates of sedimenting elongated rod-like particles (see figure 7.37). By comparing the collision rates of rods and spheres of equal volume, we find that the elongated shape leads to a several-fold enhancement of the rod collision rates. This enhancement provides a physical explanation for the time scales of collision-dependent biological processes in the ocean, such as bloom formation of slender plankton species. Self-motility has also a notable effect on collision rates of spherical particles in mild turbulence. We recover the classic Saffman-Turner collision kernel $G_{ST}$ sphere in the non-motile limit. We also derived the collision kernel for the ballistic limit, in which self-motility dominates over turbulent advection and the collision rate grows linearly with particle motility $v_s$. Furthermore, we studied spheres of different diameters $l$, and we found a collision kernel master curve, shown in figure 7.38. This master curve reveals the quantity $v_s/u_K \cdot \eta_K/l$ as the relevant control parameter, where $u_K$ and $\eta_K$ indicate the Kolmogorov velocity and length, respectively. Interestingly, the transition between the limiting cases happens at a very low swimming velocity below $u_K$. This result indicates that self-motile microscopic organisms in mild turbulence may greatly enhance their collision rates even if their self-motility is only a fraction of the typical small-scale velocities of the turbulent flow.

Figure 7.37: A We carry out DNS of turbulence and include particles, which are advected and spun by the flow. B shows sedimenting elongated rod-like particles. Their shape leads to enhanced collision rates in comparison to equal-volume spheres.

Figure 7.38: Motility significantly enhances collision rates due to increased collision velocities. A master curve for the collision rates of self-motile spherical particles of different sizes in mild turbulence starts from the Saffman-Turner collision kernel $G_{ST}$ sphere, in the non-motile limit, followed by a quick transition to the ballistic limit, in which collision rates are proportional to the motility $v_s$.

Synthetic biology takes its cue from the multiplicity of natural materials and architectures whose combination enables vital functions that lead to the living world as we know it. We can benefit from its approaches and engineering principles to develop active systems as dynamic and responsive materials with emerging and programmable functionalities. Biomaterials and bioinspired systems have great potential not only to uncover fundamental mechanisms behind complex biological functions, but also to drive progress in various fields, including medicine and environmental science.

We focus our efforts on the analysis of beating structures such as cilia or flagella isolated from biological microswimmers and used to develop synthetic swimming transporter. By using a few biological building blocks from flagella we show how synthetic cilia can be reconstituted. Furthermore, we show that synthetic tissues and cells can be assembled also by using non-biological materials with the aim of engineer materials characterized by the properties of biological systems such as self-regeneration, reactiveness and self-organization.

7.17.1 Light-powered reactivation of flagella and contraction of microtubules network: towards building an artificial cell

(A. Gholami, I. Guido) Artificial systems capable of self-sustained movement with self-sufficient energy are of high interest with respect to the development of many challenging applications including medical treatments but also technical applications. Our work demonstrates the biocompatibility and efficiency of an artificial light-driven energy module and a motility functional unit by integrating light-switchable photosynthetic vesicles with demembranated flagella that provide ATP for dynein molecular motors upon illumination. We engineered light-switchable photosynthetic liposomes (150 nm in diameter) as energy modules to generate ATP under illumination. The flagellar propulsion is coupled to the beating frequency and dynamic ATP synthesis in response to illumination allows us to control beating frequency of flagella in a light-dependent manner (Fig. 7.39A-B). In addition, we verified the functionality of light-powered synthetic vesicles in in vitro motility assays by encapsulating microtubules assembled with force-generating kinesin-1 motors and the energy module to investigate the dynamics of a contractile filamentous network in cell-like compartments.
by optical stimulation. Functionalized artificial liposomes capable of continuous production of ATP in response to light, can serve as an efficient energy source for in vitro microtubule motility assays in which kinesin-1 motors are actively engaged in generating active stresses in the network (Fig. 7.39C) [1].

7.17.2 Anomalous propulsion regime in axonemal-propelled cargoes

(A. Gholami) In our work isolated flagella from green algae *Chlamydomonas reinhardtii* as an ATP-fueled bio-actuator for propulsion of micron-sized beads have been used. *Chlamydomonas* flagella have an asymmetric waveform, which can be described as a superposition of a static component corresponding to an arc-shaped intrinsic curvature, and a main base-to-tip traveling wave component. By applying resistive force theory, we performed numerical simulations and obtained analytical approximations for the mean rotational and translational velocities of a flagellum-propelled bead. Our analysis reveals the existence of a counter-intuitive anomalous propulsion regime where the speed of the flagellum-driven cargo increases with increasing cargo size. We also demonstrate that in addition to the intrinsic curvature and even harmonics, asymmetric bead-flagellum attachment also contributes in the rotational velocity of the micro-swimmer (Fig. 7.40) [2].

7.17.3 Bio-inspired active systems assembled from the bottom-up

(I. Guido) In nature, the self-assembly of biopolymers and motor proteins leads to interesting emergent behaviour that is crucial for cellular organisation and motility. An example of such self-organisation is the rhythmic bending of cilia and flagella that promotes fluid transport or propels swimming organisms introduced in Sec. 7.17.2. Ciliary beating is powered by motor proteins, which drive a sliding motion of microtubule doublets. We investigated their mechanical interplay by analysing a minimal synthetic system that we assembled using one [3] or two microtubules and different types of motor proteins including axonemal dynein [4] (Fig. 7.41). The systems undergo rhythmic bending through cyclic association/dissociation that, despite their extreme simplicity, resembles the dynamics of more complex flagellar structures. Besides their potential for answering crucial questions about the active dynamics of ciliary beating, the synthetic cilia may encourage the technological development of molecular machines for fluid transport at micro- and nanoscale. Alongside the investigation of self-organising active systems at single filament level, we also focus on microtubule-motor protein active networks. We investigate how these active filamentous structures promote nonequilibrium processes induced by active stress at the microscale. By combining passive components that produce entropic forces and extensile and contractile forces exerted by motors, we show that the network exhibits nematic organization characterised by long-range orientational order [5, 6]. The evolution of the system over time is particularly interesting and unique. It undergoes a 3D to 2D transition by contracting into a sheet, expand-
sion in the direction perpendicular to the contraction, 3D wrinkling pattern formation, and finally, 3D active turbulence. These results show that these minimal synthetic structures can serve as new model systems for the quantitative understanding of fundamental questions about cytoskeletal self-organisation.

7.17.4 Synthetic cell fabrication with microfluidic system

(H. Kim) We develop stimulus-responsive minimal cell compartments which is in the form of thermoresponsive core–gap–shell (TCGS) microcapsules with microfluidic techniques using the thermo-responsive polymer, poly(N-isopropylacrylamide)(PNIPAm) (Fig. 7.43A). By leveraging the temperature dependent solubility of NIPAm, various bioactives are able to be directly loaded inside the cavity during the formation of the microcapsules. When temperature of external solution of the TCGS is higher/lower than lower critical solution temperature of PNIPAm (33 °C), the microcapsule is reversibly shrunken/swollen by extruding/absorbing water molecules. As an application, we developed a thermo-controlled glucose sensor which encapsulates silica nanocontainers with loaded GOX (Fig. 7.43B). According to the temperature of the external solution, the GOX reaction is suppressed or intensified. In this way, glucose detection can be controlled on-demand in our thermo-controlled microcapsule system. In the future, the proposed microcapsule with stimuli-responsiveness will provide more practical applications by incorporating various bioactive compounds [7].
7.17.5 Wound healing and active foams for hybrid tissues

(H. Kim, M. Tarantola) Shape, dynamics, and viscoelastic properties of eukaryotic cells are primarily governed by a thin, reversibly cross-linked actomyosin cortex located directly beneath the plasma membrane, which needs to be fully described before successful reconstitution in synthetic models or application to wound healing. We extract time-dependent rheological responses of various cells from deformation-relaxation curves using atomic force microscopy (AFM). We access the dependence of cortex fluidity on prestress and introduce a viscoelastic model that treats the cell as a composite shell, assuming power-law-based relaxation of the cortex. It gives access to cortical prestress, area-compressibility, and cortex fluidity independent of indenter geometry and compression velocity. By interfering with myosin activity, we find that fluidity decreases with increasing intrinsic prestress and area-compressibility modulus, in accordance with synthetic biological findings for isolated actin networks subject to external stress [8].

Polymer networks in synthetic biological applications also encompass stimuli responsive coatings. We have characterized temperature dependent adhesive properties of PNIPAm microgel coated surfaces (PMS) using various AFM-based approaches: we imaged and quantified material properties of PMS upon temperature switching using quantitative AFM imaging but also employed single-cell AFM before and after decreasing the temperature to assess the forces and work of initial cell-PMS adhesion. We performed a detailed analysis of steps in force-distance curves and applied colloidal probe AFM to analyze the adhesive properties of two major components of the extracellular matrix to PMS under temperature control, namely collagen I (col) and fibronectin (FN). In combination with confocal imaging, we showed that these two ECM components differ in their detachment properties from PMS upon cell harvesting (Fig. 7.44) involving partial ECM dissolution. These tissues finally will help to create hybrid assemblies with polymerosomes or liposomes [9]. We also studied PNIPAm polymerosomes as potential carriers for encapsulating cytokines relevant to wound healing. Their Young’s moduli were characterized via AFM upon swelling and TGF-beta encapsulation using fluorescence microscopy. Release of TGF-beta from polymerosomes to wound healing fibrotic cultures was quantified by impedance spectroscopy for various wound sizes and found to accelerate healing dynamics paving the way for their usage in hybrid tissues [10].

Figure 7.44: Adhesive forces $F_{\text{max}}$ between ECM component FN (A) or col (B) and gold or PMS. C. Confocal images of MDCK II cell sheet (nuclear DNA (blue), tight junction (TJ, green), and ECM component FN (red) on PMS) with: i) 3D image upon detachment (arrow). ii) Substrate plane with remnant PMS-attached FN (arrow). iii) Apical cell membrane showing continuous TJ distribution. Scale bar: 20 μm.

References:
[9] H. Kim et al., ACS Appl. Mat. & Int. 12, 33516 (2020)
Activity in living matter can take many different forms. Growth is special in that it generates mechanical forces between cells/particles in the absence of self-propulsion and leads to the production or – together with degradation – turnover of matter. In a multi-component system, e.g., with two different cell types, this turnover can drive the emergence of competition. In the absence of mechanisms stabilizing co-existence, and when the different cell types require the same limited resources, the winner species will grow at the expense of the other. Turnover of growing matter and the resulting competition dynamics could be relevant for cellular aggregates ranging from embryos to biofilms to tumors.

In our recent work [1], we examined competition between two cell types in confinement, where the limited resource is space itself and cells only interact mechanically, down-regulating their growth in response to pressure. We showed that passive by-products of the processes maintaining homeostasis, such as dead cells, can significantly alter fitness. Using a theoretical model and agent-based simulations, we uncovered a new mechanism whereby opportunistic cells can out-compete rivals by degrading their passive matter-remnants faster (Fig. 7.45), despite having identical growth/death rates and mechanical parameters. We reveal that interfaces play a critical role in the competition: Growing matter with a higher proportion of active cells can better exploit local growth opportunities that continuously arise at interfaces as the active processes keep the system out of mechanical equilibrium. Surprisingly, this new mechanism can determine the winner species even when the homeostatic pressures of the two species separately would predict otherwise. Our results suggest that self-organization of cellular aggregates into active and passive matter can be decisive for competition outcomes and that optimizing the proportion of growing (active) cells can be as important to survival as sensitivity to mechanical cues.

Another avenue of our work focuses on the relationship between mechanical stresses generated by growth and the resulting alignment dynamics of elongated particles under confinement. For example, in a channel, we find that stresses along the channel direction and perpendicular to it can be effectively decoupled by near-perfect alignment and exhibit strong hysteresis effects (Fig. 7.46) [2]. A comparison between different agent-based models of growing particles shows characteristic dependencies of the order parameter on particle location and on the geometry of the system [3]. These examples serve to show that growth can lead to complex self-organization phenomena in active matter.

The inside of biological cells is teeming with catalytic activity: a myriad enzymes transform their respective chemical substrates into products, which are passed on to other enzymes for further processing, in a variety of metabolic cycles and signalling cascades. At a larger scale, at the level of cellular populations (e.g. bacterial ecosystems), cells communicate with each other via the production of signalling molecules, the consumption of nutrients, etc. This kind of chemical signalling can also be mimicked in the lab using synthetic colloids that are coated with a catalyst. Interestingly, all these catalytic objects, from nanoscale enzymes to microscale cells and colloids, can also move (chemotax) in response to gradients of chemicals in their environment. While cells may actively swim towards or away from chemoattractants or chemorepellants, respectively, simpler particles such as enzymes and colloids can also move thanks to phoresis, a hydrodynamic effect that causes drift in response to gradients of a solute [1].

We have explored how catalytic activity, when combined with chemotaxis in response to the same chemicals that are produced or consumed, leads to spatial organization in mixtures of several chemically-active species [2, 3, 4]. Active chemical interactions (see also Sections 7.21, 7.24, and 7.5) are typically long-ranged and, in contrast to passive interactions, can show rather exotic features impossible in an equilibrium system, a particularly interesting example being non-reciprocity (see also Sec. 7.23). For example, if two particles 1 and 2 are both attracted to the same chemical, but 1 produces this chemical whereas 2 consumes it, particle 2 will be attracted to 1 while 1 will be repelled from 2, so that 2 effectively chases after 1, and the pair will experience net motion; see Fig. 7.47. The absence of reciprocity is a manifestation of the fact that such active interactions cannot be derived from a potential.

In order to study large scale self-organization in these systems, we constructed a minimal continuum model for an arbitrary mixture of $M$ distinct chemically-active species exchanging a single messenger chemical [2]. Each species has its own catalytic activity $a_i$ (positive and negative for production and consumption, respectively), chemotactic mobility $\mu_j$ (positive and negative for chemorepulsion and chemotraction, respectively), and average concentration $r_0i$. A linear stability analysis of the homogeneous mixture showed that it will become unstable, and macroscopic phase separation will occur, whenever

$$\sum_{i=1}^{M} a_i \mu_j r_0i < 0. \quad (7.1)$$

Moreover, we could predict that the different species will segregate according to the sign of their chemotactic mobility, those with equal
sign aggregating together, those with opposite sign separating. With this information, we could construct phase diagrams predicting the phase behaviour of specific systems: in Fig. 7.48, we show the phase diagrams for a binary mixture.

Our analytical predictions were validated by particle-based Brownian dynamics simulations, see Fig. 7.49, which also uncovered a number of surprising properties of the system. For example, non-reciprocal interactions can induce the formation of self-propelling macroscopic clusters, an observation which may be relevant to collective cell migration, see the bottom panel in Fig. 7.49. We also found that, when a chemical-producing species and a chemical-consuming species form a static mixed cluster, the stoichiometry of this cluster is self-regulated such that the cluster becomes chemically-neutral, that is, there is exactly the right amount of consumers in the cluster so that all the chemical produced by the producers is channeled to the consumers, without lack or excess. This behavior is reminiscent of that observed in cells, where clusters known as metabolons bring together enzymes that participate in the same catalytic pathway to enable better channeling of reaction intermediates.

The model just described included a number of simplifications that prevent it from being directly applied to some experimental systems. In particular, (i) we assumed a constant consumption or production rate of the chemical by the active species, whereas, in the case of enzymatic reactions, the rates of substrate consumption and product production both depend on substrate concentration (typically with a Michaelis-Menten-like dependence); (ii) all the active species were assumed to have the same diffusion coefficient, and thus similar size, whereas in real systems there may be a large polydispersity in their size; and (iii) our calculations were restricted to a single messenger chemical. In ref. [3], we addressed limitations (i) and (ii). We found that a concentration dependence of the activity can lead to a screening of the long-ranged effective interactions, resulting in a stricter condition for active phase separation. In turn, size polydispersity of the active species was found to allow for transiently-oscillatory instabilities of the mixture.

![Figure 7.48: Predicted phase diagrams for (a) a producer-consumer mixture, and (b) a producer-producer mixture. Compare (a) with the simulation snapshots in Fig. 7.49.](image)

![Figure 7.49: Snapshots from simulations of a producer-consumer mixture, showing different phases. From top to bottom: homogeneous phase; dense-dense separation; dense-dilute static aggregation; dense-dilute self-propelled cluster (blue chases red).](image)
on the way to phase separation. In ongoing work, we are addressing limitation (iii), by considering metabolic networks with any number of messenger chemicals. In particular, we have extensively explored spatial self-organization of enzymes that participate in a catalytic cycle [4], and found that the topology of the interaction network can have striking effects, for example allowing for long-lived oscillations in the system.

Our work on chemotaxis demonstrated that nanoscale systems can display exciting transport phenomena. However, chemotaxis is not the only response that chemicals can elicit in enzymes and other proteins. A particularly interesting response of proteins to certain chemical stimuli is dissociation. Indeed, many important proteins in biology are actually protein complexes, composed of several (identical or non-identical) subunits that may reversibly associate and dissociate. To reveal the role of dissociation in protein transport, we considered a minimal model of a dimeric protein, see Fig. 7.50, and studied its behavior in two different situations [5].

First, we studied the reactivity of the dissociating protein complex with a distant target, relative to that of an otherwise identical non-dissociating complex. Surprisingly, we found that dissociating complexes can react significantly faster with distant targets, but only when their concentration is at a particular “sweet spot”. At too low concentration, the protein is mostly in the non-functional monomer state and cannot react with the target, whereas, at too high concentration, the protein is mostly in the dimer state and behaves like a non-dissociating protein. At intermediate concentrations, however, fast diffusion in the monomer state coupled to frequent-enough reassociation into the functional dimer state allows the protein to reach and react with the distant target in minimal time.

Second, we considered the behavior of the protein when subject to a gradient of a chemical or any other stimulus (e.g. light) that affects dissociation, be it enhancing or preventing it. Interestingly, we found that there is a generic response to such a stimulus, which we termed “stabilitaxis”: the protein spontaneously accumulates in the region in which its multimeric form is most stable. For multimers with many subunits, the concentration in the higher-stability region can be several-fold higher than in the lower-stability region. We speculate that this may serve as a way of inducing secondary gradients of protein complexes in response to a primary “template” gradient of a chemical that regulates dissociation.

7.20 BOSE-EINSTEIN-LIKE CONDENSATION VIA DIFFUSIVITY EDGE IN ACTIVE MATTER

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In absence of long-range orientational order, a broad class of active and passive systems are described at the mean field level by a scalar density field $\rho(r,t)$ obeying a drift-diffusion equation:

$$\partial_t \rho = -\nabla \cdot J, \quad J = -D_{\text{eff}}(\rho) \nabla \rho - \rho M_{\text{eff}}(\rho) \nabla U,$$  \hspace{1cm} (7.2)

where $D_{\text{eff}}(\rho)$ and $M_{\text{eff}}(\rho)$ denote respectively the effective diffusivity and mobility, while the system may be confined by an external potential $U$. $D_{\text{eff}}(\rho)$ and $M_{\text{eff}}(\rho)$ are generally density-dependent, as they integrate various microscopic processes such as the interactions between individual agents or the effect of activity. For an active dynamics which does not satisfy detailed balance, the ratio $D_{\text{eff}}(\rho)/M_{\text{eff}}(\rho)$ is moreover arbitrary as it is not constrained by a fluctuation-dissipation theorem.

BEC-like condensation via diffusivity-edge In [1, 2] we introduced a new class of active matter, corresponding to vanishing $D_{\text{eff}}(\rho)$ for $\rho$ exceeding a threshold density $\rho_c$. We showed that, although such diffusivity edge does not lead to spontaneous phase separation, it is singular enough to induce a nonequilibrium condensation transition when the system is confined by an external potential. Namely, solving Eq. (7.2) in steady state ($J = 0$) yields

$$\frac{dU}{d\rho} = -\frac{D_{\text{eff}}(\rho)}{M_{\text{eff}}(\rho)\rho}.$$  \hspace{1cm} (7.3)

Eq. (7.3) implies that density is a decreasing function of the potential $U$, so that its maximum $\rho_0$ is reached at the ground state $U = 0$. So long as $\rho_0 < \rho_c$, $\rho(U)$ can be obtained integrating and inverting Eq. (7.3). However, for $\rho_0 \geq \rho_c$, $\rho(U)$ takes a vertical tangent in the ground state $U = 0$ (Fig. 7.51(a)), which reflects the formation of a condensate.

For the subsequent analysis, it is convenient to define the control parameter $k_B T_{\text{eff}} \equiv \lim_{\rho \to 0} D_{\text{eff}}(\rho)/M_{\text{eff}}(\rho)$, which plays the role of an effective temperature in the dilute limit. At large effective temperatures where $\rho_0 < \rho_c$, $\rho_0(T_{\text{eff}})$ is determined from the density normalization\(^1\). Denoting $T_c$ the effective temperature at the condensation threshold, when $T_{\text{eff}} \leq T_c$ the singular behavior of the density in the ground state imposes to consider separately the contribution from the condensate (see Eq. (7.5)\(^1\)). For a spherically-symmetric harmonic potential $U(r) = \frac{1}{2}kr^2$, we showed that the fraction of particles in the condensate obeys [1]

$$\frac{N_c}{N} = 1 - \left(\frac{T_{\text{eff}}}{T_c}\right)^\frac{d}{2},$$  \hspace{1cm} (7.6)

with $d$ being the dimension of space.

---

1. Denoting $N$ the total particle number, the density normalization, respectively without and with the condensate contribution, reads:

$$N = \int dr \rho(r) \quad (\rho_0 < \rho_c)$$

$$N = N_c + \int dr \rho(r) \quad (\rho_0 \geq \rho_c)$$  \hspace{1cm} (7.4)

$$N = N_c + \int dr \rho(r) \quad (\rho_0 \geq \rho_c)$$  \hspace{1cm} (7.5)
Considering a step function diffusivity profile such as given in Eq. (7.7), the distribution \( \rho(U) \) takes a simple Boltzmann weight form allowing one to calculate explicitly the thermodynamics of the system [1, 2]. Various thermodynamic functions are shown in Fig. 7.51. Due to the singular nature of the condensate, they all manifest peculiar behaviors at the condensation transition. The mean energy of the system exhibits a discontinuous slope at \( T_{\text{eff}} = T_c \), resulting in a discontinuous jump of the heat capacity (Fig. 7.51(c,d)). The plateau of pressure isotherms in the condensed phase (Fig. 7.51(e)) moreover indicates a divergence of the isothermal compressibility, while the chemical potential identically vanishes for \( T_{\text{eff}} \leq T_c \) (Fig. 7.51(f)).

All these features and Eq. (7.6) point towards strong formal similarities with Bose-Einstein condensation (BEC), despite Eq. (7.2) describing a classical system. Indeed, in both cases \( T_c \) delimits a transition to coexistence between a gas and a singular phase carrying zero energy and entropy [1], resulting in the characteristic thermodynamics presented above. Nevertheless, qualitative differences between the present condensation transition and BEC exist, as detailed in [1].

**Generalizations** The above results are qualitatively independent of the specific form of the diffusivity profile. While the thermodynamics of the system is quantitatively affected by the shape of \( D_{\text{eff}}(\rho)/M_{\text{eff}}(\rho) \), such as shown in Ref. [1] for motility activation and inhibition prior to diffusivity edge, signatures of BEC are thus expected in general.

We moreover addressed the case of multiple interacting condensates in [2] by considering periodic potentials such as sketched in Fig. 7.52. Here too, we found that the overall BEC phenomenology holds qualitatively, although quantitative differences were uncovered such as nonuniversal values for the exponents describing the transition. Interestingly, we also discovered that in this case the stationary solution of Eq. (7.2) is degenerate as it allows for different configurations with the same total number of condensed particles. This last result in particular...
implies that the system is able to show a certain degree of memory.

**BEC-like condensation in a magnetic microswimmers suspension**

So far we have described the diffusivity edge class and the associated BEC-like condensation purely on phenomenological grounds. We now present a microscopic realization of this class which was examined in [3]. We consider a model of magnetic microswimmers suspended in a three dimensional cylindrical channel such as shown in Fig. 7.53. The swimmers swim along the direction given by their magnetic dipole and experience a uniform magnetic field $B_{\text{ext}}$ aligned with the channel direction, as well as a Poiseuille flow $V_f$ oriented oppositely to $B_{\text{ext}}$.

In the limit of fast orientational dynamics, the combined effects of alignment with $B_{\text{ext}}$, flow vorticity $\nabla \times V_f$, and self propulsion result in the focusing of the swimmers at the center of the channel $r = 0$ by an effective harmonic potential $U(r) = \frac{1}{2} k r^2$ [3]. Moreover, performing a mean field treatment of the dipolar interactions between swimmers, we found that their radial dynamics decouples from the longitudinal one and is governed by an equation similar to (7.2) with $D_{\text{eff}}(\rho) / M_{\text{eff}}(\rho) = k_B T_{\text{eff}} (1 - \rho / \rho_c)$, where the expressions of the effective temperature $T_{\text{eff}}$ and the diffusivity edge $\rho_c$ as function of the model parameters can be found in [3]. From the above theoretical analysis, it follows that at high swimmer densities or low values of $T_{\text{eff}}$ the swimmers condense at the center of the channel in a BEC-like fashion. As shown in Figs. 7.54(a,b), these predictions are confirmed at the fluctuating level by parameter-free comparisons with direct Brownian dynamics simulations of the underlying microscopic model.

Additionally to the BEC-like condensation reported here, magnetic microswimmers can self-organize into clusters travelling along the channel direction. This behavior was first predicted in Ref. [4] neglecting the effect of dipolar interactions on the radial swimmer dynamics. In [3] the clustering transition was revisited taking into account such interactions, which led to the phase diagram shown in Fig. 7.54(c).

Our ongoing work focuses on characterizing further the BEC-like transition outlined here, in particular regarding its dynamical features and the treatment of short-range repulsion leading to spatially extended condensates.

7.21 NEAR FIELD EFFECTS IN PHORETIC INTERACTION OF CHEMICALLY ACTIVE PARTICLES

B. Nasouri, R. Golestanian

Over the past few decades, there has been an immense focus on understanding the mechanisms behind the motion of microorganisms; either with the aim of explaining an observed phenomenon, or devising a synthetic machine that can propel in an inertialess environment. Phoretic interactions of chemically active particles concisely sit at the interface of these two classes of studies. From the biological perspective, microorganisms, cells, and enzymes have been shown to alter their motion due to presence of a chemical gradient in their medium. Synthetically, similar chemotaxis can also be reproduced by catalytic colloidal particles which respond to gradients of the solute concentration they themselves may have consumed or produced. Manipulation of such phoretic interactions in a suspension of many particles has introduced a wealth of nontrivial behaviours from self-organization, to phase separation, and autonomous swimming [1].

The first crucial step of studying such complex phenomena is to look at the interactions of only two particles, which despite its (seeming) simplicity, is not yet fully explored. These interactions are often modelled using far-field approaches which neglect the near field effects in both chemical and fluidic medium; ones that can be of significant import especially when analyzing the clustering or self-organization of closely-packed phoretic particles. The first question here we intend to answer, is thereby quite simple: What does happen to a system of two chemically active particles when they can freely interact with one another in a viscous medium?

We begin by considering the simple interaction of two isotropically-coated spherical particles in a viscous fluid. Based on far-field approximations, the interactions between these two particles is either attractive, meaning that the particles will come together and collapse, or repulsive such that they move away from one another indefinitely. However, by
accounting for the near field chemical and hydrodynamic interactions using an exact approach, we show that the interactions are far more complex, and in fact, there can be a fixed point in the associated dynamical system [2]. Depending on the chemical properties of the particles, they may hold a non-zero gap size and move together with an equal and constant speed (stable fixed point), or create a bundle that can be broken apart under sufficient perturbations (unstable fixed point). Both of these regimes of behaviour cannot be captured via far-field approximations, and are solely due to near field effects (see Fig. 7.55).

As the next step, we explore the effect of near field interactions on non-isotropically coated particles by considering two Janus particles. Each Janus particle has two compartments (or faces), and each compartment has its own chemical properties. By accounting for near field chemical and hydrodynamic interactions, we find that the dynamical system can surprisingly have up to three fixed points, pointing to a variety of non-trivial interactions for a pair of Janus particles in close proximity [3]; see Fig. 7.56.

Based on all of these, one can conclude that near-field interactions play a crucial role in phoretic interactions of chemically active systems. We showed that near field interactions can qualitatively, and significantly, alter the behaviour of two chemically active particles. Thus, the next natural step is to evaluate the role of near field interactions on large suspension of chemically active particles. For instance, a droplet-like condensation of closely-packed chemically active particles has shown to be able to break the rational symmetry and create an internal flow [4], a phenomenon that cannot be fully explained without accounting for the near field effects (see Fig. 7.57). However, unlike the pair interactions for which an exact approach is feasible, studying the interactions of many-body systems requires a hybrid theoretical/computation approach that accounts for near field effects efficiently, and can capture the non-trivial collective behaviours that such systems exhibit.

References:
7.22 EFFICIENCY AND DISSIPATION LIMITS IN MICROSWIMMERS

A. Vilfan, B. Nasouri, A. Daddi-Moussa-Ider, R. Golestanian

Biological or artificial microswimmers propel themselves through a fluid in the low Reynolds number regime either by periodically changing their shape or by inducing an effective slip velocity along their surface. The energetic efficiency of swimming is typically defined using Lighthill’s criterion as the power that would be needed to pull the swimmer through the fluid by an external force, divided by the actually dissipated power. Lighthill’s efficiency is in principle not bounded by 1, yet it is of the order of 1% in most microorganisms [1].

We have taken a general approach and derived a minimum dissipation theorem for microswimmers. It provides a lower bound on the power needed by an active swimmer, expressed with the drag coefficients of two passive bodies of the same shape: one with a no-slip and one with a perfect slip boundary [2]. The theorem holds for swimmers of any shape, moving with any translational and/or rotational velocity. The proof involves a generalization of the Helmholtz minimum dissipation theorem, the principle of linear superposition (Fig. 7.58) and the Lorentz reciprocal theorem. We also show that the optimal swimmer has the velocity profile of the perfect slip body (e.g., a gas bubble) and the tangential traction of the no-slip body. For axisymmetric bodies, the expression for the upper limit on Lighthill efficiency takes the very simple form \( R_{NS}/R_{PS} - 1 \), which agrees with solutions for some specific shapes known from the literature.

As an application of the new theorem, we addressed the question whether an optimal swimmer of a given shape is a pusher, puller or neutral. We solved the problem for near-spherical bodies, with the departure from the spherical shape expanded in Legendre modes (Fig. 7.59). We showed that to the leading order, only the third Legendre mode determines the pusher/puller nature of the optimal swimmer [3]. The study demonstrates how the theorem allowed us to solve a problem that would otherwise not be analytically tractable.

Swimmers that propel themselves by cyclical shape changes represent a different class and so far no general theorem for their dissipation has been found. We have therefore taken the classical three-sphere swimmer as a simple model system and numerically optimized its kinematics [4]. Interestingly, optimal efficiency is achieved when the side spheres are 20% larger than the central one. The Lighthill efficiency then reaches approx. 1.2% and is of a similar order of magnitude as the propulsive efficiency of various microorganisms.

7.23 SCALAR ACTIVE MIXTURES: THE NON-RECIPROCAL CAHN-HILLIARD MODEL

S. Saha, J. Agudo-Canalejo, R. Golestanian

Pair interactions between active particles need not follow Newton’s third law. In this work [1], we have proposed a continuum model of pattern formation due to non-reciprocal interactions between multiple species of scalar active matter. The classical Cahn-Hilliard model is minimally modified by supplementing the equilibrium Ginzburg-Landau dynamics with particle number conserving currents which cannot be derived from a free energy, reflecting the microscopic departure from action-reaction symmetry. For a binary system with densities \( \phi_{1,2} \), the following equations of motion are explored

\[
\begin{align*}
\frac{1}{\Gamma_1} \partial_t \phi_1 &= \nabla^2 \left[ \frac{\delta f_1}{\delta \phi_1} + (\chi + \alpha) \phi_2 \right] - \kappa^2 \nabla^4 \phi_1, \\
\frac{1}{\Gamma_2} \partial_t \phi_2 &= \nabla^2 \left[ \frac{\delta f_2}{\delta \phi_2} + (\chi - \alpha) \phi_1 \right] - \kappa^2 \nabla^4 \phi_2, 
\end{align*}
\]

(7.8)

where \( f_{1,2} \) are the bulk free energies of species 1 and 2, chosen to be the standard double well potential (details in [1]). The strength of the asymmetry in the interactions, quantified by the parameter \( \alpha \), competes with the strength of the reciprocal interactions, \( \chi \), to determine whether the steady state exhibits a macroscopic phase separation or a traveling density wave displaying global polar order. The transition from bulk phase separation to travelling states occurs as one crosses an exceptional point in the \((\chi - \alpha)\) plane. The exceptional points (marked in red in Fig. 7.60 (b)) in the \((\chi - \alpha)\) plane are predicted by a linear stability analysis of (7.8) around a homogeneous state.

In the second part of this work, we have modified (7.8) with terms inspired by the complex Landau-Ginzburg equation. We have studied the interplay of a non-linear, non-reciprocal interaction term \( \alpha \) in the chemical potential and a non-mutual surface tension \( \beta \) by numerically studying the following equations of motion for the conserved densities \( \phi_{1,2} \):

![Figure 7.60: Travelling waves can be viewed as a field of synchronised oscillators; at a given point in space, the densities evolve into a limit cycle shown in panel (a). (b) Phase diagram in the \((\chi - a)\) plane.](image1)

![Figure 7.61: Dynamical steady states of the non-reciprocal Cahn-Hilliard model: Starting from random initial conditions, numerical simulation of (7.8) in two dimensions leads to (a) travelling waves and (b-c) moving patterns. Panel (d) shows a cross section of the travelling wave. Notice how one species chases after the other. Panel (e) shows a cross section of the micro-pattern in panels (b) and (c).](image2)
The non-reciprocal interaction term in the chemical potential depends on the fields $\phi_{1,2}$: $a = a_0 - a_1 (\phi_1^2 + \phi_2^2)$ and $f = -(\phi_1^2 + \phi_2^2)/2 + (\phi_1^2 + \phi_2^2)^2/4$ is the free energy for real Landau-Ginzburg dynamics. For vanishing non-reciprocal parameters, the underlying free energy causes the mixture to separate into micro-phase-separated domains. In addition to the travelling states that are generically present when $a_0$ is the only non-mutual interaction parameter, we find chemical turbulence and other novel steady states shown in Fig. 7.63. Eqs. 7.9 allow travelling wave solutions of the form $R \exp(i (q \cdot r - \omega t))$ where $R = \sqrt{(1 - q^2)}$ and $\omega = q^2 [-a_0 + a_1 (1 - q^2) + \beta q^2]$. These solutions are unstable when (I) $|a_1| > 1, a_1 \approx -\beta$, or for (II) $a_0 \approx a_1$. In case (I), the change from travelling waves to the turbulence state shown in panel (b) of Fig. 7.63 occurs through transition states which have been called “Oscillating domains” in panel (a) of Fig. 7.63. In case (II) travelling waves are seen in a background of nearly random fluctuations. Phase turbulence where locally well-defined waves unstable over length-scales larger than their wavelength are seen for $\beta > 1$ and $a_{0,1} \ll 1$. The power spectrum calculated as $S(\nu) = \int \Delta^2 |\phi_1(r,v)|^2$ (see Fig. 7.63, panel (e-f)) shows that the interactions generate fluctuations nearly uncorrelated in time over a large range of frequencies.

References:

Chemotaxis is a ubiquitous interaction that is known to be elemental in a range of phenomena such as morphogenesis, wound healing, and cancer metastasis. Beyond extensive studies that focus on single-cell chemotaxis, analytical approaches based on the celebrated Keller–Segel model are often used to investigate the collective dynamics of chemotactic colonies [1].

The Keller–Segel model, however, is based on mean-field assumptions and neglects the statistical correlations in the chemotactic dynamics. We instead use a stochastic description to study the fluctuations in collections of particles that interact via a generalized chemotactic mechanism that arises from their polarity [2]. In general, such polarity can represent an asymmetry in the morphology of the particles or anisotropy in their response to chemical cues, as seen, e.g., in eukaryotic chemotaxis [3]. Through scaling analysis, we show that the corresponding polarity-induced interaction is a relevant nonlinear coupling in the macroscopic dynamics of the system, and it can thus modify the scaling exponents of density correlations in the critical regime. Moreover, we show that the novel interaction is not derivable from an underlying free-energy functional; therefore, in contrast to the equilibrium Keller–Segel model, the long-time distribution of density fluctuations in the presence of polarity effects does not obey Boltzmann statistics.

The scaling exponents of density correlations are then examined using dynamic renormalization group theory and symmetry arguments. Crucially, we identify a Galilean symmetry that emerges at macroscopic scales and is protected by the gradient structure of the dynamical equations. The Galilean symmetry, together with the non-renormalization of the noise strength, allows us to obtain exact values for the scaling exponents in the presence of the chemotactic couplings. These exponents show that the density fluctuations have super-diffusive dynamics (i.e., MSD $\sim t^\alpha$ with $\alpha > 1$); moreover, the system exhibits giant number fluctuations (i.e., $\Delta N \sim N^\gamma$ with $\gamma > 1/2$) if a nonconserved noise is allowed in the dynamics (e.g., due to particles stochastically switching off their chemotactic machinery), while it becomes hyperuniform (with $\gamma < 1/2$) with a conserved noise only. These results indicate that small-scale features such as the particle polarity, which are usually ignored in studying collective behavior, can in fact change the large-scale properties of the system and should be examined using systematic coarse-graining and field-theoretical approaches.

DYNAMICS, GEOMETRY, AND INFORMATION

The ongoing COVID-19 pandemic did not only lead to an exploding public interest in virology but also reinforced the general awareness of concepts from dynamical systems and data driven science (that had already been ignited by the impending dangers from climate change). This chapter therefore begins by collecting work done at the MPI DS in the last three years on dynamics of epidemics, their spread and control, with important contributions for understanding the dynamics of COVID-19. Also transport by (complex or turbulent) flows – a recurrent concept in our research – plays an important role in the transmission of the virus, which will be addressed later in the chapter.

But far beyond the application on epidemiology, complex dynamics and its interplay with geometry and information flows are central themes in our research. The systems we are studying include biological, neural and social networks, ride pooling systems, motile algae and slime molds, heart dynamics, the immune system, turbulent flows, soft matter and music. The research on this broad scope of systems is tightly linked by common underlying concepts and methods. The interplay of topology and dynamics, optimization, memory, learning and evolution, chaos and self-organization are frequently recurrent concepts studied with contemporary theoretical and experimental methods of dynamical and stochastic modelling, statistical inference and machine learning, particle tracking and microscopy.

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The COVID-19 pandemic has challenged nearly every aspect of modern life and introduced epidemiological terms into our daily conversations from 2020 onward. While vaccination programs and non-pharmaceutical interventions (NPIs) help reduce the levels of morbidity and mortality in the population, the total eradication of COVID-19 seems utopic as of September 2021. Nonetheless, mitigation and containment of COVID-19 outbreaks have been possible, primarily due to joint efforts of theoreticians and practitioners, and have been vital to protect our societies. Mathematical models have played a crucial role in those efforts, helping policymakers allocate scarce resources and assess the effectiveness of their interventions [1, 2].

One of the preferred approaches to model disease spread is to use compartmental models, most of which derive from the well-known susceptible-infectious-removed (SIR) model. This simple model admits two dynamical regimes, depending solely on the infectiousness of the disease and the fraction of the population that remains susceptible: exponential growth or exponential decay of infections. However, incorporating NPIs or vaccination into models opens a rich range of regimes.

In our research, we extended the SIR model to incorporate test-trace-and-isolate (TTI) initiatives (and the challenges thereof) explicitly [3]. In order to study whether TTI can curb the spread of COVID-19, we modeled two modi of contagion: hidden and traced (cf. Fig 8.1 A, B). Hidden infections propagate unnoticed until they are discovered through testing. When this happens the infected persons and their close contacts are traced. However, health authorities have limited capacities to trace contacts; at a certain number of reported new cases (henceforth ‘case numbers’), TTI starts missing infected contacts, and thus their contagion chains [3]. We identified two tipping points between controlled and uncontrolled spread: the hidden reproduction number (i.e., the average number of offspring infections generated by each hidden case) becomes too large to be compensated by TTI, and the number of new infections exceeds the tracing capacity. Both trigger a self-accelerating spread and separate the dynamic phases that determine whether an outbreak is under control (Fig 8.1 C).

Analyzing the stability of our TTI model, we found a meta-stable regime at low case numbers (Fig 8.1 A). In this regime, efficient TTI, hygiene, and voluntary contact reduction counterbalance the high contagiousness of COVID-19, seasonality, and the influx of externally acquired infections. When case numbers are below the TTI capacity limit, efficient TTI can compensate for local outbreaks and allow for higher levels of contacts without rendering the system unstable (Fig 8.2 B). However, the level where case numbers stabilize depends on...
the current level of contacts and the influx of infections (Fig 8.2 C). Understanding these principles allows policymakers to design long-term strategies for epidemic control [4].

In the early stages of the pandemic, NPIs were the only means to curb the spread of COVID-19. Since 2021, mass vaccination has offered a transition path to endemicity. However, as vaccination progresses, demands to lift restrictions increase, despite fractions of the population remaining susceptible. To answer the question about the need for NPIs during vaccine rollout, we developed an age-structured model including the hospitalization of individuals, and vaccination [5]. We found that a rapid lifting of NPIs may soon overwhelm hospitals without permanent gains in freedom, as restrictions would need to be quickly reinstated, and only lifting restrictions at the pace of vaccination can minimize morbidity and mortality. In this way, case numbers will stay low, and the disease spread can be controlled with TTI at maximum efficiency. Ultimately, this means more freedom overall and offers the best preparedness to potentially emerging variants of SARS-CoV-2 [6].

Altogether, our results were highly relevant for societies and decision-makers, providing evidence for investing in TTI, keeping case numbers low, and when to implement or lift NPIs. To condense and communicate the COVID-19 response strategies to the public and politicians, we initiated a series of joint statements with dozens of experts from all over Europe and across various research fields [6, 7, 8, 9, 10, 11]. Highlighting the importance of cooperation and coordination, we advocated for strategies to keep case numbers low, especially in the face of dangerous variants of SARS-CoV-2. Our statements were further informed by our expert survey about future developments in the pandemic [12]. We concluded that the COVID-19 pandemic would continue to pose many challenges in the coming years. Pandemic surveillance and control, vaccination, good public communication, international cooperation, and a holistic One Health view will remain crucial to addressing COVID-19 and future pandemics.

Our research and European consensus letters were paralleled by extensive public outreach in radio, print, and TV, making the Max Planck Institute for Dynamics and Self-Organization highly visible in the context of COVID-19 mitigation on Germany.

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2. V. Priesemann et al, Bundesgesundheitsbl 64, 1058—1066 (2021)
8.2 FIGHTING THE PANDEMIC WITH DATA-DRIVEN RESEARCH

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The COVID-19 pandemic spurred a global effort to understand its dynamics and find the best ways for its mitigation. In Göttingen, a task force was formed spanning the university and Max Planck institutes to discuss open questions, coordinate research and exchange results. A central theme in our research group was to understand the dynamics of the pandemic with help of officially available data: We quantified (i) the effectiveness of governmental interventions, (ii) the unfolding of epidemic waves, and (iii) the emergence of variants of concern.

At the beginning of the pandemic, governmental non-pharmaceutical interventions, e.g. lockdowns, were highly disputed. Questions were asked regarding the necessity of the enacted interventions. For the case of Germany, we used the framework of Bayesian inference and a well understood epidemiological compartmental model to infer the change of the spread at the time points of the enacted interventions [1]. Indeed, each set of interventions, including the lockdown, significantly contributed to the fast decline of case numbers in Germany. Moreover, we demonstrated that even a short delay in enacting interventions would have strongly increased case numbers and fatalities (Fig. 8.3).

During fall 2020, a new wave began to unfold in Germany. However, it only manifested in the case numbers, not in deaths. Hence, it was suspected to be purely a testing artifact. We resolved this apparent contradiction using age resolved analyses: We found the young age groups to drive the wave; hence, the increase in cases hardly led to deaths [2]. However, with increasing undocumented cases [3], SARS-CoV-2 spread to older age-groups again, and the death toll rose as predicted (Sec. 8.1).

In 2021, the dynamics of the pandemic changed because of the emergence of variants of concern (VoCs). The VoCs displayed characteristics, such as increased transmissibility and higher case fatality rate. Together with collaborators in Chile, we analyzed genomic surveillance data, and with Bayesian inference inferred the relative transmissibility of the different variants (Fig. 8.4). We found a positive correlation between the transmissibility of a variant and the number of mutations in its spike gene, demonstrating an evolutionary selective pressure [4].

In future, we will explore the relation between pandemics and infodemics (c.f. Sec. 8.6), thereby improving our pandemic preparedness.

8.3 VACCINATION STRATEGIES FOR ENDEMIC DISEASES IN NEARLY CLOSED POPULATIONS

W. Reimann, S. Eule, T. Geisel

In local populations which are partially open to influx and outflux, such as in refugee transit camps, nursing homes, or livestock farms, the endemic level of infectious diseases depends sensitively on the state of health of the arriving individuals. We have introduced an appropriate epidemiological model by extending the SIR-model for such partially open populations to study the impact of the population influx on the endemic state of typical infectious diseases. The endemic disease level responds to the influx in very complex and often counterintuitive ways. The model can also be used to study vaccination coverage thresholds, e.g. the minimum vaccination coverages required for a reduction or for a complete eradication of the disease in the population. A big advantage of the model is that it can be treated analytically to a large extent.

Vaccination of a fraction \( c \) of incoming individuals represents an important alternative to direct vaccination strategies in the population itself. Since this strategy involves significantly less individuals than a vaccination of the local population itself, it requires less vaccine. Fig. 8.5a shows for the example of measles in a human population how the endemic state changes with increasing migration rates. The fraction of infected individuals exhibits a pronounced non-monotonic behavior. With increasing influx it grows up to a maximum before declining and vanishing for large migration rates. The overshoot effect in Fig. 8.5a, i.e. the seemingly paradoxical rise of the endemic level upon influx of mostly healthy individuals, becomes less pronounced with increasing vaccination coverage and eventually disappears for relatively large vaccination coverage. The transition points can be determined analytically, in particular the critical vaccination coverage \( c_{crit}(\epsilon) \) above which the disease is eradicated in the population (Fig. 8.5b).
8.4 EPIDEMIC CONTAINMENT BASED ON SMALL-NUMBER, COOPERATIVE EFFECTS

P. Bittihn, L. Hupe, J. Isensee, R. Golestanian

As seen during past two years, countries impose varying degrees of lockdowns, contact tracing and quarantines to control the spread of a pandemic, aiming at reducing the contact rate between infected and healthy individuals. As physicists used to working with fluctuating systems in the framework of non-equilibrium statistical physics, we posed the question what role small-number effects play in the dynamics of an epidemic and whether they can improve its control.

When a population mixes homogeneously, as is assumed in traditional Susceptible-Infected-Removed (SIR) models, these effects can be expected to influence the course of the epidemic only in the very beginning, when infection numbers are extremely low. However, even at higher infection numbers, subdivision of the population can lead to a low number of infected individuals in individual sub-populations. How does this alter the overall dynamics?

In an extended stochastic SIR model for the limiting case of perfectly isolated sub-populations, we found that, even if the absolute rate of individual contacts is not altered by the subdivision, peak infection numbers are significantly reduced due to two distinct stochastic effects (see Fig. 8.6): (1) extinction, the spontaneous termination of infection chains in some sub-populations despite the expected exponential increase, and (2) desynchronization, different epidemic peak times in different sub-populations. We were able to analytically estimate both effects, in excellent agreement with stochastic numerical simulations (Fig. 8.7). Our results [1] show that regional isolation can amplify stochastic effects and thereby soften the impact of an epidemic—e.g., on limited ICU capacity. In practice, on what level such isolated sub-populations would have to be created (neighborhoods, cities, counties) depends on the current infection numbers. Notably, however, the beneficial effects arise without any further contact restrictions within each sub-population, achieving relative local freedom.

In contrast to this limiting case, in reality, sub-populations cannot be perfectly isolated, and authorities react dynamically to rising in-

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**Figure 8.6:** Stochasticity can lead to extinction and desynchronization in a subdivided population. One large population (red) compared to a subdivided one with identical initial conditions, only three of which (green, yellow, blue) eventually show desynchronized outbreaks.

**Figure 8.7:** Reduction of $\gamma_{\text{con}}$, the peak number of infections as a percentage of the total population, due to extinction (yellow) and desynchronization (blue) of 100 decoupled sub-populations of 80,000 people each, as a function of the infection rate $b$. Deterministic large-population limit shown in black. Lines: analytical estimates; symbols: numerical simulations. [1]
Can small-number effects in individual regions still be exploited for effective containment? To answer this question, we obtained the regional population structure at the county level of Germany, Italy, England, New York State and Florida and set up stochastic meta-population models which were initialized with infection numbers as of June 2020, assuming a range of effective reproduction numbers $R_0 > 1$. The models distinguish between contacts within each region and cross-regional contacts, and regional lockdowns are imposed once infection numbers exceed a threshold value (Fig. 8.8a).

We then evaluated how many days the average person will experience restrictions for different proportions of cross-regional contacts and compared this restriction time with an equivalent national lockdown strategy (where contact restrictions are imposed once infection numbers in the total population cross the same relative threshold). We found a strong reduction of the restriction time required by the regional strategy compared to the national one (Fig. 8.8b), but only when the leakiness $\xi$, i.e., the proportion of cross-regional contacts, is sufficiently low—on the order of 1%.

By analysing how the restriction time depends on the regional structure itself, we found that this benefit is strictly due to small-number effects and cooperativity: Small typical regional population sizes, on the order of 200,000 people, and low thresholds for initiating local measures can increase the likelihood of eliminating the disease entirely on the local level and thus cooperatively create more and more disease-free areas if the cross-infection probability is low. Consistently, a comparison of different countries shows that regional lockdowns initiated on a county level achieve a greater reduction in the required restriction time in a country like Germany with few large counties, compared to other countries where many large counties hinder the exploitation of small-number effects (Fig. 8.9). Overall, our results show that low cross-regional contact rates and strict local lockdowns can activate these effects to greatly reduce the time the average person has to experience contact restrictions.

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Managing an epidemic requires both accurate day-by-day data on crucial parameters, such as the reproduction index, $R$, but also optimized intervention strategies. In the framework of a susceptible-infected-recovered (SIR) model, we derive rather general conditions for minimizing the costs incurred by the introduction of control measures, parametrized by $a(t)$, under the constraint that the infected fraction of the population, $I$, never exceeds the capacity of the public health system. By variational and numerical methods for a number of model cost functions, $f(a)$, we find that the optimal strategy depends on $f(a)$ only at very early times, but is universal for almost the full duration of the epidemic (cf. Fig. 8.10) [1]. Its precise control is crucial for the minimization of casualties.

This requires accurate monitoring of incidence and the reproduction index,

$$R(t) = \tau |\partial_t S| / I,$$

throughout the epidemic. $|\partial_t S|$ represents the daily incidence and can be considered known accurately. $\tau$ is the average time an infected individual is contagious. It can be derived from clinical experience with the disease, and $I(t)$ can be estimated once $\tau$ is known [2]. We propose [3] a discrete, incidence-based version of eq. (8.1) as

$$R_I(t) = \tau \left( \frac{1}{7} \sum_{j=-3}^{+3} S(t-j) \right)^{-1},$$

$$R_G(t) = \tau \sum_{j=-4}^{+4} I(t-j).$$

Publicly available data for $R$, however, usually represent the generation-time-based reproduction index, $R_G$, which is computed from incidence data taken at two different times, $t$ and $t + t_G$, where $t_G$ is
called the generation time (the Robert Koch Institute (RKI) uses \( t_G = 4 \) days). The definition of \( R_G \) is then

\[
R_G(t) = \left( \sum_{j=0}^{3} \dot{S}(t - j) \right) \left( \sum_{j=0}^{3} \dot{S}(t - j - t_G) \right)^{-1}.
\]  

(8.3)

Its mathematical meaning becomes clearer in a continuous formulation,

\[
R_G^{\text{cont}}(t + t_G) \approx 1 + t_G \frac{\partial}{\partial t} \ln |\partial_t \dot{S}(t)|,
\]  

(8.4)

where we have truncated the Taylor expansion after the first term. This is clearly not in line with eq. (8.1). The difference between \( R_I \) and \( R_G \) becomes obvious by direct comparison, as shown in the left panel of Fig. 8.11 for the SARS-CoV2 pandemic in Germany. While \( R_I(t) \) clearly shows effects of certain events and interventions (arrows, numbers count days after March 1st, 2020), these are hardly visible in \( R_G(t) \). Furthermore, the latter seems to greatly underestimate \( R \) at many points in time. This is potentially dangerous, as \( R \) marks the dividing line between decaying and (exponentially) increasing infection rates.

![Figure 8.12: Self-consistent correction of \( R_I(t) \) by determining the (slowly varying) \( \tau(t) \) from the differences between \( R_I \) and \( R_I^{\text{calc}} \). The resulting, self-consistently corrected, \( R(t) = R_I^{\text{corr}} \) is not only very accurate (e.g., as to its transitions through unity) but also contains all short time features. Furthermore, we obtain an estimate for \( \tau(t) \).](image)

We can distill more information from \( R_G \) by observing that eq. (8.4) can be rewritten into

\[
\frac{\partial}{\partial t} \left( \frac{\tau}{R(t)} \right) + \left( \frac{R_G(t) - 1}{t_G} + \frac{1}{\tau} \right) \frac{\tau}{R(t)} - 1 = 0.
\]  

(8.5)

This is a linear differential equation in \( \tau/R \), which can be solved by the method of variation of parameters. The solution is

\[
R_I^{\text{calc}}(t) = \tau e^{\int p(t) \, dt} \left( \int e^{\int p(t) \, dt} \, dt \right)^{-1},
\]  

(8.6)
where
\[ p(t) = \frac{R_G(t) - 1}{t_G} + \frac{1}{\tau}. \] (8.7)

The right panel of Fig. 8.11 shows the result for three chosen values of \( \tau \). Due to the approximations made, \( R_I^{\text{calc}}(t) \) is somewhat smoothed with respect to \( R_I \) (grey curve), and misses some of the short-time features of the latter. Since \( R_I \) is directly proportional to \( \tau \) due to its definition (cf. eqs (8.1) and (8.2)), the slowly varying difference between \( R_I \) and \( R_I^{\text{calc}} \) must be due to the (unknown) gradual variation of \( \tau \). This can be exploited to compute \( R_I(t) \) in a self-consistent manner [3], as shown in Fig. 8.12. Hence we do not only obtain very accurate values for the important parameter \( R \) from the inaccurate RKI data, but also an estimate of the slowly varying parameter \( \tau(t) \), for which usually no data are available at all.

Finally, we can exploit the so-obtained \( R(t) \), together with the incidence, \( |\partial_t S| \), to visualize the orbital structure of epidemic waves. This is shown in Fig. 8.13. The arrows next to the trajectory indicate the direction of passing time. Note that \( R \) is generally a forerunner to incidence, which stresses its importance for prediction.

**Figure 8.13:** Epidemic data in the plane spanned by \( R \) and incidence. Each dot is one day, numbers have the same meaning as in Fig. 8.11. First wave (open dots), \( t < 130 \). Second wave (filled, grey), \( t \in [130, 351] \). Third wave (filled, black), \( t > 351 \). Owing to the high sensitivity of \( R(t) \), social events immediately show up in the trajectories.


8.6 CASCADE DYNAMICS IN ONLINE COMMUNITIES

J. P. Neto, R. Carlucci, K. M. Heidemann

Social media has a large role in modern society, making studying its dynamics fundamental to understand social and political events. Reddit is one of the biggest and most influential social media platforms in the world, and some of its individual subcommunities — called subreddits — have played important roles in recent events (e.g. r/The_Donald in the 2016 US election and r/wallstreetbets in the 2021 $GME short squeeze).

Discussions on Reddit occur in individual threads, submitted to a subreddit, and generating a comment tree (Fig. 8.14). We analyze a large, almost fully-sampled Reddit dataset covering the years 2008-2021 [1]. We find that aggregate observables of subreddits (total number of submissions, comments and total score) approximately follow power-law probability distributions \( P(x) \sim x^{-a} \) spanning many orders of magnitude (Fig. 8.15). Moreover, the exponents \( a \) are close to \( a = 3/2 \), suggesting processes in the MF-DP universality class [2].

When analyzing individual subreddits, however, we observe a large heterogeneity of distributions. About 60% of the largest 1000 subreddits have comment and score distributions well-fitted by power-laws. We also find that exponents of the score distributions are both smaller and less variable than those of the comment distributions (Fig. 8.16A).

We explore the comment cascade with a preferential attachment model that takes into account both aging and fitness effects [3]. Using submission and comment rates extracted from data, the model is able to reproduce both non-power-law and power-law behavior with varying exponents (Fig. 8.16B). Together, our findings suggest that i) scores and comments are effectively generated by different processes and ii) comment distribution variability is chiefly affected by rate heterogeneity.

8.7 BOUNDED RATIONALITY IN PUBLIC-GOOD GAMES

P. Godara, D. Aléman, S. Herminghaus

The public-good game (PGG) is a frequently used game theoretic formalization of a rather general type of interactions in a human society. In each round, players contribute a fraction of their fortune to a common pot (the public good), whose contents plus some interest are then disbursed equally among the players. In experiments, one finds humans to contribute significantly, but average contributions decline over the course of several rounds of the game [1] (cf. Fig. 8.17). Recent studies have suggested that this is solely due to payoff-based learning of the players, i.e., from the contributions of the other players they learn certain habits which allows them to increase their own revenue [2].

However, game trajectories can be so erratic that learning anything useful from them appears hardly credible (cf. Fig. 8.18). Perhaps thoughtful attempts to maximize revenue, based on anticipations of other player’s behaviour, may be a better explanation of empirical data. However, fully rational players are known to generally contribute nothing (Nash equilibrium), which is at variance with observation. We have devised agents which maximizing their income using a path integral formulation, but their intellectual resources are assumed finite. We used the well-known concept of bounded rationality, which can be implemented in a mathematically sober way [3], and exclude any kind of learning. Fig. 8.19 shows that with our agents, we can simulate the playing behaviour found among humans equally well. Not only the declining trend of the contributions is well reproduced by our simulations, also the (quite substantial) variability of contributions, as expressed by the error bars, are well accounted for.

Figure 8.17: Average contributions of players in four-player PGG played in sixteen cities from all over the globe. One universally finds significant willingness to contribute, but contributions tend to decline from one round to the next. The level and slope, however, varies between different cultures.

Figure 8.18: Single trajectory of contributions in a game played in Athens over ten rounds. It is hard to believe that the quite erratic behaviour will be fruitful for any mechanism of payoff-based learning.

Figure 8.19: Average contributions in PGG for Athens (left) and Minsk (right). Agreement is similar for the 14 other cities studied.

8.8 RIDEPOOLING ON REAL STREET NETWORKS

S. Mühle, M. Sternbach, D. Bantje, K. M. Heidemann

The need for sustainable and reliable mobility is a major paradigm of the 21st century. Currently, traffic is responsible for approximately 23% of human carbon emissions while, at the same time, the lack of flexible public transport forces citizens of rural areas to travel by private car. By allowing the trips of independent users to be combined into one vehicle, demand-responsive transport (DRT) (or ride pooling) services have the potential to drastically decrease urban traffic, carbon emissions and the need for owning a vehicle.

Since optimizing a DRT system in real world settings using an experimental trial-and-error strategy is not feasible due to financial and time requirements (and public perception), the conditions under which it operates optimally remain elusive. Thus we investigate the performance of ride pooling systems on real street networks via both theory and simulations using synthetic as well as taxi data.

Figure 8.20: Efficiency. The fleet’s driven distances (in units of all users’ direct requested distances) is an efficiency measure for our system, indicating whether it effectively increases or decreases carbon emissions. Interestingly, it becomes a universal function of user demand, for high demand, independently of fleet size (supply).

Figure 8.21: Capacity. The max. demand the DRT system can serve grows with the number of buses. For many buses, this growth is well described by a superlinear power law, meaning that the demand served per bus increases when adding more buses - an indicator for cooperation between buses via the dispatch algorithm.

Figure 8.22: Service Quality. The average delay (i.e. time spent waiting for the bus or driving a detour, both in units of the direct travel time) experienced by users increases with demand (request frequency) but decreases with number of buses.

Ride pooling simulations on OpenStreetMaps Our custom simulation framework (written in the Julia language) allows us to run DRT dynamics directly on OpenStreetMaps. The vehicles move according to the local speed limit and respect one-way lanes. A dispatch algorithm orchestrates them and decides which requests are served or rejected.
In our model, the times between requests are exponentially distributed according to a Poisson process, and the dispatcher respects user constraints such as maximum-allowed detours and waiting times. A typical simulation with several thousand requests on a map such as the one displayed in figure 8.23 can be run on a single PC in less than a minute. Having access to a high-performance computing cluster, this allows us to systematically investigate e.g. the efficiency (see figure 8.20), capacity (see figure 8.21) and service quality (see figure 8.22) of our system across various system parameters (dispatcher, fleet size, request patterns etc.), user constraints and street networks. In general, we can confirm and quantify the intuition that a DRT system improves with increasing demand: A given request has a better chance of being effectively pooled with another user when there are many other users.

**Taxi request data** In order to benchmark a DRT system under realistic conditions, we performed simulations with taxi query data from taxi.de serving as incoming requests. The data set for the city of Kassel provides realistic values for the spatial distribution of pickup and drop-off locations as well as typical time intervals between requests. The performance of the DRT system is characterized in Fig. 8.24 by means of service quality and ecological efficiency. As before, higher demand improves the performance measures of the DRT system.

**Graph-based theoretical modelling** The mean-field approach in previous work [1] neglects the street network and instead describes a ride-pooling service operating in the Euclidean plane. We are currently developing further models based directly on the mathematical graph structure of a street network. An example is the following model of the waiting time statistics: For sufficiently high supply and low demand, the closest vehicle drives directly to the pick-up location of any incoming request. Assuming $N$ vehicles distributed uniformly on the street network, the (cumulative) distribution of waiting times is thus directly linked to the volume growth of the network, i.e. the fraction $\lambda$ of street length reachable within some time $t$:

$$\text{CDF}_{t(w)}(t) = 1 - [1 - \lambda(t)]^N.$$  

(8.8)

Given a street network, this expression allows for a direct comparison with simulated waiting time distributions, see figure 8.25. Despite the simplicity of this approach, it yields the correct qualitative curve and order of magnitude. For increasing demand (per bus), however, it can no longer be expected that the closest bus approaches the pickup location along a shortest path. Therefor we develop more sophisticated analytical expressions taking this into account by modelling bus trajectories as (persistent) random walks.

8.9 SCALING PROPERTIES OF BIMODAL ON-DEMAND PUBLIC TRANSPORTATION

P. Sharma, H. Heuer, S. Mühle, S. Herminghaus, K. M. Heidemann

Demand-responsive ride-pooling (DRRP), if operated efficiently, can be much more sustainable than individual traffic by private car [1]. However, since customers are only willing to incur limited pooling delays, the degree of poolability of ride requests via unimodal DRRP (single vehicle per trip) is limited. Fortunately, if we consider pooling of trip segments, instead of full door-to-door trips only, the potential for pooling increases. Imagine two villages, which are served with DRRP individually, but are connected by a dedicated line service for all inter-village requests (see Fig. 8.26).

In this project, we develop a model of bimodal on-demand transportation, where a DRRP system is combined with a fixed schedule line service. We overlay the transportation domain ($\mathbb{R}^2$) with a square grid of mesh size $\ell$ forming the line service network (see Fig. 8.27 A). Transportation requests are characterized by a distance distribution (see Fig. 8.27 B). If a requested distance is less than a cutoff distance $d_c$ it is assigned to unimodal service, to bimodal service otherwise (see Fig. 8.27 B, C).

We consider $\ell$ and $d_c$ as control parameters to optimize system performance, which is measured via emissions $\mathcal{E}$ and quality $\mathcal{Q}$. We solve this multiobjective optimization problem by computing Pareto fronts for $\mathcal{Q}$ and $\mathcal{E}$, thereby characterizing the possible tradeoffs between quality and emissions under varying demands (see Fig. 8.28).

Our model quantifies under what circumstances bimodal public transportation is feasible, both in terms of convenience and ecological footprint. Moreover, the model yields estimates for how to set up (mesh size $\ell$) and operate (cutoff distance $d_c$) a bimodal transportation system optimally (inset Fig. 8.28), and as such, may guide urban planners and public transportation services when considering the transition towards sustainable mobility.

Compressing soft elastic matter parallel to its surface leads to creasing, an instability where the surface folds sharply into periodic self-contacts. Creases are ubiquitous to nature and can readily be observed by closing one’s hand or bending one’s arm [1, 2]. The morphology of mammalian brains or tumors is dominated by creases due to tissue growth under constraint conditions. Similarly, polymer coatings in technological applications may suffer from creasing due to swelling [3, 4, 5]. Intriguingly, the unfolding of the surface upon releasing the strain is usually not perfect: small scars remain that serve as nuclei for creases during repeated compressions. Despite intense research over the last decades, the nature of these scars remained enigmatic.

In our recent research [6], we creased sticky polymer surfaces, resolving the micro- and macro-morphology with confocal microscopy (Figs. 8.29, 8.30). It is found that surface tension induces a second fold, at the edge of the self-contact, which leads to a singular elastic stress and self-similar crease morphologies (Fig. 8.31). Interestingly, these profiles exhibit an intrinsic folding-unfolding asymmetry (Fig. 8.31), and a microscopic residual crease, a “scar”, typically remains even after the strain is fully released (Figs. 8.29, 8.30 a). This small feature is of great significance, since it serves as a nucleus for creases when repeating the compression, and endows soft materials with programmable mechanical memory [4, 6].

In our work [6] we could show that these phenomena are caused by contact line pinning, in a way that resembles wetting of liquids on imperfect solids. Contact line pinning is therefore a key element of creasing: it inhibits complete unfolding and gives soft surfaces a folding memory.

The spreading of liquid drops on soft substrates is extremely slow, owing to strong viscoelastic dissipation inside the solid. A detailed understanding of the spreading dynamics has remained elusive, partly owing to the difficulty in quantifying the strong viscoelastic deformations below the contact line, the so-called wetting ridge.

Using shadowgraphic imaging, we could experimentally visualize dynamic wetting ridges at high spatio-temporal resolution (Fig. 8.32). The wetting ridge exhibits a rotation that follows exactly the dynamic liquid contact angle (Fig. 8.33, left) [1] – as was previously hypothesized [2]. This experimentally proves that, despite the contact line motion, the wetting ridge is still governed by Neumann’s law i.e., a vectorial balance of the solid and liquid surface tensions. Surprisingly, we also found that the solid opening angle increases at large speeds [3], which cannot be caused by bulk viscoelasticity. The effect prevails for moderate solid opening angles (Fig. 8.33, right; 180° corresponds to a flat surface), suggesting a surface rheological origin, rather than a geometric effect.

We therefore set up a new theory that incorporates the influence of surface strain, for the first time including the so-called Shuttleworth effect into the dynamical theory for soft wetting [1, 4]. It includes a detailed analysis of the boundary conditions at the contact line, complemented by a dissipation analysis, which shows, again, the validity of Neumann’s balance for static [4] and moving [1] contact lines on soft solids. Treating the tip region of a static wetting ridge in the framework of non-linear elasticity, we could analytically derive self-similar folding maps that admit surface shear and thus gradients in solid surface tension (Fig. 8.34) [4]. This way we could show that neither linear, nor non-linear bulk elasticity can generate concentrated line forces [4], irrespective whether the contact line is pinned or moving freely.

8.12 NETWORK HIERARCHY TO STORE MEMORIES

K. Bhattacharyya, D. Zwicker, K. Alim

Most successful networks, including economic, societal, transport and vasculature networks, are dynamic. Continuous adaptation of network links ensures optimal network performance when challenged within their environment. Yet, how can continuous adaptation in a dynamic environment be aligned with the observation that stimuli trigger permanent changes in adaptive networks?

To investigate memory of adaptive networks morphology, we use the standard model of adaptive network, where the link conductances adapt to minimise the power loss of the networks while the available material to create links remains constant. The constraint of conserved material strongly influence the hierarchy arising in networks [1]. We observe that despite the presence of fluctuating inflow, the information about applied stimuli position can be retrieved from adaptive networks Fig. 8.35. We observe that the links with conductances larger than a threshold ($C_{th}$) remain more or less constant, while conductances below the threshold decay following a power law of 1/3 (Fig. 8.37(a)). As a result of this dynamics an irreversible hierarchy is being created in the networks.

![Figure 8.35: Power loss of networks trained with a stimulus at direction $\theta_1$ vs. the memory probing direction ($\theta_2$) shows memory in trained networks. The untrained network is relaxed without any stimulus before probing the network from different directions ($\theta_2$).](image1)

![Figure 8.36: No memory in hierarchy-free networks. (a) Ratio of conductances of two subsequent time point with respect to conductance value. (b) The network architecture at time point $t_{train}$ and the network structure at $4t_{train}$. The color code represents the log of conductances.](image2)

![Figure 8.37: Memory is stored in vanishing links. (a) Ratio of conductances of two subsequent time point with respect to conductance value. (b) The network structure at time point $t_{train}$ and the network structure at $4t_{train}$. The color code represents the log of conductances.](image3)

Our analytical calculation of dynamics of link conductances ([2]) predicts the numerically observed dynamics, identifying the irreversibility as a direct consequence of the adaptation dynamics [2]. Moreover, our analytical theory faithfully predicts the role of all system parameters during memory formation [2]. As example, our calculations predict that material conservation constraint can limit memory formation by limiting the irreversibility of network hierarchy. We confirm this prediction by showing, no information about applied stimuli position can be retrieved from simulated networks with low or no hierarchy Fig. 8.36. In summary we find that irreversible hierarchy of adaptive networks, controlled by material conservation stores information about stimuli. Our work not only opens an entirely new perspective on adaptive networks such as our vasculature but provides an analytically tractable theory of memory formation in disordered systems.

In order to survive in highly complex environments, simple organisms have to be able to process and store sensory information. We studied the mechanism of memory encoding in *Physarum polycephalum*, a giant unicellular eukaryote with a body made up of soft, contractile, cytoplasm-filled tubes interconnected in a network.

The tubular network constantly reorganizes as the organism forages for nutrients, and nutrient sources taken up by the organism leave an imprint in the morphology of the network. In order to decipher the mechanism behind the observed imprinting and probe its significance for the organism’s function, we followed the process of nutrient encounter using a synergy of experimental methods and theoretical model building [1].

![Figure 8.38](image1.png)

**Figure 8.38:** The location of a nutrient stimulus is memorized in network hierarchy. Bright-field images of a foraging *P. polycephalum* network with the nutrient stimulus (red arrow) applied at 0 min. The reorganizing network changes its migration direction towards the nutrient in 45 min, consumes the nutrient (90 min) and continues foraging (310 min). Nutrient location is imprinted in the network hierarchy by thick tubes formed around the nutrient source - persisting long after the nutrient is consumed.

![Figure 8.39](image2.png)

**Figure 8.39:** Following nutrient stimulus application, hierarchy of tube diameters changes, establishing a new migration direction. (A) Bright-field images of a network before and after the application of a nutrient stimulus (red arrow). A new migration direction is being created at the top of the network. (B) Relative tube growth over the 45 min after stimulus (red dot) application. While overall mass is redistributed from the bottom to the top of the network, close to the stimulus site, initially larger tubes lose less mass, thus increasing network hierarchy.

We found that the location of the food source is imprinted in the hierarchy of tube diameters in the network. The food source triggers a release of tube-softening chemical agent which gets transported by cytoplasmic flows across the network and is readily taken up by the tubes. Tubes that receive more of the chemical agent due to their proximity to the food source grow at the expense of the other tubes, thereby updating the network hierarchy.

Strikingly, rather than experiencing a complete reset, the reorganizing network of *P. polycephalum* relies on its existing hierarchy established by previous stimuli, effectively demonstrating the ability to read out stored memories and even overlay multiple memories. This novel mechanism of self-organisation opens exciting new venues for studying associative memory formation in flow networks and is likely to contribute to bioinspired design.

8.14 THE DYNAMICS OF THE GUT AND ITS MICROBIOME: IS THE GUT SELF-ORGANIZING?

A. Codutti, J. Cremer (Stanford U.), K. Alim

The gut is of eminent importance for health, recently receiving widespread attention of its implication on brain functioning through the so called gut-brain axis. Indeed, malfunctioning of the gut and of its microbiome are associated with severe diseases such as irritable bowel syndrome, depression, obesity, anxiety. How is this possible? It was discovered that the microbiome produces metabolites, such as neurotransmitters, which can directly affect the nervous system. Even more interestingly, these metabolites do not only affect the brain functioning but also the contractility of the gut itself [1]. The gut can be viewed as a long tube, whose aim is to absorb the nutrients as efficiently as possible; this tube undergoes different motility phases, which determine the flow within the gut (see Fig. 8.40). The flow itself impacts bacterial growth and nutrients absorption, as well as metabolites dispersion and advection. Therefore, any metabolite-induced change of motility will produce a cascade of feedback connections, which would profoundly affect not only the gut functioning but also the global well-being of the individual. This leads to the following question: is the gut self-organizing to maximize nutrient absorption and to control the size and stability of its microbiome?

To answer this, we tackle how the motility of the gut, i.e. its time-dependent wall geometry, influences the gut and microbiome dynamics through the motility induced fluid flows. We pinpoint the essential parameters through which the gut can self-regulate. We focus onto well-known motility patterns, peristalsis, i.e. a sinusoidal contraction wave, and segmentation, i.e. amplitude-phase coupled waves [2]. Peristalsis provokes faster flows than segmentation; thus, changing motility pattern, flows can be regulated. We identify the fluid flow as the main regulating parameter of the bacterial and nutrients dynamics (Fig. 8.41), whose steady state is determined computationally (data points) and theoretically (lines), through means of a Taylor-dispersion approach. High flows decrease the nutrient-uptake efficiency (panel A) while inhibiting bacterial growth. Vice versa, slow flows increase the efficiency at the expense of higher bacterial growth. High absorption rates (pink curve) facilitates absorption and reduces bacterial growth, while low absorption rate (green curve) has the opposing effect. Thus, the gut regulates the efficiency of absorption and bacterial growth by changing the flow velocity through means of altered motility, or by changing the nutrients uptake rate. Therefore, metabolites that induce higher flows by changing the motility pattern could be interpreted as a self-regulatory mechanism aimed at maintaining the microbiome size to healthy levels.


Figure 8.40: The gut is a highly interconnected system, where gut wall motility determines flows, which in turn affect nutrients and bacteria transport, dispersion, and nutrients absorption. Bacteria and nutrients trigger feedback reactions on the motility itself, which could lead to self-organization.

Figure 8.41: The steady-state solution of the gut dynamics shows that the gut controls the efficiency of the nutrients uptake and the bacterial growth through the mean flow (x-axis) and the absorption rate (different colors). Higher flows decrease the nutrient uptake efficiency (panel A) while inhibiting bacterial growth (panel B); slow flows show an increase in efficiency but also a significant bacterial growth. A high absorption rate (pink curve) has similar effects as fast flows.
8.15 STATISTICAL GEOMETRY OF TURBULENT MIXING

L. Bentkamp, C. C. Lalescu, M. Wilczek
T. D. Drivas (Stony Brook)

Turbulence drives pollutant dispersion in the atmosphere, the mixing of nutrients and microorganisms in the ocean, and it helps to sustain dynamos in stars and planets. Traditionally, turbulent mixing is characterized in terms of the dispersion of tracer particles or tracer-particle pairs. However, the stretching and folding of fluid elements, which is the central dynamical mechanism underlying turbulent mixing, cannot be captured following just a few tracer particles. This rather requires a new geometric perspective, which we recently developed to uncover and explain the statistical geometry of turbulent mixing.

We focus on the simplest extended fluid elements — material loops — and track how they are stretched and folded by turbulence, see Fig. 8.42. While our simulations show that their geometry becomes unfathomably complicated over time, we reveal universal, predictable features of these complex objects. As a key quantity to characterize how much fluid elements are twisted and folded by the turbulent flow, we investigate the loop curvature, which may become extremely high at isolated points along the loop, see Fig. 8.43. The resulting curvature distributions show a clear power law (Fig. 8.44), indicating that the generation of large curvatures along material lines is a scale-free process. As a main result, we theoretically explain the curvature distribution based on just the local stretching and compression rates of the flow.

As such, our work offers a new geometric perspective on the statistics of turbulence, and it enables predictions for advected material lines in a broad range of chaotic and turbulent flows. Potential applications include polymeric flows, geophysical transport phenomena like the dispersion of nutrients, salt or heat in the ocean, as well as astrophysical dynamo problems.

8.16 PHYSICAL BIODYNAMICS

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In many cases an understanding of physical backgrounds of different biological processes is very important to optimise their dynamics or to prevent undesirable effects. In this chapter we consider examples of biodynamical processes including cilia driven flow in the brain, hydrodynamic interaction and waveform of oscillating flagellas, adhesion and migration of amoeboid cells, and spiral wave dynamics in excitable media.

8.16.1 Cilia-driven flows in the brain third ventricle

(Y. Wang, C. Westendorf) The cerebrospinal fluid (CSF) fills the cavities in the mammalian brain, known as the brain ventricular system, see Fig. 8.45(a). On a large scale the CSF is produced in a specialized tissue and then transported in a unidirectional manner from the lateral ventricles, through the third and fourth ventricle finally ending up and being reabsorbed in the spine. Almost all the surface of the ventricular system is covered with cilia bearing cells with the cilia often being arranged in bundles of up to 80 individual cilia. The continuous beating of these cilia bundles drives the CSF flow through the ventricular system. However, on a smaller scale, we have discovered that the cilia driven flow in the third ventricle (Fig. 8.45(a), green) is not a uni-directional throughflow but organized in rather complex flow patterns. Our initial analysis focused on the flow patterns itself and the polarization of the underlying tissue. We have extended the description onto several proteins, known as key players in establishing the planar cell polarity (PCP) of the tissue, as the orientation and location of the cilia bundles is likely tightly bound to the establishment of the PCP.

After describing the flow patterns, we now ask the questions, how do these patterns arise during the development of the organism and which function may those patterns serve [1]. It is very intriguing to see, that comparing by now several hundreds of investigated specimens, the large-scale organization of the flow patterns and the underlying tissue polarization is remarkably conserved. We have therefore extended our studies to include the developmental timescale as an additional dimension describing the origin of the flow patterns. We hypothesize that the flow patterns serve for directed transport of signal molecules contained in lipid vesicles (exosomes). We thus applied injections of liposomes onto the prepared samples as a surrogate for the biological cargo. This allows for a much more accurate investigation of possible biological targets of the complex flow in the third brain ventricle, see

Figure 8.45: (a) Sketch of the mouse brain ventricular system with the ventral third ventricle colored in green. (b) Integrated approach to study the architecture and dynamics of local cilia arrangement. (I) - Bead tracking, (II) - Liposome injection, (III) - Live cilia staining, (IV) - Immunostaining.
Fig. 8.45(b). The entire project was carried out in a close collaboration with the department of Prof. G. Eichele at the neighboring MPIBC. This collaboration is now further intensified, as Prof. G. Eichele recently joined the MPI DS as an emeritus group with a fully equipped laboratory.

8.16.2 Resistive force theory and wave dynamics in swimming flagellar apparatus isolated from Chlamydomonas reinhardtii

(A. Gholami) Cilia-driven motility and fluid transport is ubiquitous in nature and essential for many biological processes, including swimming of eukaryotic unicellular organisms. The-biflagellated micro-swimmer Chlamydomonas reinhardtii is a model organism to study dynamics of flagellar synchronization. Hydrodynamic interactions, intracellular mechanical coupling or cell body rocking are believed to play crucial role in synchronization of flagellar beating in green algae. We use freely swimming intact flagellar apparatus isolated from wall-less strain of Chlamydomonas to investigate wave dynamics. Our analysis in phase coordinates shows that, when the frequency difference between the neighboring flagella is high (10-41% of the mean), neither mechanical coupling via basal body nor hydrodynamics interactions are sufficiently strong to synchronize two flagella, indicating that beating frequency is perhaps controlled internally by the cell. We also examined the validity of resistive force theory for a flagellar apparatus swimming freely in the vicinity of a substrate and found a quantitative agreement between experimental data and simulations with drag anisotropy of ratio 2 (Fig. 8.46). Finally, using a simplified wave form, we have shown that by controlling phase or frequency differences between two flagella, steering can occur [2].

8.16.3 On the existence of a back-propagating wave component in isolated Chlamydomonas reinhardtii flagella

(A. Gholami) We also analyzed the motion of isolated and demembranated flagella from green algae Chlamydomonas reinhardtii, which act as ATP-driven micro-swimmers. The waveform of the Chlamydomonas beating flagella has an asymmetric waveform that is known to involve the superposition of a static component, corresponding to a fixed, intrinsic curvature, and a dynamic wave component traveling in the base-to-tip direction at the fundamental beat frequency, plus higher harmonics. We performed principal component analysis of the flagellar beat and show that the first four dominant eigenmodes describe the axonemal shapes with high accuracy. Furthermore, our mode analysis of free, pinned and clamped axonemes show the co-existence of a secondary tip-to-base wave component at the fundamental beat frequency that propagates opposite to the dominant base-to-tip wave, albeit with a smaller amplitude (Fig. 8.47). Finally, to understand the effect of calcium on the constituting wave components, we performed experiments at different [Ca^{2+}] and observed that as we increase [Ca^{2+}] from 0.0001
mM to 1 mM, the static mode drops significantly (~ 85%), triggering a transition from circular swimming path to a straight trajectory [3].

8.16.4 Cell adhesion and migration

(A. Krekhov, M. Tarantola, C. Westendorf) Amoeboid adhesion is very versatile and does not involve focal adhesion complexes. We employed model substrates to identify adhesion mechanisms of the amoeba *Dictyostelium discoideum* (*D.d.*) and recently extended this approach to study contact guidance on micropatterned polyethylene-glycol gels, which nearly exclusively restrict migration to adjacent glass stripes. Surprisingly, this allowed us also to describe substantial differences between developmental stages and laboratory strains of *D.d.*, as also confirmed by single-cell adhesion force spectroscopy (SCFS) [4].

We furthermore studied the interplay of *D.d*. adhesion and Clathrin-Mediated-Endocytosis, which controls transmembrane protein recycling. We examined LimE-labelled actin foci colocalized to spots of the adhesive protein SadA using a novel combination of SCFS and super-resolution microscopy (metal-induced energy transfer, MIET). We showed that the cell detachment process is sensitive to a loss of clathrin-light-chain (*clc*), reducing adhesion forces (Fig. 8.48A), number of adhesive points per cell and contact area. MIET allowed for quantification of the overall ventral height of *carA*-labelled cell membrane, *clc*, and actin relative to the underlying substrate (Fig. 8.48B-C). At actin foci locations coinciding with *clc* structures, the membrane is lifted and actin lifetimes increased. Cells deprived of *clc* show a significant reduction in actin-substrate distance (Fig. 8.48D) at increased foci densities. In summary, we can show that *clc* at actin foci is involved in cluster stability- and cell-substrate distance-regulation upon amoeboid cell adhesion [5, 6].

Besides the adhesome, the actin cytoskeleton and its response to external chemical stimuli is fundamental to amoeboid migration. One key player governing actin network dynamics is the motor protein myosin II. Based on experimental evidence, we have designed a model capturing three phases observed upon chemotactic stimulation by phase space embedding, which predicts a decreasing myosin II – actin coupling strength for the robust control of cell contraction upon chemotaxis [7].

*D.d.* cells also present other techniques to modulate the dynamical state of their actin cytoskeleton upon chemotaxis: In a population of cells, some specimen show noisy oscillatory cycles of actin polymerization, which we studied in response to external stimuli. These cells adopt a noisy quiescent state, before returning to their initial, oscillatory dynamics. We proposed a model based on a generic nonlinear noisy oscillator and a Hopf-bifurcation as transient termination mode [8].

Figure 8.48: A: Maximum adhesion force *F*\(_{\text{max}}\), normalized to contact area for *D.d*. wild-type cells and amoeba with *clc* deletion. B: Exemplary cellular fluorescence (left) and MIET height (right) micrographs for: actin (LimE, top), clathrin (*clc*, middle) and membrane (*carA*, bottom) and corresponding average maps (+ Error bars) for WT (C) or *clc* null cells (D, shown only for LimE), *n* = 16-20 cells/category.
8.16.5 Spiral waves within a bistability parameter region of an excitable medium

(V. Zykov) Spiral waves are a prominent and intensively studied dynamic phenomenon in excitable media of very different nature. Until now, it has been assumed that an excitable medium must have a single stable resting state in order to sustain a spiral wave. Our computations, performed with the widely used Barkley model, clearly demonstrate that the spiral waves exist in a much wider parameter range than it was previously postulated in [9], as can be seen in Fig. 8.49.

Within the bistability parameter region, where \( b < a - 1 \), no meandering spiral waves have been found. Here the spiral waves either rotate around a wave core that is at rest, or the tip trajectory orbits around a "negative" core that is located within the excited state. The obtained analytical expression \( b = (a - 1)/2 \) for the boundary between these two parameter ranges is in quantitative agreement with the results of direct numerical computations [10].

Along the most part of this line, the core size is equal to zero. However, in the upper right part of this line, where \( b > 0.7 \), this solution becomes unstable. Depending on the initial conditions used, two different rotation patterns with a common positive or an unusual "negative" core are obtained here for the same parameter set, as shown in Fig. 8.50. Therefore, in this parameter range marked by the green line in Fig. 8.49, a duality of the spiral wave core and a hysteresis phenomenon in the spiral wave dynamics have been observed [10].

Thus, the calculations performed with the Barkley model allowed us to discover many important and unknown properties of rotating spiral waves. Since the Barkley model is very general and widely used to reproduce the basic properties of spiral wave dynamics, the data reported here should be applicable to various models and excitable media of different nature. We are planning to estimate parameters of the obtained spiral waves by application of the earlier elaborated kinematical approach [11].

It should be noted that spiral waves are considered as a plausible cause of cardiac arrhythmias, if the size of the heart muscle exceed at least the core diameter. From this point of view, the observed existence of spiral waves with an infinitely small core is rather important factor because a small core size obviously increases the probability of spiral wave maintenance.

8.50: Counterclockwise rotating spirals with (a) positive and (b) "negative" core obtained for \( a = 2.4, b = 0.7 \) and \( \epsilon = 0.02 \). Within the gray regions \( u(x, y, t) > 0.5 \).

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Cellular processes manage to function with exquisite precision, even if the molecular-scale components that carry them out are subject to strong thermal (and non-thermal) fluctuations. How does robustness arise in such inherently noisy systems? A possible solution comes from the notion of topologically-protected phenomena, that is, phenomena that rely on a discrete, qualitative feature of the system rather than on finely-tuned parameters, enabling behaviors that are robust against disorder or noise.

Many biochemical processes are described by continuous-time, memoryless Markov networks representing transitions in a discrete state space. This state space may represent, for example, the internal state and location of a molecular motor along a filament, the length of a biopolymer, the conformational state of a protein complex, etc. In recent work, we explored whether topologically-protected phenomena can arise in such networks [1].

To this end, we considered processes that occur in a two-dimensional configuration space and are strongly driven out of equilibrium by the presence of ‘futile cycles’, i.e. energy-consuming transitions that loop back to the original state and leave the system unchanged. In Fig. 8.51 we show our results for one such network, which could for example represent the state of a biopolymer composed of two types of subunits. Analytical considerations and stochastic simulations demonstrated that topologically-protected currents emerge along the edges of configuration space, no matter their shape, as long as $\gamma_{\text{in}} \ll \gamma_{\text{ex}}$. In this particular example, the edge currents would manifest as oscillatory growth and...
shrinkage of the biopolymer, robust to any perturbations such as variations in the transition rates or in the availability of the monomers that make up the biopolymer. The topological nature of the effect could be identified by a novel application of tools from non-Hermitian quantum physics to classical stochastic systems. Further applications include the design of robust clocks, nanoscale swimmers, or the synchronization of subsystems through a shared pool of resources.

Much of the activity inside cells is ultimately driven by nanoscale enzymes that catalyze out-of-equilibrium chemical reactions. Often, enzymes work in close proximity of each other, be it in large clusters such as metabolons, or small multimeric complexes of just a few enzymes. While the activity of a single enzyme requires the noise-activated crossing of a chemical free-energy barrier and is thus inherently stochastic, we wondered about the effect that mechanical interactions between nearby enzymes can have on their catalytic activity [2].

By building a minimal model that captures the conformational changes experienced by enzymes during a catalytic step, and considering the enzyme-enzyme interactions mediated by the surrounding viscous environment (see Fig. 8.52), we showed that physical proximity can couple the catalytic activity of two enzymes. For weak coupling, the two enzymes still perform single noise-activated catalytic steps, although they start to happen in tandem, i.e. the two enzymes begin to synchronize. For strong coupling above a critical value, however, a single thermal fluctuation can trigger long catalytic ‘runs’, where the two enzymes perform dozens of perfectly-synchronized catalytic steps in one go. This transition could be explained by a topological bifurcation of the dynamical system describing the two catalytic phases of the enzymes, which is defined on the torus. While for weak coupling all trajectories are attracted to the fixed point corresponding to the chemical free energy minimum of each enzyme, for strong coupling a ‘running band’ of periodic trajectories emerges that winds around the torus and allows for deterministic catalysis, see Fig. 8.53. It is interesting to speculate, although it remains to be seen, whether enhanced catalysis and synchronization are at work in biological enzyme clusters.

Figure 8.52: (a) Two enzymes undergoing conformational changes may interact with each other hydrodynamically through the surrounding viscous fluid medium. (b) Two enzymes embedded in a lipid membrane might interact elastically. (c) The catalytic cycle of each enzyme is represented by a phase \( \phi_a \) evolving in a biased free energy landscape \( V(\phi_a) \) (solid blue). The enzyme elongation adapts to a phase-dependent rest length \( L(\phi_a) \) (dotted red).

Figure 8.53: Topological bifurcation on the torus with increasing coupling. White regions are basins of attraction of the stable point. Beyond the critical coupling, a ‘running band’ (grey) of periodic trajectories emerges.

We have been interested in transport, information and navigation in flow-fields, especially as pertains to small particles for which fluctuations are important. Here, we will discuss new relations for passive particles that undergo stochastic motion in fluids [1, 2] as well as active microswimmers [3].

Flow-fields are ubiquitous systems that are able to transport vital signalling molecules necessary for biological system function. While information regarding the location and transport of such particles is often crucial, it is not well-understood how to quantify the information in such stochastic systems (Fig. 8.54). Using the framework of nonequilibrium statistical physics, we develop theoretical tools to address this question [1], defining information as differences in entropy. We observe that rotation in a flow-field does not explicitly appear in the generalized potential that governs the rate of system entropy production. Specifically, in the local region around a flow-field, rotation contributes to the information content only in the presence of strain – and then with a comparatively weaker contribution than strain and at higher orders in time. Indeed, strain, and especially the flow divergence, contribute most strongly to transport properties such as particle residence time.

Figure 8.55: (A) A tracer particle undergoes diffusion and drift in a force-field whose non-conservative component is generated by a vortex line (thick green), tracing out a stochastic trajectory (thin irregular loop). The force-field has the same rotational component throughout but varying irrotational components (the cross-sections depict force-field streamlines) – however the distribution of closed loops depend only on the rotational component. (B) Different particle trajectories around a single vortex line (green) can be characterized by the winding number n. The leftmost two are topologically equivalent with n = 1, while the rightmost two have the opposite sign and winding numbers n = −1 and n = −2, respectively. (C) Force-fields can contain multiple vortex-cores (thick green lines or rings), around which particles can trace closed trajectories (thin irregular loops).
and the rate of information change. These results shed light on how information can be analyzed and controlled in complex artificial and living flow-based systems.

Separately, fluctuation theorems specify the non-zero probability to observe negative entropy production, contrary to a naive expectation from the second law of thermodynamics. For closed particle trajectories in a fluid, Stokes theorem can be used to give a geometric characterization of the entropy production. Building on this picture, we formulate a topological fluctuation theorem that depends only on the winding number around each vortex core and is insensitive to other aspects of the force (Fig. 8.55). The probability is robust to local deformations of the particle trajectory, reminiscent of topologically protected modes in various classical and quantum systems. We demonstrate that entropy production is quantized in these strongly fluctuating systems, and it is controlled by a topological invariant [2]. We demonstrate that the theorem holds even when the probability distributions are non-Gaussian functions of the generated heat, which are most relevant for non-equilibrium systems.

![Figure 8.56](image)

**Figure 8.56**: (a) Microswimmer trajectory $r(\tau)$ (blue dashed line) on a Riemannian manifold $M$. The microswimmer moves in the tangent space $TM$ under the influence of the force $f$ (black arrows) and its self-propelling velocity whose direction $\hat{e}$ is marked with cyan arrows. (b) Fraction of a spherical surface enclosed in the optimal forward-backward loop as a function of the maximum force on the sphere. There is a jump when the vortex is enclosed in the loop, also seen in the change in the scaling behavior, which is essentially linear (black dashed) for small values of the force.

Lastly, finding the fastest path to a desired destination is a vitally important task for microorganisms moving in a fluid flow. We study this problem by building an analytical formalism for overdamped microswimmers on curved manifolds and arbitrary flows (Fig. 8.56). We show that the solution corresponds to the geodesics of a Randers metric, which is an asymmetric Finsler metric that reflects the irreversible character of the problem. A study of the shape of isochrones reveals features such as self-intersections, cusps, and abrupt nonlinear effects. Our work provides a link between microswimmer physics and geodesics in generalizations of general relativity.

Controlling an evolving population is an important task in modern molecular genetics, including in directed evolution to improve the activity of molecules, in breeding experiments, and in devising public health strategies to suppress pathogens. An optimal intervention should be designed by considering its impact over an entire evolutionary trajectory that follows. Thus, a seemingly suboptimal intervention at a given time can be globally optimal as it can open opportunities for desirable actions [1].

In a recent work, we developed a population genetics based optimal control formalism for stochastic and in general out of equilibrium systems to direct the evolution of multi-variate molecular phenotypes [2]. We showed that artificial selection should counter evolutionary trade-offs among multi-variate phenotypes, such as the stability and catalytic activity of an enzyme, to avoid undesirable outcomes in one phenotype by imposing selection on another. Evolutionary control is challenged by the limited predictability of evolution due to stochastic effects at the molecular or environmental level. Evolutionary predictability depends on how far into the future we want to predict [3, 4], as seen in models forecasting the evolution of influenza [5, 6]. We developed an information theoretical approach to gauge the efficacy of an evolutionary control based on the degree of predictive evolutionary information [2]. Notably, we showed that molecular time-scales for evolution under natural selection can inform how to monitor a population to acquire sufficient predictive information for an effective intervention (Fig. 8.57).

The interplay between prediction and control is a key in devising optimal strategies against evolving pathogens. Currently, we are developing a predictive approach for HIV escape against broadly neutralizing antibodies (BnAbs). HIV therapy with passive BnAb infusion has become a promising alternative to anti-retroviral drugs for suppressing the disease in patients without a need for daily administration. The current obstacle is the frequent escape of the virus seen in mono- and even combination BnAb therapy trials [8, 9, 10]. The key is to identify BnAb cocktails that target multiple vulnerable regions on the virus, to reduce the likelihood for rise of resistant variants with escape-mediating mutations in all of these regions. Identifying an optimal BnAb cocktail can be a combinatorially difficult problem, and designing patient trials for all the potential combinations is a costly pursuit.

In a recent work, we have proposed a computational approach to predict the efficacy of a BnAb therapy trial based on population genetics of HIV escape, which we parametrize using high-throughput HIV sequence data collected from a broad cohort of BnAb-naive patients [7]. Specifically, we characterize evolutionary fate of escape mutations to predict patient outcomes in recent mono- and combination therapy trials with 10-1074 and 3BNC117 BnAbs [8, 9, 10]. Given that our predictions are done solely based on the genetic data from a cohort of ART-naive patients, we can use our approach to assess the efficacy of
a broader panel of BnAbs, for which no clinical trial data is available. Interestingly, we infer that escape from mono-therapies is almost certain and a combination of at least 3 antibodies is necessary to the probability of early rebound below 1%. In addition, we can propose optimal combination therapies that can efficiently curb an HIV infection and sustain viremia at low levels and suppress evolutionary escape of HIV within patients (Fig. 8.58).

Our approach showcases that, when feasible, combining predictive population genetics models with control approaches can have surprisingly broad applicability, and their interpretability can shed light into the complex dynamics of populations with applications for therapy against evolving pathogens.

![Therapy ranking diagram]

**Figure 8.58:** Therapies with 1, 2, and 3 BnAbs, ranked by the predicted probability of late viral rebound is shown. BnAbs for each therapy are listed under the corresponding data point.

8.20 INFERENECE OF FUNCTIONAL SELECTION IN IMMUNE REPERTOIRES

G. Isacchini, Z. Montague, & A. Nourmohammad

The adaptive immune system develops during the lifetime of an organism and consists of highly diverse B- and T-cells, whose unique surface receptors are generated through genomic rearrangement, mutation, and selection. This diverse repertoire of receptors can mount specific responses against a multitude of evolving pathogens and keep a memory of past infections for future encounters. Pathogens in return, evolve to escape the immune challenge, forming a rapid coevolutionary arms race during the life-time of an organism.

Each B and T cell recombines its receptor chain to express a unique receptor. An additional process of selection, which happens in the thymus for T cells, selects for receptors with higher affinity to foreign antigens and tolerance to self-antigens. During selection T cells also differentiate into separate subtypes that perform distinct functions. The resulting potential diversity of their sequences due to this process has been estimated to be approximately $10^{17}$ amino acid sequences [1]. The realized diversity in a individual is approximately $10^9$ unique receptors. Thanks to advancements in high throughput sequencing we have access to $10^5$ unique receptor sequences on average from an experiment. These three numbers define orthogonal dimensions of complexity in the analysis of immune receptor repertoires: on one hand an individual typically carries a repertoire of receptors that is mostly personal, on the other hand we have access only to an under-sampled snapshot of its repertoire. For these reasons mathematical modeling and computational approaches are needed to characterize the statistical properties of these repertoires and extract information about an active immune response. In a series of studies, we have developed statistical inference approaches to characterize the statistics and dynamics of functional B- and T-cell repertoires in response to immune challenges.

Statistics of immune receptor repertoires. Initiation of the immune response relies upon the recognition of foreign pathogens by B and T cells. Recognition is mediated by an highly specific interaction between their receptor and the pathogenic epitope. Properly characterizing this process is of particular importance in order to better understand the dynamics of the immune response and subsequently develop novel diagnostic tools and better therapies.

In a recent work [1] we combined the best of model-based statistical inference and the flexible deep learning approaches to infer functional selection models for immune repertoires. In recent years we have seen growing popularity in machine learning approaches to immune repertoires [2]. However, black box machine learning techniques often lack interpretability and require a very large amount of data for training [3]. On the other hand, biophysical models [4] are more interpretable and easier to train, yet they are limited by the prior assumptions that define their structures. We introduced an inference framework to integrate
the interpretable knowledge-based models with more flexible but powerful deep learning approaches \[1\]. This framework enabled us to characterize signatures of differential functional selection on immune receptors. The identified the differential sequence features between distinct cell types (e.g. CD4+ helper, CD8+ cytotoxic, or regulatory T-cells) in different tissues (Fig. 8.59). We characterized the sequence properties that encode synergistic selection on paired chains of T-cells and B-cells. Finally, we demonstrated that biophysical selection models can be used as simple classifiers to successfully identify T-cells specific to distinct pathogenic target—a problem that is of significant interest for clinical applications.

**Short-term dynamics of immune receptor repertoires.** Acute infections (e.g. the common cold) or vaccinations can trigger transient adaptive immune responses, resulting in proliferation of immune cells. Tracking the clone size (i.e., the number of immune cells with a common receptor) or expression level of a clone (i.e., mRNA count for a given receptor) over time can be informative of such response. In a recent study with the group of Chris Mok at the University of Hong Kong, we used our selection inference for immune repertoires \[1\] to establish a principled statistical approach to study the statistics and dynamics of B-cell receptor (BCR) repertoires in COVID-19 patients, and to characterize repertoire features in patients with different disease severities \[5\].

By combining information from the statistics of sequence features in plasma and bulk BCR repertoires, the expanding dynamics of clonal lineages during infection (Fig. 8.60), and sharing of BCRs among COVID-19 patients, we identified 38 clonal lineages that are potential candidates for response to SARS-CoV-2. Using single-cell sequencing, we verified reactivity of BCRs shared among individuals to SARS-CoV-2 epitopes. Moreover, we identified cross-reactive responses to SARS-CoV-1 in some of the COVID-19 patients, and have identified natural emergence of a SARS-CoV-1 reactive antibody.

Our work showcases that robust statistical modeling is a key in interpreting the complex organization of the immune repertoires. We are currently leveraging our expertise in this area to characterize the features of repertoires that permit emergence of BnAbs in HIV patients to characterize the feasibility of eliciting these highly potent antibodies by vaccination.

8.21 MEMORY STORAGE IN EVOLVING BIOLOGICAL NETWORKS

O. Schnaack & A. Nourmohammad

Biological systems, ranging from the brain to the immune system, store memory of molecular interactions to efficiently recognize and respond to stimuli. However, the strategies for encoding a memory vary largely across biological systems. For example, in the olfactory cortex, synaptic connections form when stimulated by an odor and establish associative distributed memory that can be retrieved upon re-exposure to the same odors. In contrast, the adaptive immune system encodes specialized memory by diverse sets of cells whose unique surface receptors can readily recognize and mount a specific response against a multitude of pathogens upon a re-infection. Despite the vast mechanistic differences between memory storage in the olfactory and the immune system, these processes can still be viewed as different information encoding strategies.

In a recent study, we present a theoretical framework with artificial neural networks to characterize optimal memory strategies for both static and dynamic (evolving) patterns. Our approach is a generalization of the energy-based Hopfield-like neural networks in which memory is stored as the network’s energy minima. Our proposed model can adopt different memory encoding strategies, including distributed memory, similar to the classical Hopfield network, or specialized memory in separate compartments. The learning rate and the number of compartments in a neural network define a memory strategy, and we probed the efficacy of different strategies for static and dynamic patterns.

We found that while classical Hopfield networks with distributed memory can efficiently encode and retrieve a memory of static patterns, they are inadequate against evolving patterns. To follow an evolving pattern, we showed that a Hopfield network should use a higher learning rate, which in turn, can distort the energy landscape associated with the stored memory attractors, leading to pattern misclassification (Fig. 8.61). To remedy this problem, we demonstrated that compartmentalized networks with specialized subnetworks are the optimal solutions to memory storage for evolving patterns.

The contrast between these memory strategies is reflective of the distinct molecular mechanisms used for memory storage in the adaptive immune system and in the olfactory cortex. In particular, the memory of odor complexes, which can be assumed as static, is stored in a distributed fashion in the olfactory cortex. On the other hand, the adaptive immune system, which encounters evolving pathogens, allocates distinct immune cells (i.e., compartments) to store a memory for different types of pathogens (e.g., different variants of influenza or HIV). We postulate that evolution of pathogens may be one the key reasons for the immune system to encode a focused memory, in contrast to the distributed memory used in the olfactory cortex that interacts with mixtures of static odors.
Memory is a hallmark of adaptive immunity and enables organisms to respond more readily upon re-infections. However, memory differentiation especially in antibody secreting B-cells is one of the least understood cell fate decisions in the adaptive immune system. In a recent study, we incorporated kinetics and biophysics of immune memory response as ingredients of a non-equilibrium decision-making between an adaptive exploration to mount a specific and novel response or exploitation of existing memory that can be activated rapidly yet with a reduced specificity against evolved pathogens [2]. Our theory makes concrete predictions about the functionality of immune memory and the strategies that are likely to be selected over evolutionary time scales, and therefore, are hard-wired in our immune system as rules of memory differentiation. To achieve a long-term benefit for the host, we showed that memory generation should be actively regulated and dependent on immune receptors’ affinity, with a preference for cross-reactive receptors with a moderate affinity against pathogens as opposed to high affinity receptors (Fig. 8.62)— a recipe that is consistent with recent experimental findings.

Moreover, we predict that an organism’s life-expectancy should impact the extent of cross-reactivity in their memory repertoires, and that organisms with shorter life expectancy and fewer pathogenic encounters should carry more cross-reactive memory. This prediction can guide comprehensive cross-species comparisons of immune systems, which are currently missing from the field of immunology. Lastly, we showed that sudden changes in an organism’s life-span (e.g. in humans), can have dire consequences for the efficacy of the immune memory. Specifically, the abundance of cross-reactive memory in this case can limit novel responses, necessary for protection against evolutions by evolving viruses—a problem known as original antigenic sin, presently observed in human immune response to influenza [3].

In a recent collaboration with Prof. Peliti at the Santa Mariella Institute, we explored more general models of memory for out-of-equilibrium systems with evolving patterns to uncover the principles of memory storage in biological networks [1].

As a whole, our framework provides a baseline to gauge the efficacy of immune memory in light of an organism’s coevolutionary history with pathogens.

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After decades of development in biophysics and biomedical engineering, we now understand far more about the physics of living matter and are rapidly developing new technologies for human health and safety. This is a topic central to the department of Prof. E. Bodenschatz. On the one hand we investigate problems in cardiac function, like fibrillation mechanisms and their avoidance, mechanics of the contracting heart, and helping in the development of Engineered Heart Muscle (EHM) and its placement on a patient’s heart. To this end based on cellular electrophysiology, we studied how spiral waves in cardiac tissue can be controlled with light and temperature. In the German Centre for Cardiovascular Research (DZHK) funded project "Alliance for the Regeneration of the Heart", we developed a computational model for the heartbeat and investigated the mechanical properties of heart muscle both theoretically and experimentally, in collaboration with the group of Prof. W. Zimmermann at the University Medical Center Göttingen (UMG). In the Federal Ministry for Education and Research (BMBF) funded project IndiHEART, we are helping developing with our partners fibre-based 3D bioprinting for patient specific EHM. On the other hand the pandemic has shown that we know too little about the mechanisms and pathways of airborne disease transmission, a topic which has been studied deeply by us over the past 1.5 years. In collaboration with Prof. S. Scheithauer from the UMG we have measured the human exhaled particles from more than 130 volunteers, have investigated aerosol emission from wind instruments and mask efficacy in collaboration with R. Müller and Dr. K. Wogram from the Institute for Music and Aerosols. We have developed the web app HEADS, https://aerosol.ds.mpg.de, that allows the calculation of the infection risk by human pathogens. HEADS relies on a new theoretical model for poly-pathogen infection risk. In collaboration with MPI-C and Fraunhofer IKTS we measure the constituents of human droplets.
8.22.1 Human exhaled particles and risk of infection from airborne diseases

(G. Bagheri, F. Nordsiek) The COVID-19 pandemic has demonstrated how little we know about the mechanisms and pathways of airborne disease transmission and prevention strategies, despite decades of research. Uncertainties and knowledge gaps about the size and concentration of exhaled particles during various activities, the suitability of infection models used, the effectiveness of masks in preventing disease transmission, and the dispersion and dilution dynamics of infectious particles indoors or outdoors, to name a few, have severely compromised our ability to contain the spread of the virus. The physics of infectious particle dispersion carried by turbulent exhalation flow is reminiscent of cloud physics, for which we have developed sophisticated analytical and experimental tools. We have measured directly the size and concentration of exhaled particles from more than 130 subjects aged 5-80 years using aerosol size spectrometers and in-line holography from nanometres to millimetres. With this we have filled the most important knowledge gap, i.e. the source term, for assessing the risk of infection in airborne disease transmission. We have found age to be an important parameter influencing the concentration of particles &lt; 5 µm, while gender, body mass index, smoking and exercise habits had no discernible influence. We have also investigated the physics of the exhalation flows during different respiratory manoeuvres using size-resolved three-dimensional particle tracking imaged at 10-15 kHz, which are furthermore complemented by two-dimensional optical flow measurements. We have collected and analysed 200 h of exhalation samples with the spectrometers, 12000 holograms, and more than three million images from the high-speed cameras. From this data and direct measurements we obtained the shrinkage of particles by drying. With this knowledge, we are now able to predict risk of infection from human exhaled particles in well-mixed indoor environments in our web application HEADS. We have further improved risk assessment models to account for particles containing multiple pathogens [1]. We also assessed dispersion of aerosols in two German hardware stores. It was found that in such environments near field exposures are dominant [2]. We find for a typical SARS-CoV-2 parameters that social distancing alone, even at 3 meters between two talking individuals, leads to a more than 90% infection risk after a few minutes. With surgical masks, the upper bound on the person-to-person risk of infection with infectious speaking remains below 26% even after 60 minutes. For well-fitting FFP2 mask, this is reduced by 60% compared to surgical masks. We conclude that wearing appropriate masks in the community provides excellent protection for others and oneself and makes social distancing less important [3].

8.22.2 From cardiac mechanics simulations and printing of engineered heart muscle towards repairing a patient specific failing heart
(Y. Wang) The human heart is one of the most important organs of our body, responsible for pumping oxygenated blood and receiving deoxygenated blood. Heart failure is a common and potentially fatal condition in which the heart muscle cannot pump sufficient blood to meet the body’s needs. Current options for patients with end-stage heart failure include mechanical support devices and heart transplants. Alternatively, EHM may offer new avenues to repair the failing heart. Within the IndiHEART project with our collaborators from the UMG, the German Primate Center (DPZ) and the Leibniz University of Hanover, we won second place (out of three) in the national innovation competition "Organ Replacement from the Laboratory" of the BMBF. In IndiHEART we aim to build a patient specific organ-like engineered myocardium consisting of porous, interwoven and microfiber-based tissue by using different micro-fluidic technologies. In this way we create a tissue that has optimized fibers. Cells and extracellular matrix are incorporated into a Ca-alginate shell and extruded via bioprinting (Fig. 8.64). Employing fiber-based tissue not only increases nutrient and oxygen exchange throughout thick constructs but also may induce cell orientation via contact guidance and enhance cell maturation. After being very promising in animal studies the first successfully in man studies have been conducted by our collaborator Prof. W. Zimmermann and his colleagues.

To obtain a functionally synchronized native heart muscle tissue, both deep understanding of cardiac mechanics and muscle fiber orientation are required. Myocardium, as a complex active soft matter, typically displays anisotropic mechanical behavior due to their fibrous nature. In constitutive modeling, fiber families are often assumed to be unidirectional. However, recent related studies show the need to incorporate dispersion of fiber orientation. Taking fiber dispersion into account, we have proposed a new class of constitutive laws, which compute faster, are easier to implement, and more stable than their counterparts [4]. The proposed laws are used with the finite element method to model the infarcted heart. In silico EHMs are introduced and how the pump function changes with different EHM configuration is evaluated (Fig. 8.65). Within the DZHK, we also study the mechanical properties of myocardium with rheometer (Prof. W. Zimmermann) and understand the fiber architecture using phase-contrast micro-CT (Prof. T. Salditt, U Göttingen) and DT-MRI (Prof. S. Boretius, DPZ). All of these, enable us to provide a directed orientation for extruded cell-loaded microfibers into the patch. The personalized EHM design generated in modeling will be used to guide the production of personalized patch, which will be produced by 3D bioprinting.

8.22.3 Control of electric turbulence in the heart

(Y. Wang, V. Zykov) Self-organisation in complex excitable systems often results in the formation of spiral waves or vortices. In the heart they can cause lethal rhythm disorders which predispose to sudden cardiac death. Restoration of normal heart function requires the timely termination of these singular structures. This is best possible by
tools that allow precise, safe and at best painless control of the wave dynamics. Optogenetics offers such a possibility. We have shown in silico with numerical simulations that inhomogeneous illumination of optogenetically modified cardiac tissue can detach anchored spirals from inhomogeneities [5], and global, time-periodic, light-based sub-threshold perturbations lead to the controlled triggering of wave breaks [6]. The spatio-temporal modulation of tissue excitability by moving zebra-like illumination patterns at sub-threshold light intensity over optogenetically modified tissue can suppress spiral wave activity in a domain by way of transient chaos. In line with our previous findings [6], we observe reshaping of the spatial profile of the wave as we illuminate the stripes (Fig. 8.66). The initial state of the spiral in the domain is shown in Fig. 8.66(A). Here blue highlighted stripes indicate illuminated regions moving upwards. Wave breaks occur at a boundary between the illuminated and non-illuminated regions (Figs. 8.66(B-D)). Bold green arrows indicate the positions of the wave breaks. The created spirals are then constrained to propagate along the moving light stripes towards the in-excitable domain boundary and disappeared. Finally, the self-sustained spiral wave activity can be completely suppressed, as shown in Fig. 8.66(E) [7]. Thus, we have found a robust method to suppress spiral wave activity without prior information about the location and dynamics of the spiral. The method relies on introducing a transient chaotic state that survives for about 1-2 s.

With an alternative approach, we study numerically how temperature can be used to remove scroll waves from the heart, i.e. defibrillation of the atria by temperature. Ambient temperature has a profound influence on cellular electrophysiology through direct control over the gating mechanisms of different ion channels. We performed the first, detailed, systematic in silico study of the electrophysiological characterization of cardiomyocytes from different regions of the human atria ([8], Fig. 8.67), based on the effects of ambient temperature (5 – 50°C) and the Courtemanche-Ramirez-Nattel cellular model. Our studies show that different parts of the atria react differently to the same changes in temperature. We show how this heterogeneous response can provide an explanation for the development of a proarrhythmic substrate during mild hypothermia. We use the above concept to propose a treatment strategy for atrial fibrillation that involves severe hypothermia in specific regions of the heart for a duration of only ~ 200 ms (Fig. 8.67).

Figure 8.66: Termination of spiral waves by transient break-up with spatio-temporal modulation of tissue excitability using a moving zebra-like pattern.

Figure 8.67: Scroll wave dynamics in the remodeled human atria, under the effect of global cooling at 5°C.

The mechanical contraction of the pumping heart is driven by electrical excitation waves running across the heart muscle due to the excitable electrophysiology of heart cells. With cardiac arrhythmias these waves turn into stable or chaotic spiral waves (also called rotors) whose observation in the heart is very challenging. While mechanical motion can be measured in 3D using ultrasound (see Sec. 6.15), electrical activity can (so far) not be measured directly within the muscle and with limited resolution on the heart surface, only. To bridge the gap between measurable and not measurable quantities we use machine learning, to solve relevant data modelling tasks in cardiac dynamics like recovering excitation patterns from noisy, blurred or undersampled observations and reconstructing complex electrical excitation waves from mechanical deformation. Using synthetic data generated with mathematical models of cardiac activity the performances of two machine learning methods, echo state networks (ESNs) and convolutional autoencoders (CAEs), have been evaluated [1]. Figure 8.68 shows reconstructions of membrane voltage from undersampled data. Also, the membrane voltage can be reconstructed from the mechanical deformation (see [1]). For both applications predictions with CAEs turned out to be more exact. Further improvement of ESNs may be achieved, for example, by gradient based optimization of hyperparameters [2].

Figure 8.68: Exemplary visualization of the reconstruction of the membrane voltage of the BOCF model from undersampled data. The first column shows input with different levels of coarsening. The second column is the ground truth (with full resolution) and the third and fifth column show reconstructions obtained with CAEs and ESNs, respectively. Differences shown in columns four and six are largest at the fronts of the waves.

Besides cross-prediction of variables that are difficult to observe temporal forecast of the spatio-temporal chaotic dynamics during fibril-
ulation is a challenging but crucial task for novel diagnostics and control methods. Straightforward nearest neighbors prediction based on local states and nonlinear dimension reduction provides very good results without any computationally expensive training phase [3]. Excellent results in terms of very long prediction horizons have been obtained with a hybrid algorithm consisting of a CAE and a conditional random field describing temporal evolution in the latent space of the CAE [4].

Machine learning has also been used for unsupervised feature extraction of anterior chamber OCT images for ordering and classification [5] and for predicting the locations of phase singularities [6] by using a UNet architecture (Fig. 8.69).

High-performance GPU computing provides new efficient tools for simulating and investigating nonlinear systems [7] and have been used to develop a novel feedforward attractor targeting method using a dual-frequency driving [8, 9]. This approach has been applied to periodically driven oscillators (well studied for a long time, see for example [10]) and provides means for changing between coexisting attractors with directly manipulating state variables.¹

[8] F. Hegedüs et al., Chaos 30, 073123 (2020)

¹https://bmp.ds.mpg.de/research/machine_learning/
8.24 CHAOTIC TRANSIENTS

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During life-threatening ventricular fibrillation we observe complex and chaotic excitation wave propagation inside the heart (see Sec. 6.15). This dynamics is governed by spiral or scroll waves which can be studied in numerical simulations of the electrical excitation wave propagation in cardiac tissue. In both, the numerical simulations of chaotic spiral waves, as well as in experimental studies of rabbit or pig hearts we observe, that the complex dynamics is often not persistent, but returns to the “resting state” without any active intervention (e.g. the application of a high energy defibrillation shock, which comes along with severe side-effects, see Sec. 6.14).

Figure 8.70: Example of how chaotic spiral wave dynamics can be controlled by an exceptionally small perturbation. The perturbed (left column) and unperturbed (right column) trajectory of the same episode is shown (different rows are separated in time by 150 ms). The chaotic dynamics can in this case be controlled by only three spatially localized perturbations (marked by white circles in the first row).

Figure 8.71: Sketches of the exemplary state space structure in the case of persistent chaos (left) and transient chaos (right). The existence of a chaotic attractor in the first case or a chaotic saddle in the latter can have significant implications for the control of these systems, for example (see Ref. [3]).

In various studies, we investigated the governing mechanisms underlying self-termination in numerical simulations of cardiac tissue [1] and other systems [2]. Furthermore, we demonstrated that controlling systems which exhibit chaotic transients can be fundamentally different to systems with persistent chaos [3]. The essential differences of the underlying state space structure in both cases may play a significant role here (see Fig. 8.71). In detail, we showed that chaotic transients can be terminated (thus kicked to the desired state) by exceptionally small interactions with the system (example shown in Fig. 8.70). Also, we studied how the duration of chaotic transients can be estimated, based on (measurable) quantities [4].

Furthermore, we are using state of the art deep learning algorithms, aiming at a suitable characterization of the dynamics [5], which potentially opens up the way towards applications in experiments and life sciences.2


2https://bmp.ds.mpg.de/research/chaotic_transients/
The seamless integration of structural and functional measurements with unprecedented resolution (Sec. 6.15), data driven modeling, and machine learning (Sec. 8.23) opens new paths to the understanding of dynamical diseases in heart and brain (Sections 6.13, 6.14, 8.24). However, the reproducible management of entire workflows from data acquisition to analysis and publication within heterogeneous, interdisciplinary research environments remains a major challenge, that hinders scientific progress and contributes to the translational gap. To address these challenges, we designed and implemented the flexible semantic research data management system CaosDB [1] that enables FAIR management of research data and algorithms. Figure 8.72 illustrates an example from our heart & brain research, where ordinal patterns were used to obtain biomarkers from multichannel EEG recordings [2].

The Open Source software CaosDB integrates with existing research software, tools and workflows [3]. CaosDB is an active research project that provides essential concepts and tools to enhance dynamic scientific workflows and self-sustainable data infrastructures for a fast growing community of users within and outside the MPG. The CaosDB project receives funding from the Else Kröner-Fresenius Foundation, the Volkswagen Stiftung and the Max Planck Digital Library.

Figure 8.72: CaosDB research data management of the entire workflow from EEG measurement and analysis to publication [2]. The CaosDB crawler synchronizes objects on the file system with the flexible semantic data model in the database. Indexed objects can be searched expressively and interacted with through scriptable programming (e.g., Python) or web interfaces.

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4https://www.bmp.ds.mpg.de/research/caosdb/
8.26 STOCHASTIC PROPERTIES OF MUSICAL SEQUENCES

C. Nelias and T. Geisel

Music theorists since Leonard Meyer [1] have emphasized the importance of the interplay and balance between expectation and surprise in musical compositions. It would be desirable to quantify this interplay comparing different composers, musical genres, etc. on the basis of information theoretical concepts. Unfortunately the length of compositions is by far not sufficient to reliably estimate e.g. entropies and redundancy of melodies. A somewhat related concept is the autocorrelation function. It can also describe the amount of innovation, and it is feasible to determine its properties through detrended fluctuation analysis (DFA) and power spectral densities (PSD).

Various authors since Voss and Clarke [2] have arrived at controversial conclusions, however, on the functional form of the PSD, claiming $1/f$-noise, $1/f^2$-noise, or power-laws ending in plateaus at low frequencies. These discrepancies might be due in part to numerical artifacts or large errors in the PSD-estimates. We wanted to clarify the situation by a very careful analysis of the PSD of pitch sequences in musical compositions as well as in improvised performances. Using a multitaper PSD-method we aimed to reliably extend the PSD-estimates down to the smallest possible frequencies (given by the bandwidth).

Our results show that the PSDs typically follow power-laws with different exponents in a certain frequency range (corresponding to a slow decay of correlations) and reach a plateau at small frequencies (corresponding to a lack of correlations) (Fig. 8.73). We conclude that inverse power-laws with plateaus are the typical shapes of pitch PSDs of musical sequences and we determine the range of power-law behavior. The "scale-free" regime of musical timeseries typically is quite narrow and extends only up to times of less than 24 measures, beyond which the timeseries are uncorrelated as indicated by the plateaus in the PSD.


Figure 8.73: Multitaper PSD-estimation of a) complete violin sonata in G minor by J.S. Bach and b) Mozart's 15th string quartet. The shaded grey areas represent 95% confidence intervals encompassing the fitted PSD (grey line). For convenience dashed vertical lines denote corresponding time periods in quarter note units.
"What is this thing called swing", is a question raised already by Louis Armstrong in a well-known song. The swing feel certainly is one of the most salient features of jazz music and is considered an essential ingredient of jazz performances. Yet astonishingly, a century after jazz musicians like Armstrong and Ellington came on stage, it is still controversial what is the nature of the swing feel and what are its main musical and psychoacoustical components. Among these components only one is established unambiguously so far, the conspicuous uneven subdivision of quarter notes. It is measured by the so-called swing ratio, i.e. the length ratio of consecutive long and short eighth notes known as "downbeats" and "offbeats". Listening to computer-generated jazz music that was "swingified" by merely implementing a swing ratio, it is obvious that this is not sufficient and that there must be other components. But which are these components, and which ones are important?

It has long been speculated that rhythmic effects, in particular microtiming deviations (MTD), play the other major role for the swing feel. However, while the importance of the swing ratio is generally accepted, the role of rhythmic microtiming deviations has been a subject of controversy for many decades. Various authors have emphasized the importance of participatory discrepancies; i.e. "little discrepancies within a jazz drummer’s beat, between bass and drums, between rhythm section and soloists, that create 'swing' and invite us to participate”[1], or other kinds of microtiming deviations. Others, however, contested their influence and rather stressed the importance of rhythmic accuracy.

Many of these claims were based on observational analyses of extracts from individual jazz musicians, which may explain the origin of the controversial claims, as MTD are not used equally by all musicians. It is not clear, however, that MTD - even if they occur - are specifically related to and enhance the swing feel. Is there a way to prove that MTD do contribute substantially to the swing feel?

Adopting an operational definition of swing we have carried out the first study which is able to clarify the controversy and to rigorously demonstrate a positive effect of certain microtiming deviations on the swing feel. [2] By manipulating the timing of original piano recordings and measuring the swing feel of different manipulated versions as rated by jazz musicians we demonstrated that a playing style with systematic microtiming deviations, slightly delaying downbeats of the soloist with respect to the rhythm section while synchronizing offbeats, considerably enhances the swing feel (Fig. 8.74). We compared these versions with downbeat delays of the order of 30 ms or 9% of a quarter note to the quantized original recordings and to versions in which both, downbeats and offbeats, are delayed. As the soloist’s offbeats need to remain synchronized with the rhythm section, this playing style has an influence on the swing ratio. If the downbeat onsets of
the soloist are delayed (their durations thus shortened) and offbeats remain synchronized, this implies a somewhat smaller swing ratio for the soloist than for the rhythm section and may create a perceived friction between them.

That’s a nice experiment, but to which extent do jazz musicians actually make use of this phenomenon? We also analyzed a large set (456) of full solo performances and determined the average downbeat delays. We found downbeat delays of jazz soloists as a general trend and we found that their magnitude decreases with tempo (Fig. 8.75). Taken together the results of our experimental and our observational study lead to the conclusion that downbeat delays are a key component of the swing feel in jazz. They underline the general importance of timing and rhythmic effects for the swing feel and resolve the long-standing controversy on the role of microtiming deviations by demonstrating that certain systematic microtiming deviations enhance the swing feel, while involuntary random microtiming deviations do not. In previous work [3] we had shown that such random timing fluctuations present in every human performance do not enhance but rather tend to inhibit the swing feel.

That downbeat delays could play such an important role for the swing feel was widely unknown. Professional and semiprofessional jazz musicians participating in our online experiment reported a pleasant friction between soloist and rhythm section, but were unaware of the effect and could not determine its nature. (cf. "you can feel it but you just can’t explain it" [4]).

Our findings are of interest to various fields, from the physics of social interactions and human behavior to psychoacoustics and the perception of musical rhythms. They also have implications for music education and music production. Many modern digital audio workstations offer options for “swingifying” computer-generated music. So far these features are of limited value, as they mainly serve to introduce a suitable swing ratio. Adding downbeat delays according to our findings would help improve these features for digital music production.

![Figure 8.75: Average downbeat delays of soloists as a function of tempo.](image)

Each point in the scatter plots corresponds to one of 456 jazz solos and represents the average downbeat delays in milliseconds as a function of tempo in beats per minute. The red line delimits the tempo range of pieces used in our experiment.

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Neural networks in both biological settings and artificial intelligence distribute computation across their neurons to solve complex tasks. A number of computational properties are maximized when the dynamics of a network are at a critical point [1]. Therefore, the critical state has been hypothesised to be the optimal regime for recurrent neural networks to solve many computationally demanding tasks. A competing hypothesis is that of the asynchronous irregular regime, which has maximal entropy in its spike patterns and supports fast network responses - it might thus be optimal for tasks that necessitate fast reaction times [1]. Here, we experimentally assess these two hypotheses by evaluating the performance of a spiking recurrent neural network tasks of varying complexity at – and away from critical dynamics [3].

We instantiated such a network on a prototype of the analog neuromorphic BrainScaleS-2 system and equipped it with homeostatic plasticity [3], which we have previously shown can set the dynamical regime by adapting the mean input strength [2] (cf. Sec. 8.31). With this implementation, we demonstrated a clear relation between the dynamical regime, task-performance, and information-theoretic fingerprints. In particular, we show that information-theoretic measures are maximized at criticality, only the complex, memory intensive tasks profit from that state, whereas simple tasks suffer. Thereby, we challenge the general assumption that criticality would be beneficial for any computationally demanding task, and instead provide an understanding of how the collective dynamics should be tuned to task requirements. This finding may explain why biological neural networks operate not necessarily at criticality, but in the dynamically rich vicinity of a critical point, where they can tune their computational properties to task requirements.

As a next step, we now study the impact of the spiking network’s working point on classifying artificial and real-world spoken words. In related lines of work, we are applying the analysis methods developed here to experimental data spanning different behavioural states: First, mouse data from the Packer Lab at Oxford University to assess the how the perception of direct cortical stimulation depends on the dynamical state of the somatosensory cortex [4] and second human data from the Mormann Lab at Bonn University to assess how different sleep stages influence the dynamical state of hippocampus. These projects will demonstrate the real-world advantages of tunable recurrent neural networks in silico and the link between network dynamics and behavioural state in vivo.

In biological neural networks, information is represented using a variety of different strategies. However, the optimization principles that guide the development and self-organization of neural networks remain unclear. We infer information-theoretic neural goals that underlie the development of living neural computation, derive learning rules analytically from first principles, and then put them to use in artificial neural networks.

To study neural information processing, we use a recent extension of information theory, Partial Information Decomposition (PID). PID allows to disentangle the information contribution of several neurons (or variables) about some target variable: how much of the information is redundantly encoded, what is unique to one of them, and which neurons encode information synergistically (see Figure 8.77A). Thereby, PID lends itself perfectly to study information encoding in multiple neurons.

To investigate the formation process of neural representations, we measured the information-theoretic properties of neural networks during development in vitro. Using PID, we were able to show that these networks increase their synergistic encoding (Figure 8.77B); however, eventually encoding becomes highly redundant, potentially because of the isolation of these networks in vitro [1, 3].

Complementary to this experimental work, we showed that it is possible to unify previously proposed information-theoretic goal functions such as the Infomax Principle and the Predictive Coding framework with the help of PID and derived a generalized way of designing other goal functions [2]. Currently we are building on this unified framework to study the effectiveness of different goal functions by applying them for learning in artificial neural networks [4].

Taken together, information theory enables us to quantify neural representations and infer coding strategies in a principled manner from an information-theoretic perspective. Thereby, we will shed light on living computation, and eventually make its efficiency and robustness available for artificial neural networks.

Figure 8.77: A (upper): Venn diagram of the mutual information of neural activity of two neurons with a target variable Y. (lower): Partial Information Decomposition (PID) into unique, synergistic and redundant information of multiple variables N about a target variable Y. B: In a developing neural culture in vitro, information modification - measured as synergistic information - increases significantly over the first four weeks of development, but breaks down later. (Figure from [1])

Neural systems possess impressive capabilities to learn regularities in their environment, despite facing severe constraints. First, neural learning orchestrates biological processes using only locally available information. Second, neural learning uses very limited resources, and third achieves surprising robustness in the face of noise. Our goal is to understand the neural plasticity mechanisms that enable learning in these conditions.

First, to understand how the constraint of locality influences learning, we derived neural plasticity rules from first principles of neural population coding (Fig. 8.78). Importantly, we found that learning in realistic scenarios requires global information about the population activity. Yet, previous plasticity mechanisms do not incorporate this global information, because it is thought to not be locally available to synapses. We could overcome this limitation by introducing the novel mechanism of dendritic balance [1], which does not only substantially improve learning, but also proposes a unified explanation for a range of experimental observations in neural dendrites.

Second, neural learning and processing face severe resource constraints. In collaboration with the experimental lab of Silvio Rizzoli, we found that neural activity has to be closely matched by the costly generation of synaptic vesicles to ensure transmission of information via the synapses [2]. On the other hand, these costly internal synaptic dynamics greatly shape the function of the neurons they connect to. Currently, we investigate how this trade-off between resource budget and function can be optimized by synapses, and how this can be achieved with local plasticity rules.

Third, we investigate how neural and external noise influences learning in recurrent neural networks. We found that under homeostatic or spike-timing-dependent plasticity, the strength of external input tunes the distance to a critical phase transition of the resulting recurrent dynamics [3], and thus crucially shapes the information processing capabilities of the network [4] (see also Sec. 8.28). Strikingly, we found that this pre-shaping by noise can substantially improve sequence memory in plastic recurrent neural networks [5] (Fig. 8.79). Thus, although noise is thought to be an obstacle, we found that it can crucially shape function in self-organizing recurrent neural networks.

**Figure 8.78:** Learning of efficient representations in a recurrent spiking network. To this end patches of images are presented to spiking neurons, which encode these images in their activity. Local plasticity rules optimize the encoding and neurons form receptive fields similar to neurons in visual cortex. Figure adapted from [1].

**Figure 8.79:** Spike-timing dependent plasticity pre-shapes network memory performance under noisy input. First, development under noise for time $T_{\text{pre}}$. Then, development under sequence input ($t = 0$, dashed vertical line). Pre-shaped networks ($T_{\text{pre}} > 0$) initially maintain higher sequence memory performance than those starting from random initial conditions ($T_{\text{pre}} = 0$). Figure from [5].

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8.31 EMERGENT DYNAMICS IN SELF-ORGANIZED AND STRUCTURED NEURAL NETWORKS

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Recent experimental results suggest that information processing in the brain would profit from specialized neural network dynamics across different brain areas (cf. Sec. 8.32). At the same time, across all brain areas the single-neuron properties (e.g. the mean activity) are fairly conserved. Neural networks hence require mechanisms that leave single-neuron properties invariant but shape their collective dynamics according to computational needs. We identified two mechanisms that can shape emergent network dynamics: homeostatic plasticity [1, 2] and tailored network architectures [4].

To preserve their mean activity, neurons can regulate their coupling strength via homeostatic plasticity. We demonstrated that, in addition, homeostatic plasticity enables neural networks to self-organize towards different collective dynamics. In particular, we derived a mean-field theory that predicts an increasing emergent network timescale for decreasing input strength [1] (Fig. 8.80). We verified our theory in experiments on neuromorphic hardware and found that homeostatic pre-shaping can be beneficial when timescales are optimized for task complexity [2] (cf. Sec. 8.28). Our results suggest that homeostatic plasticity is a key mechanism in adapting emergent dynamics to task requirements [3].

In addition to local adaptation, the brain processes information within highly tailored network architectures. But it is unknown how to tailor architectures for flexible information processing. We found that flexible encoding of a broad range of input stimuli can be achieved with a modular architecture, tailoring emergent local timescales to produce synergistic collective responses for relevant stimulus ranges [4] (Fig. 8.81). However, we further found that emergent timescales in networks of biologically plausible neurons require heterogeneous synaptic weights. This suggests that deviations from the common choice of homogeneous synaptic weights will reveal more synergistic effects in modular architectures of realistic neurons.

Combining both tailored network architectures and homeostatic tuning via stimulation promises to unfold rich emergent dynamics. Thus, we now study collective dynamics when stimulating modular cultures in collaboration with the experimental lab of Hideaki Yamamoto (Fig. 8.82); first results show that stimulation indeed induces dynamic richness in the collective dynamics.

8.32 INTRINSIC TIMESCALES PROVIDE A WINDOW INTO NEURAL INFORMATION PROCESSING

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Even with exciting advances in recording techniques of neural spiking activity, experiments only provide a comparably limited and short glimpse into the activity of neurons. Thus, investigations of how neural information processing is organized in the brain remain a challenge. In our work, we exploit that certain properties of information processing leave distinct footprints on the collective dynamics of neural activity. In particular, we quantify how long neural information depends on its own past, which is often called the intrinsic timescale. Because this timescale describes for how long information is stored in the activity of the network, it also serves as a proxy for memory and response times: Whereas a short time scale is considered beneficial for fast responses to stimuli (and fast forgetting alike), a long timescale facilitates information storage and integration [1].

To measure intrinsic timescales, we use two complementary approaches. One builds on linear correlations and their (subsampling invariant) decay (Fig. 8.83, cf. Sec. 6.17). In order to account for non-linear dependencies, we generalized the ansatz using information theory (Fig. 8.83). This enables us to quantify an intrinsic timescale, but also, closely related, the history dependence within the spiking of a single neuron [2]. To make both approaches easily applicable, we provide open-source toolboxes [3, 4], and keep improving our framework. For example, we recently derived an analytical solution to overcome non-stationarities, which are typical in experiments [5]. Noteworthy, our approaches have been adopted by a number of colleagues already.

We measured for the first time intrinsic timescales of spiking activity in human medial temporal lobe. We found extended and highly variable intrinsic timescales, ranging from tens to hundreds of milliseconds [6]. Interestingly, intrinsic timescales differed between sleep stages, with longest timescales during slow wave sleep (Fig. 8.84 b). Moreover, timescales differ among brain areas [6], but apparently are not predictive for epileptic seizures [7]. We also measured timescales in macaque cortex, finding differences between sensory and higher brain areas (Fig. 8.84 a). Together, this suggests that intrinsic timescales are not a static network property, but can vary depending on the functional role of a brain area, on cognitive state, and depending on task.

Cells sense mechanical signals using force-gated ion channels in the perception of touch, sound, and pain. In development, internally generated forces and stresses are the signals that travel fastest [1], and force-gated ion channels can transduce them into intracellular response variables virtually instantaneously. Here, we demonstrate using tissue-wide analysis of cell-cell synchronization together with data-driven modeling, optophysiological perturbation [2] and subcellular calcium imaging that the force-gated ion channel Tmc mediates active synchronization of contractile oscillations in Drosophila morphogenesis.

Figure 8.85: Synchronized cellular oscillations are concentrated in a self-organized tissue-scale contractile ring. Both synchronization and tissue patterning are selectively abolished by genetic ablation of the force-gated calcium channel Tmc.

Tmc-dependent synchronization is required for establishing an isotropic tissue morphology and isotropic force balance, and mediates the emergence of a tissue-scale ring-like array of synchronously contracting cells. A data-driven model for cell synchronization by Tmc-mediated calcium signals confirms the presence and Tmc-dependence of calcium signals in vivo. Force-gated ion channels in this active epithelium thus function to transduce internally generated forces into intracellular calcium signals that synchronize cell behavior. The evolution of mechanotransduction in metazoa presumably dually tailored force-gated ion channels for the detection of environmental and morphogenetic forces.

8.34 DYNAMICS OF NEURAL CIRCUIT TURNOVER

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M. Kerschensteiner (LMU), K. Willig (MPIEM), M.A. Busche (UCL), D. Huber (U Geneva), Y. Hayashi (Kyoto University)

Synaptic turnover and volatility are considered a main feature of the reorganisation of neuronal circuits [1, 2] and can result in extensive representational drift. In the hippocampus, locations associated with salient features are represented by a disproportionately large number of neurons, but the dynamics and molecular mechanisms underlying this over-representation remain elusive. Using longitudinal calcium imaging in mice learning to navigate in virtual reality, we studied the emergence of the over-representation of reward and landmark locations [3]. The dynamics involved persistent and separable subsets of neurons, with distinct time courses of emergence and differing underlying molecular mechanisms.

Strikingly, we find that in mice lacking Shank2, an autism spectrum disorder (ASD)-linked gene encoding an excitatory postsynaptic scaffold protein, the learning-induced over-representation of landmarks was absent whereas the over-representation of rewards was substantially increased, as was goal-directed behavior. These findings demonstrate multiple hippocampal coding processes. Anomalous neural circuit turnover may also underlie memory dysfunctions such as Alzheimer’s disease [4].

8.35 A LOCALIZATION TRANSITION IN NEURAL CIRCUIT CHAOS

M. Soltanipour, A. Schmidt, A. Neef, F. Wolf
A. Palmigiano, R. Engelken (Columbia University)

Nerve impulses, the currency of information flows in the brain, are generated by an instability of the neuronal membrane potential dynamics. Spiking neural circuits exhibit collective chaos [1, 2, 3] that appears essential for learning, memory, sensory processing and motor control. What controls the nature and intensity of collective chaos in neuronal circuits, however, is not well understood [4, 5]. Using computational ergodic theory we discovered that basic features of nerve impulse generation profoundly affect collective chaos in neuronal circuits.

Figure 8.87: Localization transition of the leading covariant Lyapunov vector in a large-scale model of cortical neuronal circuits. The covariant Lyapunov vector is delocalised below (A) and localised above (B) the transition. Local Lyapunov exponents demonstrate that above the transition intense chaos is restricted to short episodes, facilitating external control of network states. (C) Localization transition coincides with peak maximum Lyapunov exponent.

Lyapunov spectra, Kolgomorov-Sinai entropy, and upper and lower bounds on attractor dimension show that changes in nerve impulse generation in individual neurons, while moderately modifying single neuron information flow, qualitatively transform phase space structure by a localization transition. Beyond this transition, the networks exhibit sparse chaos: extended periods of near stable dynamics interrupted by short bursts of intense chaos. Our results demonstrate a tight link between fundamental features of single neuron biophysics and the collective dynamics of cortical circuits and suggest that the machinery of nerve impulse generation is tailored to enhance circuit controllability and information flow.

Collective rhythmic activity is implicated in brain functions from sensory information processing to memory consolidation and depends on the interplay between inhibitory and excitatory neuronal populations [1]. Fast-spiking (FS), parvalbumin-positive but not adapting (AD) interneurons appear closely associated with the initiation and maintenance of high-frequency oscillations (30-150 Hz). But is the spectral sensitivity of different interneuron populations fixed or state-dependent? To answer this question, we characterized the spectral sensitivity of cortical GABAergic interneurons at different in vivo-like working points by measuring their dynamic gain. To probe the potential impact of different brain states on spectral sensitivity, we used different types of background inputs that mimic the strength and timescales of correlations in background input across brain states [2].

Figure 8.88: Spectral selectivity of AD neurons drastically shifts for different background fluctuations. Neurons were driven with inputs of different correlation times. Under fast background, AD neurons modulate their firing rate strongest in response to lower frequencies. Under slow background, the frequency preference shifts (arrows) and the firing rate is modulated mainly by high frequencies.

We find that both FS and AD interneuron populations have remarkably wide bandwidths (up to about 500 Hz), making them capable of tracking fast input frequencies well into the range of sharp wave-ripples. Moreover, our results uncover an unanticipated flexibility in AD neurons, which can massively shift their frequency preference. In particular in the presence or absence of slowly correlated input, such as during slow-wave sleep or active wakefulness respectively, AD neurons specifically engage or disengage with high-frequency rhythms, such as gamma and sharp wave-ripples.

PART III

SUPPORT
# FACILITIES

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The microscopy facility of the MPI DS combines a set of advanced light- and laser based microscopes. It is operated by the LFPB department (Bodenschatz), but is open to users from the other departments as well as external users from the neighboring MPIBPC. The current focus of the biophysical subgroups within the LFPB department are quantitative and synthetic biology. Therefore, the selection of the microscopes applies techniques of life cell imaging aided by sensitive cameras/detectors (fig. 9.3). The backbone of the facility are the confocal laser scanning microscopes (Olympus FV1000) and a confocal spinning disk microscope (Olympus), which serve for a broad range of experiments, such as single cell stimulation and fast 3D imaging of migrating Dictyostelium discoideum. These are complemented by a high precision light microscopy set-up (Deltavision), which achieves its z-resolution by deconvolution of epifluorescence z-stacks.

After substantially enlarging the facility in the period 2016-2019, we now finalized the necessary upgrades and programming of the microscopes as well as the attached auxiliary hardware. Furthermore, we recently integrated multiple light and fluorescence microscopes of the now Emeritus group of Gregor Eichele. The different set ups allow for a variety of experiments such as large scale and long time unsupervised recordings, high speed video capture, dynamic light scattering and surface roughness measurements (see figures 9.1, 9.2, and 9.4 for examples). As in the previous period, the service of the microscopy facility also comprises the training of new users and the education of apprentices.
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 realize flows with various spatial and temporal large scale properties. These well defined flows must go hand in hand with precise measurements. In addition one must have the ability to adjust the conditions in various ways, so that dependencies can be uncovered. The facilities at the MPI DS 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. To match our achievements in controlling turbulent flows, we have advanced measurement technologies, and have even adapted these to field experiments of natural flows.

The Variable Density Turbulence Tunnel (VDTT) [1] is a recirculating pressurised 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 maximum flow speed is approximately 5.5 m/s. 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 sulphur hexafluoride (SF$_6$) up to a pressure of 15 bar. In its current configuration, an active grid consisting of 111 individually controllable flaps creates turbulent wakes of variable size and intensity [2, 3]. This ultimately influences the homogeneity, isotropy, and intensity of the turbulent fluctuations. The active grid allows us to reach Reynolds numbers up to 6000 compared to maximally 1700 when a classical grid of crossed bars is used to inject turbulent kinetic energy. There exists no other wind tunnel facility that can achieve comparable Reynolds numbers. Additionally, the active grid gives us precise control over the turbulence forcing. Recently, a stationary particle-tracking system was implemented and tested successfully. With this, the facility has tripled the Reynolds number of Lagrangian measurements available to international turbulence research. Key elements include a 300W laser illumination, an in-house particle disperser, and a vibration-damped platform holding four state-of-the-art high-speed cameras.

The Prandtl tunnel is an open-circuit wind tunnel dating to the 1930’s. The wind tunnel is 11 meter long with a measurement section of 1.2m x 1.5m and maximum wind speed of 12 m/s. It can be equipped with hotwire anemometers and thanks to the large measurement section it is suitable for a large variety of experiments. A version of the active grid implemented in the VDTT is also available for flexible turbulence generation.

The High Pressure Convection Facility (HPCF) [4] utilizes a general-purpose pressure vessel called the “U-Boot”, which is 5.3 m long and has a diameter of 2.5 m and can be filled with SF$_6$ up to a pressure of 19 bar. We precisely control both the temperature and the pressure in the vessel. Within the vessel is a rectangular Rayleigh-Bénard (RB)
experiment of large aspect ratio (height 0.7 m, length 3.5 m and width 0.35 m) that can reach Rayleigh numbers as high as $5 \times 10^{13}$. With its transparent sidewalls, the experiment allows for optical velocity measurements at unprecedented large Rayleigh numbers.

The “Cigar” is a general-purpose pressure vessel with a length of 4 m and an inner diameter of 1.5 m. It can be filled with SF$_6$ up to a pressure of 19 bar to perform smaller convection or turbulence experiments or to test equipment for the other pressurized facilities.

Two von Kármán mixers generate high Reynolds number turbulent water flows between two counter-rotating baffled disks. 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 $R_L$ can be as high as 1200. Large glass windows provide optical access for imaging techniques. The apparatus can be pumped down to reduced-pressure for the study of bubble dynamics. A frequency doubled high-power (50 W), high-repetition-rate Nd:YAG laser is devoted to measurements in this apparatus.

Theoretical knowledge is most developed for turbulence that is stationary and isotropic. But real flows are neither. Three novel apparatuses [5, 6], make it possible for the first time to control the degree to which a turbulent flow is anisotropic both, in gases and in water. We produce cloud-like conditions in one soccer ball.

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 ultra high-speed cameras viewing the same particles from different angles, with megapixel resolution and kilohertz frame rates. Recently we have developed a techniques that enables us to measure the 3D vorticity in water flow. 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 is typically produced by Nd:YAG lasers or argon-ion lasers. The systems produce data at rates that necessitate high-performance computing and storage clusters.

The Max Planck Turbulence Facilities (MPTF) are open to visiting researchers. For example it has been used in the European High-Performance Infrastructures in Turbulence (EuHIT) project\(^1\). It aims to integrate cutting-edge European facilities for turbulence research across national boundaries [7, 8].

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\(^1\)The European Commission supported the project European High-Performance Infrastructures in Turbulence (EuHIT, Grant Agreement Number 312778)

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The requirements for experimental work at the Max Planck Institute for Dynamics and Self-Organization are versatile and very demanding. They require the highest quality in mechanical engineering from design and verification/certification to construction. The sizes of mechanical parts employed in the scientific experiments range from micrometers to many meters. They are used in various environments from the laboratory, to mount Zugspitze, and on research vessels like the Maria S. Merian. Parts are uniquely designed and manufactured for highly specialized experiments. Designs are conducted by the mechanical engineer, who heads the facility, in tight collaboration with the scientists. CAD 3D construction software is used not only to construct and develop the parts but also to conduct Finite Element Structural Analysis. The components created in the designs are then processed quickly, flexibly, and with high quality in the mechanical workshop according to the drawings or directly from the CAD design data with the help of a CAM interface. With a simulation integrated in the CAM software, potential errors occurring during the production process can be detected and eliminated before the actual part is machined. In addition, the 3D-CAD output can be used in scientific presentations and publications.

Many of the unique experiments employ automated, integrated, computer-controlled systems. Very often, actuators, sensors, etc. with the associated control and testing devices are integrated into the mechanical components. In close cooperation with the Scientific Electronics Facility, the mechanical constructions are finetuned with the electronics.

Mechanical production is accomplished with computerized turning, milling, grinding, 3D printing, and other machines which cover the full area of precision mechanics. In order to produce precision parts with geometrically complex shapes, we have 5D-milling machines and 3D-printers.

The training of apprentices has also been an important part of the work of the facility from the very beginning. In the last ten years, our trainees have passed these examinations with distinction.
9.4 RESEARCH ELECTRONICS FACILITY

L. N. Diaz-Maue, H. Nobach

The outstanding experimental research projects of the MPI DS often require measuring devices, communication techniques and human-machine interfaces, which are commercially not available. In order to better meet these challenges, in 2018 the Research Electronics facility has been founded, making the expertise in electronics available to the entire institute. Recently, a newly remodeled $139 \text{ m}^2$ office and workshop area and another $57 \text{ m}^2$ storage and machine area have been finished and handed over to the Research Electronics facility, bundling the institute’s human and material resources.

The available machine pool allows to develop and build highly specialized, unique electronic circuits for measurement and control tasks incl. the electronic interfaces between computer and measurement technology for scientific apparatuses all-in-house. The Research Electronics members work closely together with the scientists during the specification and design of the circuits. Later they assist the scientists in implementing and operating the circuits in their experiments. This enables a focused and fast response in improving the devices incl. on-site repair in failure cases and short development cycles in optimizing and adapting them with the highest professional support. Some projects, in which we are especially engaged are:

- Cloudkite / Physics of clouds and atmosphere,
- Active Grid and Hot-Wire Anemometers / Turbulent Flows,
- Optical Particle Counters / Aerosol Dynamics,
- Low-Energy Amplifier Pulse Generators / Low-Energy Anti-Fibrillation Pacing,
- Digital Light Processing and Micro LEDs / Optogenetics,
- Programmable Current Source / Current Density Measurements by Magnetic Resonance Imaging,
- Microscope Light Sources / Biological Systems.

With the current Research Electronics members, we are able to develop a wide range of components beyond commercial devices for the experiments running at the institute. However, in order to fulfill the demands of all scientific groups, and to achieve the concept of maintaining the acquired knowledge and skills, our short-term demand is to obtain an additional permanent engineer position and in a near future to apply for one more engineer, one more technician and further apprentices.

Furthermore, the group members also pursue own research projects, namely on the development of measurement devices, signal processing and novel technologies for cardiac research [1, 2].

9.5 MICROFABRICATION FACILITY

S. Romanowski (lab manager)

The Microfabrication Facility provides space, equipment, and assistance to design and manufacture devices for several groups within the institute and for other research institutions. The clean room (35 m2-Class 1000) is used to develop silicon masters via photo-lithography and it is equipped with a spin coater for depositing thin layers of SU-8 photoresist, hotplates for baking the resist and two mask aligners (EVG-620, UV-KUB 3) for exposing the wafers to UV illumination. Structures with features of 7-10 micrometers can be fabricated and a white light interferometer (Wyko NT1100) is used to accurately measure film thickness, surface roughness and surface features.

Microfluidic devices are assembled outside of the clean room environment after replica molding of the fabricated silicon master.

The facility is also equipped with a 3D laser lithography system (Photonic Professional GT) used to build unique 3D structures and devices with submicron resolution. Starting from the CAD model of the structure, using embedded software it is possible to rapidly print the structures with high degree of complexity via two photon polymerization of a UV curable photoresist.

Beside lithography, a high precision milling machine (DMU 50, DMG Mori Seiki) is used to pattern microchannels in hard plastic and metals for fabricating structures from 150 microns up to 10 cm.

![Figure 9.14: Working in the clean room.](image)

![Figure 9.15: 3D printer.](image)

![Figure 9.16: SU-8 wafer used for replica molding.](image)

![Figure 9.17: CAD Model of a snow crystal with hexagonal prism shape (a) and the fabricated 3D printing (b). Scale bar 70 microns. 3D printed elliptic particles (c) and hot wire probe (30 microns long and 4 microns thick) from measuring small-scale turbulence. Scale bar 100 microns.](image)

![Figure 9.18: Microfluidic device fabricated by replica molding of PDMS.](image)

The facility plays a pivotal role in developing microfluidic platforms for generating compartments that mimic cellular systems within the Max Planck Network on Synthetic Biology (MaxSynBio/cors), a joint Max-Planck-BMBF initiative. Training and assistance in microfabrication at all levels, from design to the use of microfluidic devices, is provided by the facility.
The field measurement laboratory is a facility operated by MPI DS at the research station Schneefernerhaus near the peak of Zugspitze mountain at an altitude of 2650 m. Location of the laboratory provides easy access to the two topmost outside platforms of the station, which are best suited for study of atmospheric turbulence and cloud dynamics. On the top platform, we have installed a mast with a set of 3D sonic anemometers to conduct long-term year-round measurements of the wind and turbulence conditions at the UFS. Also situated on the top platform is a Lagrangian particle tracking apparatus dubbed the “Seesaw”, consisting of a 6 m-long set of rails along which a vibration-damped box housing a set of high-speed cameras that can be driven at speeds of up to 7.5 m/s by two electromagnetic motors. Precise control of the translation velocity and tilt of the rail with respect to the horizontal make it possible to match the west-east and vertical components of the mean flow and follow cloud particles over time intervals longer than those achievable with a stationary setup. Illumination is provided by a 300 W green laser housed in the laboratory. A dual phase-Doppler interferometry probe allows measurement of cloud droplet size distribution and individual velocities. The set of tools and equipment stored at the laboratory, together with the in-house machine shop, allows rapid development of new field experiments.

9.7 MOBILE CLOUD LABORATORY

O. Schlenczek, G. Bagheri, P. Höhne, F. Nordsiek, M. Schröder, E. Bodenschatz

Each Cloudkite carries a suite of instruments to measure fluid properties and particle properties in clouds. But to interpret the time series of wind speed and other quantities measured by the Cloudkite as well as evaluating flight safety, we need additional instruments on the ground to get the big picture in terms of cloud and boundary layer dynamics. Additionally, we need to transport the Cloudkite to the field, have a location to repair instruments, and bring some computing power to do data analysis in the field. To accomplish this, we are building the Mobile Cloud Laboratory (MCL), an instrumented van to transport the Cloudkite and function as a mobile weather station. A CAD visualization is shown in Figure 9.21. The quantities measured on the ground are basic meteorology (temperature, pressure, relative humidity, wind speed and direction), dewpoint via chilled mirror, precipitation rate, hydrometeor size distribution, cloud ceiling and backscatter, and the atmospheric electric field via field mill. Specifically, the wind and electric field measurements are important to evaluate the risk of high winds and potential lightning.

Figure 9.21: Customized MCL van.
The need for computing power and data storage space at MPI DS originates from both numerical computations and simulations as well as from data acquisition and evaluation in experiments. For both purposes the HPC group provides file servers for personal and project data, HPC clusters with fast local data storage space for parallel computing and HPC systems for GPU accelerated codes. The necessary computing infrastructure scales way beyond single workstations, but well below large computing centers. As a mid-sized HPC facility it has to allow for interactive use, e.g. for developing large-scale parallel applications or directed parameter space exploration. The Linux workstations are part of the HPC systems at MPI DS. Scientists can directly work on their data and control their jobs from their desktop systems.

The HPC group puts a lot of effort in keeping hardware as homogenous as possible in order to minimize the maintenance workload and maximize interoperability between the scientific working groups. Currently, the HPC hardware at MPI DS is mainly built of Lenovo systems using Intel Omnipath network interconnects for the parallel clusters. A few older DELL clusters with Mellanox Infiniband networks are still being maintained. Scientists at MPI DS have direct access to HPC clusters with an overall size of about 1000 HPC systems (more than 26,000 CPU cores, approximately 160 TB RAM, and 20 PB of data storage capacity).
Hosting computing facilities of this size requires a very dense packing of servers which is ensured by using multicore machines and efficient system designs like blade server enclosures. Corresponding power densities of more than 20kW per square meter cannot be cooled by traditional open air flow cooling with false floors. An efficient cooling system is required from an environmental perspective, but is mandatory from a budget point of view too, as electricity costs for cooling can be as high as one third of the total electricity costs with traditional cooling. MPI DS was among the first institutes of the Max Planck society to solve this issue by using optimized water cooled cabinets in order to cool the necessary parts of the server rooms only, as shown in fig. 9.22.

To improve service reliability half of the MPI DS HPC systems are located in a server room in the institute’s building at Fassberg, whereas the other half is located at an external computing center site in the former ‘Fernmeldezentrale’ (FMZ) of Göttingen University. The smaller department server rooms at Fassberg were recently refurbished and can now be used for project data file servers and infrastructure servers of all groups.

In order to manage such a complex facility at different sites, MPI DS uses provisioning, configuration and monitoring systems based on open source software. The monitoring system collects important health data of the HPC hardware and the cooling facilities on a frequent basis. This data is summarized into a comprehensive overview and its history can be viewed for further diagnostics. In case of a cooling failure the monitoring system is able to perform an emergency shutdown autonomously in order to prevent machine damages by overheating.
INFRASTRUCTURE

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The scientific creation of value at the Max Planck Institute for Dynamics and Self-Organization (MPI DS) is supported by an efficient, high-performance and flexible infrastructural service. The so-called infrastructure management is divided into the two core areas of Administrative Service and Scientific Technical Service. The administrative service includes the areas of personnel, budget and finances, and building and operational technology, which ensure the basic operational processes. The Scientific and Technical Service includes the areas of: IT, Scientific Electronics and Scientific Mechanical Engineering, which essentially provide direct, technical services for science.

In view of their characteristically overarching service role for the scientific organizational units and infrastructure management, the areas of Quality Management, Press and Public Relations, Driving Service and General Service have been organized as staff units and assigned directly to the Chief Operations Officer. The Quality Management unit acts in a process-oriented manner and scrutinises existing organizational processes together with the existing organizational units in order to continuously ensure the quality of existing processes with regard to internal and external influencing factors.

Press and public relations work is essentially characterized by a close proximity to the scientists of the MPI DS. This is a key factor for the success of press and public relations work at the MPI DS. The Institute’s own driving service supports travellers in keeping appointments over short and long distances despite tight schedules in a dynamic and internationally oriented environment. The reception of our guests at the Institute location and in the WBZ (Wissenschaftliches Begegnungszentrum, Scientific Meeting Center) is ensured by the General Service. In addition to this, they take on general assistance tasks.

In recent years, Infrastructure Management has been able to grow increasingly in terms of its quality but also in terms of its scope of services for the promotion of science. With its flat hierarchies, it does not only provide an optimal research environment, but also noticeably relieves the Institute’s management and scientists of the increasingly growing daily tasks.

10.1.1 Administrative Services

The Institute’s administrative service covers a wide range of responsibilities and tasks. Until August 2021, the administrative service was divided into the areas of personnel, budget and finance, building and operating technology and IT service. With the reorganization of the entire IT at the MPI DS (IT Service, HPC and Department Administration), the IT Service was combined with the other two units to form an overall IT and assigned to the Scientific Technical Service.

Based on various legal regulations and standards, funding guidelines and federal guidelines, it is the task of the administration to ensure a comprehensive, legally secure, science-promoting and sustainable organization of all administrative processes. The administration acts as
an advisor and service provider for science in all personnel-related but also financial issues, as well as for all areas of infrastructure.

In all its activities, the MPI DS is supported in internal and external communication by press and public relations work, with a value-added focus on external communication on scientific successes and processes.

The creation of an internal monthly newsletter "MPI DS Aktuell" and the organization of a lecture series entitled "Wissenschaft vorm Wochenende" (Science before the Weekend) promote internal communication. By this way bridges are built between science and administration. Through professional press work, which includes press conferences, website maintenance and the organisation of high-profile events for specific target groups, the staff unit makes a valuable and important contribution to the external image of the MPI DS and to the identification and motivation of the Institute’s staff.

As an important anchor for a sustainable institute organization, the MPI DS has a staff unit for quality management. Starting from the moderation of numerous meetings with the directors and senior scientists to create a common Institute vision, the staff unit accompanies and controls all Institute processes. By analyzing the individual processes, their interfaces and their respective outputs, the processes can be clearly defined and implemented in accordance with current legal regulations and standards. The standardized documentation ensures a legally compliant institute organization in the scientific and non-scientific areas. For the MPG’s risk management system, the staff unit identifies the risks for all areas with the Institute’s respective risk experts, draws attention to them and finally promotes the development of suitable preventive and emergency measures.

The General Service staff unit welcomes the guests of our Institute at the Faßberg and the WBZ. In addition to this, the General Service assists with standardized processes in all departments of infrastructure management, or takes over the catering for the entire Institute within the framework of internal events. In addition to this, the post office service and the cash desk service are also provided.

The Institute’s own transport service is an important service, especially in times of tight schedules and processes between the Institute’s location, the numerous cooperation partners, the WBZ and the general travel locations (e.g. event venues or airports), so that deadlines can be met while those travelling can concentrate on their work.

10.1.2 Personnel

The Human Resources Division advises and supports scientists in all matters relating to employment and at all career levels, as well as infrastructure staff. This includes all personnel, legal and organizational issues such as work permits, health insurance and tax and social security benefits.

In March 2020, face-to-face operations at the MPI DS were reduced to an absolute minimum due to the pandemic. Based on the virtual workstation introduced at the MPI DS at the beginning of March, all essential personnel processes were converted. This ensured an almost
smooth service even during the pandemic, while maintaining data protection. Based on the framework created by the general administration of the MPG, the Human Resources team was able to make valuable contributions to the extension of employment contracts of our scientists due to the restrictions of the pandemic, and at the same time to enable the administratively secured start of fellowships abroad in order to avoid delays in the promotion of science due to embassies closed due to the pandemic.

10.1.3 Budget and Finances

The Budget and Finances section includes accounting, budget planning and taxation, asset management and annual accounts, all purchasing and customs procedures, export control, and manages third-party funds, the scientific meeting centre, the vehicle fleet, guest hospitality, event organization and all business trips.

Within the administration, there were some changes on the digital level. In March 2020, all SAP-based workstations were converted to virtual workstations (vAP). The importance of this conversion became particularly apparent with the start of the pandemic and the lockdown in 2020. Since the vAP can be operated from any place with Internet connection, the desired HomeOffice regulation of the federal government during the pandemic period made a seamless transition to mobile level possible even outside our institute. The optimization of workflows in the ordering system already took place in 2017 with eProcurement. It enables electronic orders via catalog or free text and links to the virtual level with digitization. With the expansion of eProcurement and the establishment of e-Invoicing in 2021, we have created a successful combination for digital-based transaction processing. In addition to flexibility, as described above, another major advantage is the minimization of paper masses and the associated folder archiving. Digitized processes are archived in digital form.

In the field of third-party funding, the acquisition of third-party and project funding continues to be successful. The experienced employees provide professional support and advice in the application and administration of the acquired funds at national and international level.

10.2 BUILDING AND OPERATING TECHNOLOGY

The service area "building services and operating technology" is divided into electrical and plant engineering. The Building Services and Operating Technology is responsible for the maintenance and repair of the entire technical infrastructure of the institute, including heating, cooling, plumbing and ventilation, electrical engineering, fire alarm systems, telecommunications, gas detection systems, and emergency call systems. While small and medium-sized repairs and maintenance are carried out by team members, larger measures are outsourced and coordinated by the team. The service unit also takes care of all janitorial and cleaning tasks.
10.3 INFORMATION TECHNOLOGY

The IT group consists of the HPC group, which is responsible for the HPC networks, HPC clusters, HPC file and project data servers and the Linux workstations (see section 9.8 High-Performance Computing Facility for details), and the IT service (ITS) group. The ITS group operates the normal institute network including the central network core and router, the firewall systems and the wireless LAN. It also runs the basic server infrastructure of the institute, which includes central file and authentication servers for Windows workstations and notebooks, and a virtualization cluster that is used to implement a broad spectrum of different IT services. The ITS group also provides Windows and macOS desktop and laptop support for the infrastructure groups and the scientific departments. Furthermore, the ITS group is responsible for the maintenance and operation of the printers and print servers.

In addition to providing IT systems, services and support the provision and licensing of software is also centrally handled by the IT group. In the case of the ITS group, this primarily involves commercial software, whereas the HPC group also handles the installation and maintenance of a wide range of open source software packages that usually need to be compiled and tailored to the existing HPC clusters. The setup of experiments is supported by both groups, depending on the respective IT requirements. This also includes the data management, backup and archiving and the provision and maintenance of the corresponding IT systems.

The IT group participates in the apprenticeship program of the institute. Few other institutions in Göttingen have got such a large variety of different IT systems that can be used in IT training courses. The current apprentice started his professional training in September 2019 and will complete it in the summer of 2022.

10.4 CORONA IMPACT - HOW THE CORONA VIRUS CHANGED LIFE AT THE INSTITUTE

The spread of the corona virus at the beginning of 2020 also presented our institute with new, unknown challenges to continue work and research projects.

On January 29th, 2020 we received a first information from the General Administration of the MPG regarding a new type of corona virus from the Hubei region in China. We started the preparation of a (pandemic) crisis plan for safe handling of the daily life at the institute including various operational restrictions up to temporary shutdown of the institute. The first version of this Pandemic Plan and Hygienic Concept has been published on March 12th, 2020. It describes and specifies the conditions to be complied with and the measures to be taken. It has been updated and adapted to the laws and regulations in force at the time. In order to comply with infection control, large parts of the employees worked from home for extended periods of
time. To make this possible, the management of the MPI DS adapted the applicable working time regulations and rules on mobile working and equipped employees with the necessary hardware for setting up a home office and for mobile working. Meetings and lectures thus took place predominantly in virtual space. These measures ensured a high level of safety, while the institute’s operations were temporarily restricted. However, as people became accustomed to the new situation, all necessary and central functions were able to continue without interruption.

A crisis team consisting of Institute management and members from many departments around the institute has been established to enforce the rules and adapt all measures to the current needs. This combination of strict rules and enforcement has been very successful: In the 22 pandemic months to date (until December 2021), we have had a total of seven Covid 19 cases among institute employees, all of which occurred in a private environment. There were no chains of infection in the workplace.
OUTREACH

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11.1 PUBLIC RELATIONS

Public outreach and media relations are recognized as an important part of the institute’s responsibility. This is shown not only by 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.

11.1.1 Press releases

Press releases and news articles continue to be an important mean 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 MPI DS scientists, and advertise special events the institute organizes or takes part in.

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

11.1.2 Media presence

The activities of the institute are regularly featured in regional and national newspapers and magazines. Along the same lines, experts of the MPI DS frequently appeared in TV and radio shows to present scientific models and findings which could enable a prediction and containment of the spread of the Covid-19 disease. An overview of the media reports is collected by the press office and communicated to the employees in the internal newsletter.

11.1.3 Government consultation

During the Covid-19 pandemic in 2020 and 2021, our institute played a substantial role in providing evidence-based advice for decision makers on the governmental level. Experimental investigations of the aerosol distribution in the breathing air as well as epidemiological modelling of the spread of the disease provided scientific expertise to contain the pandemic.

The MPI DS continues to play a key role in the assessment of the pandemic and is frequently consulted by regional and national media. Likewise, the Federal Constitutional Court in Karlsruhe contacted the institute several times for an expert assessment in the context of the pandemic.
11.1.4 Guided Tours

The MPI DS offers school and student groups regular tours of the Institute. Young participants get the opportunity to learn more about the scientific work at the institute. Visits can include the experimental hall, the computer cluster or the various laboratories. Upon request, the public relations office can involve scientists to present the scientific content in a clear and target-oriented manner.

11.1.5 Future Day

Once a year in spring, 30 students from Göttingen and the surrounding area visit us for our future day. It is lively and turbulent for the 5th to 10th graders. They get the impression of a working day in a basic research institute. During their visit, girls and boys experienced research on dynamics and self-organization up close: currents such as those found on a small scale in the brain or heart, or currents on a large scale such as those found in clouds. The Future Day is always a major success, not only for the young visitors, but also for the scientists involved. Although the event unfortunately had to be suspended in 2020 and 2021 due to the global pandemic, we are looking forward to resume the visits from interested students at the Future Day as soon as the situation allows it.

11.1.6 The EcoBus-project

To improve and facilitate public transportation, back in 2018 the EcoBus-project has been initiated. The aim of the mobility project is to connect the outer areas of a city to the public transportation system via on-demand busses. After a promising trial period in the Harz region, the concept has already successfully been implemented in the city of
Leipzig. Currently, additional cities, including Göttingen, are considering the implementation of the EcoBus algorithm to promote low-cost and environmentally friendly transportation in rural areas.

11.1.7 Online presence

During recent years, the MPI DS expanded its online presence and continues to do so. Amongst other content, this includes videos on the YouTube channel of the institute, featuring news and press releases on LinkedIn as well as several accounts on Twitter, which are administered by the individual group leaders. With a clean and modern design, the website of the MPI DS aims to provide information to all stakeholder groups in both, English and German.

11.1.8 Max Planck goes to school

In a joint project together with the other Max Planck Institutes in Göttingen, the initiative ‘Max Planck geht zur Schule’ was resumed in 2021. Scientists from the institutes visit local schools on a dedicated date using one of the lessons to explain their research to the pupils. In total, around 30 different subjects were offered to the schools from which they could select. By this, not only the visibility of the Max Planck Institutes is increased, but also scientific thinking and interest for contemporary research topics are promoted already at an early stage.

11.1.9 Night of Science

Due to the Covid-19 pandemic, the Night of Science organized by Göttingen campus, was suspended in 2020 and 2021, along with many other public events. However, the MPI DS continues to maintain close contact with the organizers and further research institutes in Göttingen to take part in the next edition of the event in compliance with the general hygienic requirements.
11.1.10 Summer festival

Each summer we usually celebrate our annual summer festival, together with our neighbor institute MPIBPC. Informal discussions, sporting activities, a “Brain Match Quiz” and musical highlights turn the summer day into a happy event. However, the summer festival recently had to be cancelled due to the pandemic but will be resumed as the sanitary situation allows it.

11.1.11 Göttinger Literaturherbst

The MPI DS takes part in the annual literary festival in Göttingen, called “Göttinger Literaturherbst” which is organized each autumn. Traditionally, the event is initiated by 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, with the aim of stimulating a vigorous exchange of ideas. In addition, among the invited speakers the Science Communication Medal is awarded for strong commitment to communicate current scientific results to the general public. In recent years, Prof. Martin Wikelski and Prof. Maja Göpel were awarded with the medal in 2019 and 2021, respectively.

11.1.12 Future press/public relations work

The scientific output of the institute will continue to be accompanied by press releases and news articles. As science communication is of increasing importance, also further communication channels will be used. In addition to existing videos, audiovisual portraits of individual researchers or research groups are planned. By this the scientific topics will be introduced in more depth and detail. By establishing a local Alumni-Network, the institute will also maintain contact with former members provided a network for exchange with current employees.

11.2 INTERNAL COMMUNICATION

11.2.1 Intranet

Following the central administration of the Max Planck Society, the MPI DS also relaunched their intranet platform MAX based on MS SharePoint as of October 2021. The new interactive platform does not only allow communication and formation of working groups within the institute, but also enables the connection to all employees of the Society using MAX. The Intranet also serves as a repository for documents such as forms, documentations and standard operating procedures as well as an archive for the MPI DS newsletter.
11.2.2 Science before the weekend

The lecture series “Wissenschaft vorm Wochenende” (“Science before the weekend”) has shown to be an efficient and well-received tool in order to explain the scientific work of the institute to the administrative and technical staff. In quarterly intervals, the departments of MPI DS identify speakers who present their topics in a comprehensive and understandable manner in German language. This way, also the employees with a non-scientific background easily gain access to scientific topics from their colleagues which supports both the mutual understanding and the team spirit. Typically, the audience consists of up to 50 people from all over the institute, indicating a high appreciation for this internal communication project.

11.2.3 Internal newsletter

The internal newsletter ‘MPI DS Aktuell’ has been re-designed and is now send as a digital version embedded into the mail client of the institute. This way, all legal regulations can be met while improving the design and style of the newsletter to a more appealing and handier format.

The newsletter is sent out towards the end of each month and serves as a major source of information on news, developments and changes around the institute and beyond. Regular topics include: important dates and deadlines, news teasers with direct links, section ‘in the spotlight’ where particular topics are highlighted, newcomers and guests, job offers, final theses, publications, press review and the ‘beyond research’ category. Suggestions for topics can be sent to the press office which will compile the newsletter on a monthly basis.

11.2.4 Crisis communication

In face of the Covid-19 pandemic, a crisis management team was formed under the lead of the managing director. As the German government introduced and constantly adapted legal requirements to contain the pandemic, this committee is responsible for both ensuring the health and safety of the MPI DS employees and to communicate decisions regarding internal regulations. Due to regular meetings and short communication loops, the team supported the continuation of the scientific work even throughout the pandemic.

11.2.5 Sustainability group

In 2019, several employees of the MPI DS initiated a task group to promote and encourage a more sustainable and environment-friendly behavior at the institute. This includes regular discussions on waste and energy management as well as regular communication of recommendations via the internal news channels. The group is open to all employees and seeks to support the mutual exchange on future-oriented topics.
11.3 THE GÖTTINGEN CAMPUS

The Göttingen Campus Council (GCC) was established by the university in 2006 in order to coordinate campus wide activities with the non-university institutes. The main task of the GCC is the consultation between the executive committees of the University (Presidential Board, University Medical Centre Board, Senate) and the non-university institutes. Topics range from joint teaching and research activities, towards the identification of research foci for the development of the Göttingen Campus. The Campus Marketing Group exists since 2016 and exchanges information once a quarter about joint activities such as the Night of Science, the Göttingen Literaturherbst, joint advertising products, the Göttingen Campus website, the Göttingen Campus Calendar or activities such as the “Belebten Schaufenster” (lively shop windows).

11.4 MAX PLANCK CAMPUS

Together with the Gesellschaft für wissenschaftliche Datenverarbeitung mbH Göttingen (GWDG) and the neighbor Max Planck Institute for Biophysical Chemistry (MPIBPC), the MPI DS forms the Göttingen Max Planck Campus. 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 between Max Planck Institutes and create synergistic projects. This includes regular meeting on scientific, but also on organizational and infrastructural topics.

11.4.1 Ecological projects on campus

During recent years, several ecological projects were initiated and conducted around the Max Planck Campus. A recent example is the creation of a meadow orchard at the rear side of the MPI DS. Together, these projects aim to support a sustainable ecology, provide living space for animals and insects and raise the consciousness for environmental care, also supported by the sustainability group of the MPI DS.

11.4.2 Further Max Planck Campus Activities

In recent years, several tools have been established to foster the scientific exchange between researchers from the Max Planck Institutes in Göttingen. This is e.g. realized via the Campus Seminar, a biweekly lecture series. Here projects and results can be discussed with colleagues, thus allowing for a preliminary exchange of ideas with the aim of triggering scientific cooperation. A more unofficial framework for getting to know other colleagues on campus is possible during the annual summer festival.
HOW TO REACH US AT THE MAX PLANCK INSTITUTE FOR DYNAMICS AND SELF-ORGANIZATION

_Fassberg site (main building)_

Address:
Am Fassberg 17
D-37077 Göttingen
Germany

Departments: Fluid Physics, Pattern Formation, and Biocomplexity (Prof. Eberhard Bodenschatz)
Dynamics of Complex Fluids (Prof. Stephan Herminghaus)
Living Matter Physics (Prof. Ramin Golestanian)

Max Planck Research Groups:
Biological Physics and Morphogenesis (Dr. Karen Alim)
Biomedical Physics (Prof. Stefan Luther)
Statistical physics of evolving systems (Dr. Armita Nourmohammad)
Neural Systems Theory (Dr. Viola Priesemann)
Turbulence, Complex Flows and Active Matter (Dr. Michael Wilczek)
Theory of Biological Fluids (Dr. David Zwicker)

Independent Research Units:
Dynamics in mesoscopic systems (Dr. Ragnar Fleischmann)
Theory of Turbulent Convection (PD Dr. Olga Shishkina)

Emeritus Groups:
Nonlinear Dynamics (Prof. Theo Geisel)
Rhythms – Beating Cilia and Ticking Clocks (Prof. Gregor Eichele)

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 Hanover 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 (20 minutes). At platform D take the bus No. 21 (direction: »Nikolausberg«) or No. 23 (direction: »Faßberg« or »Universität Nord«). After about 20 minutes 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 (Scientific Meeting Center)**

**Emeritus Group:** Molecular Interactions (Prof. Jan Peter Toennies)

**Services:** Scientific Meeting Center

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**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 Hanover 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, 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 MPI DS 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.