Interdisciplinary Challenges in Non-equilibrium Physics

10-13 April 2019
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WELCOME

Non-equilibrium processes play important, and often vital, roles at many length- and time-scales, ranging from those relevant in the cell nucleus to those for the swarming of birds. Non-equilibrium statistical mechanics is a critical tool that is being developed and refined to understand these complex behaviours. A key step to improve our understanding of universal non-equilibrium mechanisms at play across scales is to discuss and compare ideas coming from research fields. At the same time, given the richness of phenomena that are being discovered at the interface between biology (where non-equilibrium processes play a major role) and physics, it is natural to expect that future research efforts, e.g. in terms of grants, collaborations, papers between the next generation of researchers will be critical to address outstanding problems in this field and maintain research excellence in fascinating interdisciplinary areas of the Physical and Life Sciences.

For these reasons, this meeting aims to bring together enthusiastic, talented and motivated early career researchers (post-docs and junior group leaders) working on interdisciplinary topics which have the common theme of non-equilibrium physics. The meeting will focus on a broad spectrum of inter-related topics: biophysics, polymers, ecology and population dynamics, active matter, non-equilibrium statistical mechanics and glasses and disordered systems.

Davide Michieletto, Gianmaria Falasco, George Constable, Elsen Tjhung

VENUE INFORMATION

This event will take place at the University of Edinburgh in the James Clerk Maxwell Building, Lecture Theatre C (marked with ★, building no. 24 on bottom map) on the King's Building Campus.
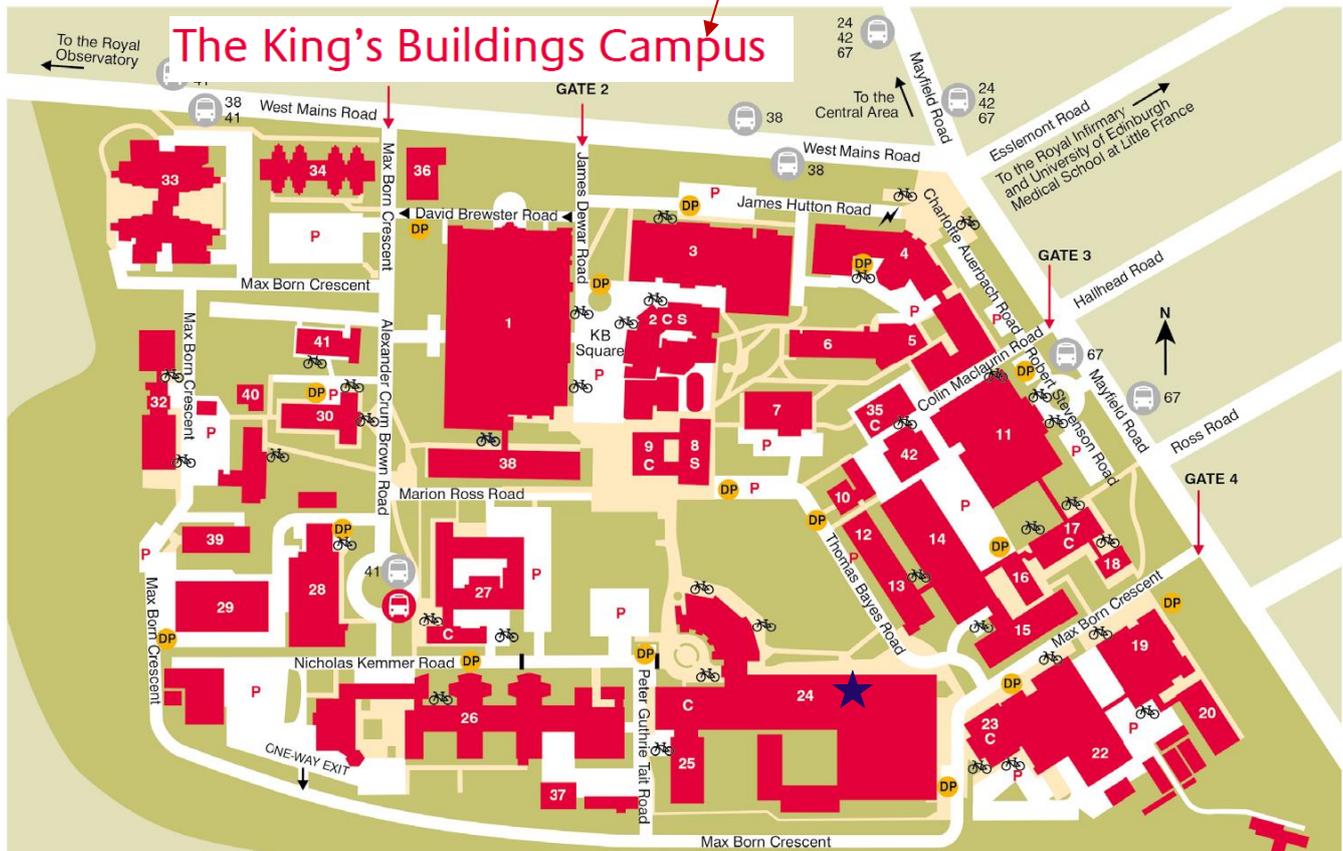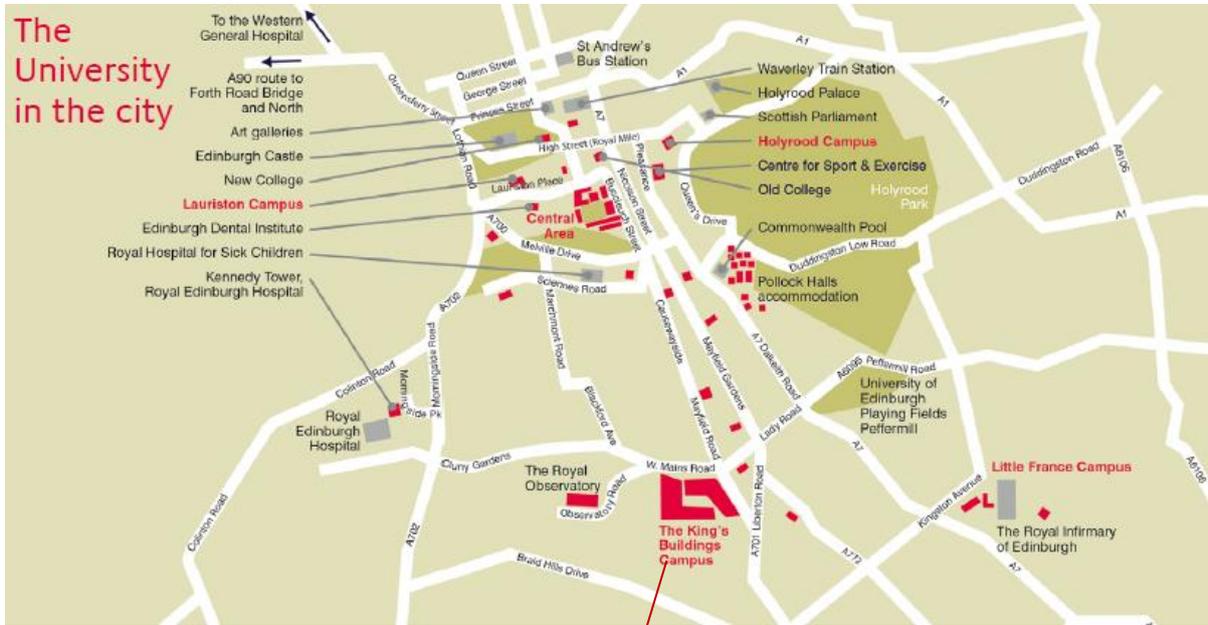
PROGRAMME

Day One	Wednesday 10 April
13.00	Registration
Session 1	**Noise Driven Systems**
14.00	Stefano Bo, *Can microscopic systems exploit noise? The case of driven anisotropic diffusion at boundaries*
14.30	Grant Rotskoff, *Nonequilibrium importance sampling with a driven dynamics*
15.00	Alexandre Lazarescu, *Large deviations and dynamical phase transitions in stochastic chemical networks*
15.30	**Break**
Session 2	**Active Polymers**
16.00	Tom Ouldridge, *Biological copying of polymers: a necessarily non-equilibrium process*
16.30	Aleksandre Japaridze, *The role of spatial confinement in DNA organization: From single molecules to bacterial chromosomes*
17.00	Jan Smrek, *Active-passive polymer mixtures in relation to chromatin conformation and dynamics*
Day Two	**Thursday 11 April**
Session 3	**Topology**
9.30	Lucia Coronel, *Dynamics of supercoiled knotted DNA: large-scale rearrangements and persistent multi-strand interlocking*
10.00	Amin Doostmohammadi, *Active Thin Structures*
10.30	Dan Pearce, *Controlling active matter with curvature and topology*
11.00	**Break**
Session 4	**Rheology**
11.30	Nicoletta Gnan, *The microscopic role of deformation in the dynamics of soft colloids*
12.00	Jan Meibohm, *Catastrophes and Large deviations in turbulent aerosols*
12.30	Romain Mari, *Dynamic vorticity banding in discontinuously shear thickening suspensions*
13.00	**Lunch**
Session 5	**Slow Relaxation**
14.00	Beatriz Seoane, *Spin-glass-like dynamics in highly compressed colloidal and granular glasses*
14.30	Misaki Ozawa, *Numerical Investigation of Ideal Glass Transition in Glass-Forming Liquids*
15.00	Elisabeth Agoritsas, *Out-of-equilibrium dynamics of particle systems in infinite dimension*
15.30	Francesco Turci, *Structural-dynamical correlations and rigid response*
16.00-17.30	Poster Session/Social Event

Day Three	Friday 12 April
Session 6	**Swimmers**
9.30	Raphael Jeanneret, *Pairing in planktonic elongated diatoms, or how synchronized-sinking favours cell encounter for sexual reproduction*
10.00	Fanlong Meng, *Magnetic swimmers in a microfluidic channel*
10.30	Joakim Stenhammar, *Correlations and collective behaviours in suspensions of swimming microorganisms*
11.00	**Break**
Session 7	**Physics of Motion**
11.30	Kirsty Wan, *Non-equilibrium and critical behaviour in biological micro-swimmers*
12.00	Demian Levis, *Activity induced synchronization in chiral active matter*
12.30	Ariana Bottinelli, *Predicting collective motion in high-density crowds*
13.00	**Lunch**
Session 8	**Tissues and Biofilms**
14.00	Diana Khoromskaia, *Active surface models for cell and tissue morphogenesis*
14.30	Ananyo Maitra, *Unusual stability of oriented active suspensions on substrates*
15.00	Silke Henkes, *Universal motion patterns in confluent cell monolayers*
15.30-17.30	Poster Session/Social Event
Day Four	Saturday 13 April
Session 9	**Ecology and Evolution**
9.30	Andrea Giometto, *Mechanical interactions reduce the power of natural selection in growing yeast colonies*
10.00	Hye Jin Park, *Population size and interaction structure driven by mutant interactors*
10.30	Matthieu Barbier, *Are complex ecosystems ever simple? Disorder in competition experiments*
11.00	**Break**
Session 10	**Inference and Optimisation**
11.30	Barbara Bravi, *Characterizing and inferring epistasis via direct evolutionary couplings in models of allostery*
12.00	Caterina De Bacco, *A physical model for efficient ranking in networks*
12.30	Silvia Zaoli, *Trip Centrality: walking on a temporal multiplex with non-instantaneous link travel time*

TALK ABSTRACTS

Out-of-equilibrium dynamics of particle systems in infinite dimension

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Dense assemblies of particles are prototypes of structurally disordered systems, such as amorphous solids or yield stress fluids. In infinite dimension their mean-field description becomes exact, and solving their equilibrium dynamics in this limit has been remarkably fruitful in capturing static properties of finite-dimensional systems as well. Here we address their out-of-equilibrium dynamics, paving the way to obtaining a similar infinite-dimensional benchmark for the mechanical or rheological properties of structurally disordered systems.

More specifically, we derive the mean-field dynamical equations that describe a system of pairwise interacting particles, in infinite dimension and in the thermodynamic limit, in a generic setting with arbitrary noise and friction kernels, and possibly under a global shear. We show that the complex many-body dynamics can then be exactly reduced to a single one-dimensional stochastic process, with three effective kernels that have to be determined self-consistently.

In this talk, I will sketch the derivation of this effective dynamics, highlighting in particular the few key ingredients of the high-dimensional physics and their possible relevance for finite-dimensional systems. Since we consider a very general setting, we can model a broad range of situations — equilibrium, quasi-statics, transients or steady-states — such as liquid and glass rheology or active self-propelled particles.

A physical model for efficient ranking in networks

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Our work addresses the problem of taking a network of directed interactions and inferring a real-valued ranking of the nodes. This problem arises in many fields, including ecology (animal dominance networks), anthropology (social support networks), computational social science (prestige signaling networks), the ranking of sports teams, Chess, or Go players, and other pairwise interactions.

This model (SpringRank) uses both the existence and direction of edges to find real-valued ranks. It does so by mapping the ranking problem to a physical system of directed springs, in which the optimal ranking minimizes the energy of a convex Hamiltonian. Due to the convexity of this problem SpringRank can be solved uniquely and rapidly for networks of millions of edges in seconds. Moreover, unlike many other methods, SpringRank takes into account the fact that both the direction and the existence of a link gives us information about the entities' relative position in a hierarchy. For example, many animals tend to interact with others of similar rank, and humans tend to claim friendships with others of slightly higher status. As a result, in addition to being extremely fast, we find that SpringRank is able to accurately model both synthetic and real-world datasets, and in particular to predict the direction of missing edges more accurately than existing methods.

To complement this method of rapid rank inference, we introduce a corresponding generative model to create networks with embedded hierarchies. This model can be used to create benchmark datasets with various amounts of hierarchical structure and noise levels, which we hope will be widely useful in studying real-world systems.

We use this model to test the statistical significance of hierarchical structure in a principled way, allowing researchers to avoid overfitting based on popular techniques such as minimum violation ranking.

Are complex ecosystems ever simple? Disorder in competition experiments

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While ecology and statistical mechanics have met repeatedly over five decades, physics-like representations (e.g. networks) have crossed over much more than physics-like results (universality, mean-field theories, etc.).

In particular, little work has been done to determine when generic high-dimensional behaviours emerge in ecological networks, when their detailed structure matters or not, and when minimal models can predict real ecosystem dynamics quantitatively.
I will argue that disorder captures important facets of how species interactions shape ecosystems, as shown by precise agreement with data from plant competition experiments. I will also propose that ecological interactions could be better modelled as a combination of disorder and low-dimensional order, and suggest new and interesting directions for statistical physics tools.

Can microscopic system exploit noise? The case of driven anisotropic diffusion at boundaries

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Microscopic systems at room temperature are subject to fluctuations, which play a significant or even dominant role. On the one hand, noise plays a disruptive role, hampering the possibility to reliably perform tasks. On the other hand, systems suitably driven out of equilibrium can exploit fluctuations to achieve transport and efficient energy conversion using mechanisms that have no macroscopic counterpart. I will briefly overview the key concepts behind some noise induced transport mechanisms and present our recent findings concerning the diffusive dynamics of a Brownian particle diffusing close to a flat surface under non-equilibrium conditions.

I will show how the interplay between anisotropic diffusion and hard-core interaction with the plain wall rectifies the thermal fluctuations and induces directed particle transport parallel to the surface.

In closing, I will suggest a concrete experimental set-up to observe this novel noise-induced transport mechanism, and discuss how it can be used for sorting particles of different size.

Predicting collective motion in high-density crowds

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During mass events such as concerts, sporting events, and pilgrimages, crowd density can become exceptionally high, causing the emergence of sometimes deadly collective motion such as crowd turbulence and density waves. Inspired by the physics of soft and active matter, we adapted mode analysis to understand the basic mechanisms underlying the emergence of injurious collective motions in crowds [1,2]. I will give an overview of mode analysis techniques and present the main results obtained by applying them to a crowd video footage from a rock concert [3]. I will show that these techniques offer the opportunity to predict real crowd's motion, and discuss the potential of this approach in preventing crowd disasters.

1. A. Bottinelli, D.T.J. Sumpter, J.L. Silverberg, "Emergent structural mechanisms for high-density collective motion inspired by human crowds", PRL (2016)
2. A. Bottinelli, J.L. Silverberg, "How to: using mode analysis to quantify, analyze, and interpret the mechanisms of high-density collective motion", Frontiers (2017)
3. A. Bottinelli, J.L. Silverberg, "High-density human collective motion can be forecasted by spatiotemporal fluctuations", in preparation

Characterizing and inferring epistasis via direct evolutionary couplings in models of allostery

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In allosteric proteins, the binding of a ligand modifies function at a distant active site. Such allosteric pathways can be used as target for drug design, generating considerable interest in inferring them from sequence alignment data. Currently, different methods lead to conflicting results, in particular on the existence of long-range evolutionary couplings between distant amino-acids mediating allostery. Here we propose a resolution of this conundrum, by studying epistasis and its inference in models where an allosteric material is evolved in silico to perform a mechanical task. We find four types of epistasis (Synergistic, Sign, Antagonistic, Saturation), which can be both short or long-range and have a simple mechanical interpretation. We perform a Direct Coupling Analysis (DCA) and find that DCA predicts well mutation costs but is a rather poor generative model. Strikingly, it can predict short-range epistasis but fails to capture long-range epistasis, in agreement with empirical findings. We propose that such failure is generic when function requires subparts to work in concert. We illustrate this idea with a simple model, which suggests that other methods may be better suited to capture long-range effects.

Dynamics of supercoiled knotted DNA: large-scale rearrangements and persistent multi-strand interlocking

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In bacterial plasmids, catalytic processes involving DNA strand passages introduce knots and supercoiling. The effect of on plasmid organisation has been separately and extensively studied, however much less is known about their concurrent action. Therefore, to study the kinetic and metric changes introduced by complex knots and supercoiling in 2kbp-long DNA rings; we use molecular dynamics simulation and oxDNA, a mesoscopic DNA model, finding several unexpected results. First, two distinct states dominate the conformational ensemble, they differ in branchedness and knot size; secondly, fluctuations between these states are as fast as the metric relaxation of unknotted rings. Nevertheless, certain boundaries of knotted and plectonemically wound regions can persist over much longer timescales. These regions involve multiple strands that are interlocked by the cooperative action of topological and supercoiling constraints. Their long liver character may be relevant for the simplifying action of topoisomerases.

Active Thin Structures

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Monolayers of cells in tissue and bacterial colonies growing on substrates are ample examples of thin structures that are continuously driven out of equilibrium by the activity of their constituent elements. One generic property of these active layers is the spontaneous emergence of collective flows which often leads to chaotic flow patterns characterised by swirls, jets, and topological defects in their orientation field [1]. In this talk I will discuss recent works on cell monolayers and growing bacterial colonies, where we find interesting correlations between liquid crystal-like features of these active systems and their biological functionality.

I will explain our recent finding on the role of topological defects in regulating the morphology of growing cell colonies [2] and represent evidence on spontaneous formation of singularities in cellular alignment in the form of nematic topological defects, as a previously unidentified cause of cell apoptosis and extrusion, suggesting that such defects govern cell fate in epithelial tissues [3]. In addition, I will use theory of active liquid crystals to explain how motility of Pseudomonas aeruginosa bacteria leads to a slower invasion of bacteria colonies, which are individually faster. Moreover, the ability to achieve structured flows and ordered disclinations is of particular impor- tance in the design and control of active systems [4]. By confining an active nematic fluid within a channel, we find a regular motion of disclinations, in conjunction with a well-defined and dynamic flow structure. As pairs of moving disclinations travel through the channel, they continually exchange partners producing a dynamic ordered state, reminiscent of Ceilidh dancing [5]. I will show that this state is an intermediate state governing the transition to meso-scale turbulence in living fluids and that the transition belongs to the directed percolation universality class [6].

1. A. Doostmohammadi, et al., Active nematics. Nature Communications, 9:3246, 2018.
2. A. Doostmohammadi, S. Thampi, J. M. Yeomans, Defect-mediated morphologies in growing cell colonies. Physical Review Letters, 117: 048102, 2016.
3. T. B. Saw, A. Doostmohammadi, et al., Topological defects in epithelia govern cell death and extrusion. Nature, 544.7649: 212-216, 2017.
4. A. Doostmohammadi, M. F. Adamer, S. P. Thampi, J. M. Yeomans, Stabilization of active matter by flow-vortex lattices and defect ordering. Nature Communications, 7:10557, 2016.
5. T. N. Shendruk, A. Doostmohammadi, K. Thijssen, J. M. Yeomans, Dancing disclinations in confined active nematics. Soft Matter, doi:10.1039/C6SM02310J, 2017.
6. A. Doostmohammadi, et al., Onset of meso-scale turbulence in active nematics, Nature Com- munications 8:15326, 2017.

Mechanical interactions reduce the power of natural selection in growing yeast colonies

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Microbial populations often assemble in dense populations in which proliferating individuals exert mechanical forces on the nearby cells. Here, we use yeast strains whose doubling times depend differently on temperature to show that physical interactions among cells affect the competition between different genotypes in growing yeast colonies. Our experiments demonstrate that these physical interactions have two related effects: they cause the prolonged survival of slower-growing strains at the actively-growing frontier of the colony and cause faster-growing strains to increase their frequency more slowly than expected in the absence of physical interactions. These effects also promote the survival of slower-growing strains and the maintenance of genetic diversity in colonies grown in time-varying environments. A continuum model inspired by overdamped hydrodynamics reproduces the experiments and predicts that the strength of natural selection depends on the width of the actively-growing layer at the colony frontier. We verify these predictions experimentally. The reduced power of natural selection observed here may favor the maintenance of drug-resistant cells in microbial populations and could explain the apparent neutrality of inter-clone competition within tumors.

The microscopic role of deformation in the dynamics of soft colloids

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Unraveling the glass transition and jamming in soft colloidal systems remains a challenge for modern soft matter physics. An important open question is whether softness controls the dynamics in such dense conditions [1]. Numerical simulations represents a strong ally to elucidate this problem, but in most cases softness is tuned by modifying the pair-potential parameters allowing particles to overlap to a certain extent, while neglecting crucial aspects that contribute to the elastic properties of realistic particles. This makes the concept of "softness" in simulations and experiments very different. To fill this gap, I will discuss a new model of 2D polymer rings with tunable softness which undergo substantial deformation at high densities. The ability to deform has a strong impact on the dependence of the relaxation time on the packing fraction which change from fragile to strong. In addition, dynamics is controlled by an intermittent particle motion which gives rise to a compressed exponential decay of the self-intermediate scattering function. This behavior can be rationalized in terms of deformed rings that act as stress dipoles [2]. This simple model thus provides microscopic insights into two mechanisms which are of a deep interest in soft matter: the fragility dependence on softness and the occurrence of a compressed exponential decay in dynamical correlation functions [3].

1. J. Mattsson et al. Nature **462**, 83 (2009)
2. L. Cipelletti et al. PRL **84** (10), 2275 (2000)
3. N. Gnan et al. arXiv:1806.04788 (accepted for publication by Nat. Phys.)

Universal motion patterns in confluent cell monolayers

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Epithelial cell monolayers show remarkable long-range displacement and velocity correlations reminiscent of supercooled liquids and active nematics. Here we show that many of the observed features can be understood within the framework of active matter at high densities. In particular, we argue that uncoordinated but persistent cell motility coupled to the collective elastic modes of the cell sheet is sufficient to produce characteristic swirl-like correlations. This includes a divergent correlation length in the limit of infinite persistence time.

We derive this result using both continuum active linear elasticity and a normal modes formalism, and validate analytical predictions with numerical simulations of two agent-based models of soft elastic particles and in-vitro experiments of confluent corneal epithelial cell sheets. Our analytical model is able to fit measured velocity correlation functions without any free parameters.

The role of spatial confinement in DNA organization: From single molecules to bacterial chromosomes

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The bacterial chromosome a are spatially organized under the combined influence of protein-mediated condensation, supercoiling, and the cell-boundary confinement, but their roles have not been resolved independently. In my talk, I will discuss two methods, one based on atomic fore microscopy [1] and the other based on live cell fluorecent imaging [2], to study the influence of spatial confinement on single DNA molecules and single *Esherichia coli* chromosomes.

In our in vitro experiments, we successfully combined slits of various sizes with the nanometre high resolution of atomic force microscopy to study circular DNA under spatial confinement [1]. Our findings, supported by numerical simulations, indicated that confinement imposed a large mechanical stress on DNA as evidenced by pronounced anisotropy with respect to non-constrained molecules. For the strongest confinement, we observed nanometer sized hairpins and interwound structures associated with nicked sites in the DNA sequence. Based on these findings, we propose that spatial confinement can promote the formation of localized defects at mechanically weak sites of DNA molecules.

Next, we studied the intrinsic structure of chromosomes in live *E.coli* cells through cell shape manipulation and quantitative fluorescence imaging [2]. We used drugs and molecular genetics tools to disrupt the cytoskeleton of bacteria, leading to cell sizes far larger than the rod-like wild type cells. This enables us, to visualize for the first time the circular nature of single *E.coli* chromsomes. Surprisingly, the chromosomes displayed high heterogeneity in compaction and large dynamics at sub-minute timescacles.

Our findings provide an architectural basis for the understanding of the spatial and dynamic organization of bacterial genomes in live cells.

1. Japaridze, A., Orlandini,E., Smith,K.B., Gmür, L., Valle, F., Micheletti, C. & Dietler, G. Spatial confinement induces hairpins in nicked circular DNA. *Nucleic Acids Res.* 45, 4905–4914 (2017).
2. Wu, F., Japaridze, A., Zheng, X., Kerssemakers, J. W. J. & Dekker, C. (2018) Direct Imaging of the circular chromosome of a live bacterium. *bioRxiv* 246389

Pairing in planktonic elongated diatoms, or how synchronized-sinking favors cell encounter for sexual reproduction

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Cell division in diatoms, a large group of non-motile phytoplankton, is accompanied by a slow reduction in cell size due to their rigid silica shell. Once in a while therefore (i.e. ~ once a year) cells need to reproduce sexually to restore a sufficiently large body size and resume a life cycle based on mitosis and cytokinesis. However, pairing for sexual reproduction in an inherently turbulent and three-dimensional system, such as the planktonic marine environment, is a difficult task for non-motile organisms having poor control over their position and orientation. In this talk I will show how the sinking of populations of elongated diatoms in calm waters favors cell encounter via a hydrodynamically-mediated density instability. Starting from uniform suspensions, the time scale for the development of this instability depends on both the diatoms sinking speed and their concentration: this promotes the encounter between healthy kins that sink synchronously. This process is also accompanied by a preferential vertical orientation of the cell body due to gravitational torques induced by intracellular density heterogeneities. Because the cells need to make contact along their long-axis to reproduce sexually, this feature appears crucial for an efficient pairing. In conclusion our field observations and laboratory experiments suggest that elongated diatom populations need to sink from surface turbulent waters to more stable environments (i.e. below the pycnocline, the region of high water density gradients) in order to reproduce sexually and seed genetically renewed populations.

Active surface models for cell and tissue morphogenesis

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The ability of cells to actively generate forces is crucial for cell shape control during division, motility, and adhesion. At the level of tissues, coherent shape changes and rearrangements of a group of cells can lead to large-scale deformations of the whole tissue. Morphogenesis of epithelia, which are two-dimensional tissues, can be described within a recently developed framework that incorporates a variety of active effects into a mechanical model for a curved surface (Salbreux and Jülicher, 2017). We study in simulations the morphogenesis of epithelia as elastic shells endowed with internal tensions and torques, which lead to various classes of invaginated or folded shapes.

Large deviations and dynamical phase transitions in stochastic chemical networks

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We are all relatively familiar with the standard (macroscopic) description of chemical reactions in a well-mixed dilute solution, as a set of coupled first-order differential equations in time on the concentration of every species in solution. A natural way to describe the same system at a microscopic scale (i.e. for a priori finite numbers of chemical particles, rather than finite concentrations) is through the chemical master equation, which is a Markov jump process on probability distributions of chemical compositions (the number of particles of each species), which is consistent with the macroscopic description in the appropriate limit.

Large deviation functions, sometimes called dynamical free energies, are the natural language to describe fluctuations around the typical behaviour of such stochastic systems in the limit of either a large size, or a long observation time. In this talk, I will present recent results obtained in collaboration with Tommaso Cossetto and Gianmaria Falasco, on the structure of large deviations for stochastic chemical networks with mass-action dynamics. We will see how, in the limit of a large volume with finite concentrations, the stochastic evolution of the system can be described through a path integral with a non-quadratic action that can be calculated explicitly. We will then look at probabilities of observing certain unlikely averages of concentrations and chemical currents over a long time, which can be recast as solutions of Hamilton's equations of motion for an appropriate finite-dimensional Hamiltonian. We will see how those distributions generically exhibit dynamical phase transitions if the macroscopic set of coupled differential equations has several stable attractors, and we will illustrate this fact on the Schlögl model, which is one of the simplest bistable chemical systems.

Activity induced synchronization in chiral active matter

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Synchronization, the temporal coordination of coupled oscillators, allows fireflies to flash in unison, neurons to fire collectively and crowds of people to fall in step on the London Millennium Bridge. The emergence of synchronized states in populations of mobile entities is widely observed in very different contexts; however, previous studies have focused on, either immobile oscillators, or mobile oscillators which phase does not directly influence the way they move in space.

Here, we interpret active (or self-propelled) chiral microswimmers (particles such as asymmetric Janus colloids or bacteria close to walls), as motile oscillators and show that they can synchronize over very large distances in 2D, as opposed to non-active oscillators on static or time-dependent networks, usually leading to synchronized domains only. One consequence of this activity-induced synchronization is the emergence of a "mutual flocking phase", where chiral active particles cooperate to form superimposed flocks moving at a relative angle to each other, providing a chiral active matter analogue to the celebrated Toner Tu phase. This new synchronization scenario generates a second phase where particles of opposite chirality segregate into two macroscopic structures. Both phases feature activity-induced macroscopic synchronization in 2D, which is not achievable for the typically considered cases of immobile oscillators in low dimensional systems. For comparatively high frequencies, chiral active particles hosts a complex world of unusual patterns, including microflock patterns, featuring two coexisting length scales, and microflock patterns formed in one species, while particles of opposite chirality phase separate, forming a macroscopic cluster. The underlying mechanism responsible of such rich collective phenomena hinges on a positive feedback between phase and motility, which has been ignored so far.

Unusual stability of oriented active suspensions on substrates

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Standard theories of incompressible active suspensions predict that enhancing internal driving inevitably destroys the orientationally ordered state of anisotropic active units eventually leading to incoherent motion. However, we demonstrate that this view is simplistic for orientationally ordered active suspensions in contact with a substrate. Re-examining the symmetries of an apolar active system we uncover an additional coupling between activity and motion due to which the apolar active phase may be stabilised, even beyond its passive counterpart, upon enhancing the internal drive while preserving other hallmarks of non-equilibrium physics such as giant number fluctuations. Turning to polar suspensions, we demonstrate that motility may lead an even greater degree of stability, via an active Anderson-Higgs-like mechanism, with orientational fluctuations at zero wavenumber relaxing in a finite time. This leads to the suppression of giant number fluctuations and banding instability at the immotile-motile transition.

Dynamic vorticity banding in discontinuously shear thickening suspensions

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The phenomenon of discontinuous shear thickening is a step increase of the viscosity with increasing shear rate observed in some dense suspensions of hard particles, the most well-known example of being cornstarch suspensions. It is associated to an underlying shear stress versus shear rate constitutive curve which is S-shaped. While a S-shaped flow curve generically leads to flow instabilities such as banding, it has recently been argued that steady-state bands cannot arise in shear thickening suspensions, because the normal stress imbalance across the interface between the bands will set up particle migrations. In this talk, I will introduce a simple continuum model that couples shear thickening to particle migration. Linear stability analysis shows that homogeneous flow is unstable towards vorticity banding in the regime of negative constitutive slope. In full nonlinear computations, the resulting vorticity bands are unsteady, with spatiotemporal patterns governed by stress-concentration coupling. I will furthermore show that these dynamical bands also arise in direct particle simulations, in good agreement with the continuum model.

Catastrophes and Large deviations in turbulent aerosols

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Heavy particles suspended in turbulent fluids, so-called turbulent aerosols, are common in Nature and in technological applications. A prominent example is the suspension of rain droplets in turbulent clouds. Due to their inertia, ensembles of aerosol particles distribute inhomogeneously over space and can develop large relative velocities at small separations. Caustics are mathematical catastrophes that arise because the particle phase-space manifold folds over with respect to real space, and are believed to play an important role in aerosol systems.

Statistical models that mimic the turbulent fluid at small scales by smooth Gaussian random velocity fields have been successful in describing turbulent aerosols. Compared to systems with actual turbulence, these statistical models are simpler to study and allow for an analytical treatment in certain limits. Despite their simplicity, statistical models qualitatively explain the results of direct numerical simulations and experiments.

In my talk, I will discuss how methods of non-equilibrium statistical mechanics and large deviation theory are used to study statistical models of turbulent aerosols. The one-dimensional version of the models will serve as a simplified playground to create intuition for, and give important insights into the behaviour of higher dimensional particle systems. I will discuss in detail the universal effects of caustics on the observables of the models.

Magnetic swimmers in a microfluidic channel

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Magnetotactic bacteria can be focused to the radial centre of the channel when swimming in a microfluidic channel under an external magnetic field, and found to form clusters if the external magnetic field is strong or the flow speed is large [1]. However, the underlying mechanism was missing. We showed in our recent work [2] that the magnetic microswimmers (not only for magnetotactic bacteria, but also applicable synthetic magnetic microswimmers) can form interesting large-scale clusters when the magnetic attractive interaction dominates thermal fluctuations. By applying analytic techniques and conducting Brownian dynamics simulation, we provide the critical condition for clustering of magnetic microswimmers, which matches well with the experiment. Hydrodynamic interactions between the microswimmers are also incorporated as a generalisation. Understanding the physics of magnetic active matter will help advance the cause of studying matter out of equilibrium, and provides new insight for technological applications of synthetic magnetic microrobots (for drug delivery, solution stirring, etc.) with desired collective properties.

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Biological copying of polymers: a necessarily non-equilibrium process

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Producing copies of molecular polymers is an essential process within life, occurring during replication, transcription and translation, the three key steps of the central dogma of molecular biology. In such a process, monomer units (eg. nucleotides or amino acids) assemble into a specific sequence determined by the sequence of a template polymer. Traditional analyses of this process have focused on the challenge of assembling the copy accurately on the template. This perspective, however, neglects the need to separate the copy from its template once copying is complete. In this talk I will demonstrate that the requirement to separate has fundamental consequences for the copy process: the final state is necessarily out of equilibrium, constraining the underlying biophysics of copy processes, and shaping the design space of basic copiers that we might wish to engineer.

Numerical Investigation of Ideal Glass Transition in Glass-Forming Liquids

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The central question of the glass transition study is to understand the mechanism behind the dramatic slowing down of supercooled liquids approaching the kinetic glass transition. One possible scenario assumes the existence of a genuine thermodynamic "ideal glass transition" and that its singularity causes the divergence of structural relaxation times. Proving or disproving this scenario is extremely difficult as standard experiments and computer simulations fail to approach the putative ideal glass transition temperature due to ever-growing sluggishness. We have tackled this problem by using advanced computer simulation techniques and developing efficient simulation schemes: i) Random pinning: This approach induces an ideal glass transition by freezing the positions of randomly selected particles permanently. We demonstrated this idea computationally and sampled an ideal glass state through the combination with parallel tempering simulations [1]. ii) Swap Monte-Carlo (MC) algorithm: We developed an extremely efficient simulation scheme applying particle-swap MC updates for models with continuous size polydispersity. This scheme is more than 10 orders of magnitude efficient than the standard MC simulations and allows us to investigate extremely deep supercooled liquid state relevant for the ideal glass transition [2].

In this talk, I will introduce the above-mentioned question/theoretical scenarios, and present our recent numerical investigations to answer the question.

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Population size and interaction structure driven by mutant interactors

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Spontaneous random mutations are an important source of variation in populations. Many evolutionary models consider mutants with a fixed fitness, chosen from a fitness distribution without considering microscopic interactions among the residents and mutants. Here, we go beyond this and consider "mutant interactors," which lead to new interactions between the residents and invading mutants. We model microscopic interactions between individuals by using a dynamic interaction matrix, the dimension of which increases with the emergence of a new mutant and decreases with extinction. The new interaction parameters of the mutant follow a probability distribution around the payoff entries of its ancestor. These new interactions can drive the population away from the previous equilibrium and lead to changes in the population composition. Thus, the population composition is an evolving property rather than an externally controlled variable. We calculate how the population size changes over time [1] and how the interaction structure evolves in the high mutation regime.

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Controlling active matter with curvature and topology

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Active nematic liquid crystals are achieved experimentally by combining high concentrations of microtubules, kinesin and ATP. These active nematic suspensions can then be localized to a 2D interface, such as the surface of a water droplet suspended in another medium. We will discuss the distribution of topological defects within an active nematic liquid crystal confined to the surface of a toroidal water droplet. Due to the topology of the surface, it is possible to coat a torus in a nematic material with no topological defects. When the activity of the nematic is sufficiently high, topological defects will spontaneously form, but they must preserve the net topological charge of the system, which is zero. Through experiment and simulation we confirm that the local distribution of topological defects is proportional to the Gaussian curvature. As the activity of the system is increased the reliance on the Gaussian curvature is diminished and the available area on different regions of the torus dictates the behaviour.

Non equilibrium importance sampling with a driven dynamics

Grant Rotskoff

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Non equilibrium sampling is potentially much more versatile than its equilibrium counterpart, but it comes with challenges because the invariant distribution is not typically known when the dynamics breaks detailed balance. Here, I will discuss a generic importance sampling technique that leverages the statistical power of configurations transported by non equilibrium trajectories, and can be used to compute averages with respect to arbitrary target distributions. The method can be viewed as a generalization of the annealed importance sampling (AIS) method and the related Jarzynski equality. Unlike AIS, our approach gives an unbiased estimator, with provably lower variance than directly estimating the average of an observable. We also establish a direct relation between a dynamical quantity, the dissipation, and the volume of phase space, from which we can compute quantities such as the density of states and Bayes factors. I will illustrate the properties of estimators relying on this sampling technique in the context of density of state calculations, showing that it scales favorable with dimensionality---in particular, I will show that it can be used to compute the phase diagram of the mean-field Ising model from a single non equilibrium trajectory. I will also demonstrate the robustness and efficiency of the approach with an application to a Bayesian model comparison problem of the type encountered in astrophysics and machine learning.

Spin-glass-like dynamics in highly compressed colloidal and granular glasses

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In my talk, I will discuss the off-equilibrium dynamics of colloidal or granular glasses at high pressures. I will show evidences of the existence of a sharp threshold in pressure, deep in the glass phase, above which the dynamics become highly anomalous displaying very large equilibration time scales, aging, and a constantly increasing susceptibility. I will also discuss that this situation is strongly reminiscent of the one observed in three-dimensional spin-glasses in an external magnetic field. Both results, support the mean field prediction of the existence of a Gardner phase transition between a "normal glass" and a "marginally stable glass", and confirm the theoretical expectations about its universality class.

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Active-passive polymer mixtures in relation to chromatin conformation and dynamics

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Mixtures of identical particles maintained at different temperatures, arrive at phase-separated steady states for large temperature ratios [1,2]. If the particles are polymers the critical temperature ratio decreases with polymer length, which allows to reach the energy scales relevant for microphase separation of active and passive chromatin segments [3]. I will discuss also other interesting non-equilibrium phenomena in active-passive polymer mixtures and their similarities to equilibrium physics [4].

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Correlations and collective behaviours in suspensions of swimming microorganisms

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Many microorganisms, such as bacteria and algae, have developed swimming strategies to aid them in search for food in their aqueous environments. From a hydrodynamic perspective, these organisms are interesting since swimming on the micron scale is radically different from in the macroscopic world, due to the absence of fluid inertia. Two intriguing hydrodynamic phenomena occurring in suspensions of swimming microorganisms are the transition to so-called ``bacterial turbulence'', whereby bacterial suspensions of sufficiently high density exhibit large-scale flocks and coherent flows, and the enhanced diffusion of passive tracer particles compared to the expected value from Brownian motion alone. In this talk, I will present results obtained from large-scale lattice Boltzmann simulations of a simple model of hydrodynamically interacting microswimmers that capture both these phenomena accurately enough to draw quantitative conclusions. The results will furthermore be compared to analytical predictions from a stochastic kinetic theory of microswimmer suspensions that goes beyond mean-field, and thus takes into account swimmer-swimmer correlations, showing their importance even far below the transition to bacterial turbulence.

Structural-dynamical correlations and rigid response

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Glass-forming liquids are globally disordered but show emergent signatures of local structural reorganisation in the supercooled regime, that can be observed in colloidal experiments [1] and predicted via liquid state theory [2]. We show that employing an approach rooted in the thermodynamics of trajectories, time-integrated structural observables correlate with slow dynamics. In particular, we reveal a temperature-dependent phase transition between liquid and arrested trajectories which are respectively poor and rich in local structure [3,4]. The energy landscape of the liquid splits into a high entropy and a low entropy metabasin. Mechanically probing the two basins in numerical simulations at zero temperature, we show that the increase in local structure corresponds to an enhanced rigid response, mostly localised in well-equilibrated, long-lived structural motifs [5].

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Non-equilibrium and critical behaviour in biological microswimmers

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Biological microswimmers navigate complex micro-environments using slender propulsion-generating appendages, which exemplify diverse strategies for overcoming reversibility of locomotion at low Reynolds number. In the case of bacteria, these arise in the form of rigid helices, which are actuated by a rotary mechanism, while algal flagellates such as Chlamydomonas propagate rhythmic, coordinated bending waves of activity to pull themselves through the fluid. Increasingly, certain biopolymers inside these free-living unicellular organisms have been implicated in the active coordination of multiple motile appendages. We focus on model algal flagellates and their robust yet changeable swimming dynamics to reveal the extent to which gait-control of motility exhibits highly non-equilibrium features, and suggest that this departure from equilibrium allows such microswimmers to achieve a heightened level of sensitivity than might otherwise have been possible.

Trip Centrality: walking on a temporal multiplex with non-instantaneous link travel time

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In complex networks, centrality metrics quantify the connectivity of nodes and identify the most important ones in the transmission of signals on the network. In many real world networks, especially in transportation systems, links are dynamic, i.e. their presence depends on time, and travelling between two nodes requires a non-vanishing time. Additionally, many networks are structured on several layers, representing, e.g., different transportation modes, service providers, or lines of a transportation service. Temporal generalisations of centrality metrics based on the counting of walks on the network, like Katz centrality, exist, however they do not account for non-zero link travel times and for the multiplex structure. We propose a generalisation of Katz centrality, termed Trip Centrality, counting only the walks that can be travelled according to the network temporal structure, i.e. "trips", while also differentiating the contributions of inter- and intra-layer walks to centrality. In particular, the introduction of one secondary node per link allows to describe the non-zero travel time between two (primary) nodes as the residence time in the secondary node, while still using a formulation with null link travel time. Additionally, considering a copy of each node for each layer and introducing a weight for links between copies on different layers permits to weight differently intra- and inter-layer walks, reflecting the level of interaction of the layers. We show an application to the US air transport system, specifically computing airports' centrality losses due to delays in the flight network.

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