Abstracts of Invited Talks

Gareth Alexander University of Warwick

Dynamics of Defects in Shells of Active Nematics

Active liquid crystals are a novel form of biologically inspired materials in which microscopic hydrolysis of ATP generates bulk fluid flows and drives macroscopic non-equilibrium dynamics. We describe the macroscopic dynamics of shells of active nematics within a thin film approximation in terms of the flows created by defects in the nematic director and the consequent motion of the latter. At low values of the activity we reproduce the oscillatory dynamics of four +1/2 defects between tetrahedral and planar configurations seen in recent experiments [Keber et al. Science 345, 1135 (2014)]. At higher activity there is flow induced attraction and coalescence of the like-charge defects. +1 defects may further coalesce to a single +2 defect depending on their distortion type. Finally, we show how the surface flows generated by the active nematic lead to squirming motion of the drop and describe the bulk flows that are created. This is joint work with Diana Khoromskaia.

Hans C. Andersen Stanford University

Why is the Verlet algorithm so useful for molecular dynamics simulations?

Eva Y. Andrei Rutgers University

Artificial Atom at a Supercritically Charged Vacancy in Graphene

Graphene is known for its many superlatives, but some of its notable properties are transformed in the presence of defects. I will discuss the effect of single atom vacancies on graphene's magnetic and electronic properties as revealed by scanning tunneling microscopy and spectroscopy1.

1 J.Mao, Y.Jiang, D.n Moldovan, G. Li, K. Watanabe, T. Taniguchi, M. R. Masir, F.M. Peeters, E.Y. Andrei, Tunable Artificial Atom at a Supercritically Charged Vacancy in Graphene, Nature Physics 2016, doi:10.1038/nphys3665

Igor Aronson Argonne National Lab and Northwestern University

Computational model of substrate-based cell motility

Cell motility and collective migration are among the most important themes in cell biology, mathematical biology, and bioengineering, and crucial for morphogenesis, wound healing, and immune response in eukaryotic organisms. It is also relevant for the development of effective treatment strategies for diseases such as cancer, and for the design of bioactive surfaces for cell sorting and manipulation. Substrate-based cell motility is, however, a very complex process as regulatory pathways and physical force generation mechanisms are intertwined.

To understand the interplay between adhesion, force generation and motility, we propose a computational model based on the phase field method, which is especially suited to treat the moving and deformable boundaries involved in both individual and collective cell motility. We investigate by the means of large-scale GPU computations how cells navigate on substrates with patterned adhesion properties and modulated stiffness, situations currently under technological development to collect or sort cells. For multiple cells, the model is able to predict that collective cell migration emerges spontaneously as a result of inelastic collision-type interactions of cells. In the conclusion, I will discuss possible future extensions of the modeling framework and its applications.

Angelo Bassi University of Trieste

Models of spontaneous wave function collapse: an update

Models of spontaneous wave function collapse (collapse models) modify the Schrödinger equation by including nonlinear and stochastic terms, which describe the collapse of the wave function in space. These spontaneous collapses are "rare" for microscopic systems, hence their quantum properties are left almost unaltered. At the same time, they become more and more frequent, the larger the object, to the point that macroscopic superpositions are rapidly suppressed. I will briefly review the main features of collapse models. Next I will present an update of the most promising ways of testing them in interferometric and non-interferometric experiments.

Bruce Berne Columbia University
TBA

Peter Bolhuis University of Amsterdam
Surprises in patchy particle association

Francesco Cellarosi Queen's University
Autocorrelation functions for quantum particles on a nilmanifold
The ergodic properties of Heisenberg nilflows are well understood, and the mixing properties of time-changes of such flows were recently described by Avila, Forni and Ulcigrai. Instead of classical flows, we consider quantum particles moving freely in a Heisenberg nilmanifold, and study their autocorrelation function. Our main result is a limiting theorem for the autocorrelation function (at random time) for particles that are a superposition of N eigenmodes, as N tends to infinity. Our methods use some recent results of J. Marklof and the speaker.

Paul Chaikin New York University
Random Organization, Hyperuniformity and Photonic Bandgaps
A periodically sheared non-Brownian suspension undergoes collisions which allow the particles to explore new configurations. Below a critical strain the system evolves and arranges itself until collisions no longer occur and an absorbing state is reached. A simple model "Random Organization" well describes the process. We have studied similar phenomena in granular systems where limit cycles rather than reversible paths are found as absorbing states. Recent work by Hexmer and Levine show that at criticality absorbing state systems produce hyperuniform particle correlations. Together we have most recently found that reactivating, "kicking", the absorbing state leads to hyperuniformity approaching that of a crystal but with no periodicity or long range order.

Arup K. Chakraborty Massachusetts Institute of Technology
Statistical mechanical problems at the interface of virology and immunology
No medical procedure has saved more lives than vaccination. But, today, some pathogens have evolved which have defied successful vaccination using the empirical paradigms pioneered by Pasteur and Jenner. HIV is a prominent example, and over 60 million people have been infected by this scourge on the planet. I will describe how bringing together approaches from statistical physics with basic/clinical immunology is beginning to confront this challenge. In particular, I will describe how the pertinent problems at the intersection of immunology and evolutionary biology can be addressed by such approaches, and why the conceptual framework of statistical mechanics is a key to rational design of vaccines against highly mutable pathogens.

Gavin Crooks
On the thermodynamics of strongly coupled systems

I'll talk about the non-equilibrium thermodynamics of a pair of driven systems that are strongly coupled to one another. If we look at the problem in the right way, we get deceptively simple expressions for the local entropy production, local fluctuation theorems, and local second laws. These expressions subsume feedback fluctuation theorems and various other special cases.

Christoph Dellago University of Vienna

Simulating water and ice with neural network potentials

While the interactions between water molecules are dominated by strongly directional hydrogen bonds, it has become clear that the relatively weak, isotropic van der Waals forces are essential for understanding the properties of liquid water and ice. This insight was mostly gleaned from ab initio computer simulations, which provide an unbiased description of water at the atomic level and yield information on the underlying molecular forces. However, the high computational cost of such simulations prevents the systematic investigation of the influence of van der Waals forces on the thermodynamic anomalies of water. In my talk, I will report on a neural network potential we have recently developed for liquid water and ice. This approach, in which reference data obtained from electronic structure calculations are used to train a neural network for the prediction of energies and force, yields the accuracy of ab initio simulations at a fraction of their cost. Using neural network potentials parametrized for several density functionals with and without van der Waals corrections, we have shown that van der Waals interactions are crucial for the formation of water's density maximum and its negative volume of melting. Both phenomena can be explained by the flexibility of the hydrogen bond network, which is the result of a delicate balance of weak van der Waals forces, causing a pronounced contraction of the second solvation shell upon cooling that induces the density maximum.
Joint work with Jörg Behler, Tobias Morawietz, and Andreas Singraber

Colin Denniston University of Western Ontario

Hydrodynamic Effects on Confined and Adsorbed Polymers

Hydrodynamics can have a profound effect on the dynamics of confined and adsorbed polymers, but including them in a theory or simulation can be very challenging and costly, leading to many simplifications. Problems arise when different simplifications lead to contradictory results. For example, simulations of polymers near attractive surfaces using Langevin dynamics typically find adsorption is enhanced by shear flow, whereas simulations using hydrodynamic interactions implemented at the Rotne-Prager-Blake level (multipole-like expansion) find desorption is enhanced by shear flow. Experiments on the other hand appear to have seen both results, and in some cases an enhanced adsorption rate under strong shear that is absent at low shear rates. I will first discuss our hybrid Lattice-Boltzmann (LB) molecular dynamics (MD) scheme that elastically couples the LB-fluid to the MD-particle nodes. Then our work using the method to examine polymers confined between parallel plates in the presence and absence of hydrodynamic interactions. Finally, I will describe our recent work on the effect of shear on polymers adsorbed onto molecularly flat surfaces.

Carl Dettmann Bristol University

Spatial networks with random connections

Many networks of current interest have a spatial structure, in that the nodes and/or links are located in physical space. Examples include climate, communications, infrastructure, nanowire, neuronal and transport networks. An early and still popular model of spatial networks is the random geometric graph, where nodes are located randomly and links formed between sufficiently close nodes. Recent studies have considered random connection models, in which there is a link probability depending on distance. Applying Laplace's method to relevant multidimensional integrals, we find that the overall connection probability can be estimated from just a few moments of the link probability function for a wide variety

of domain geometries. Furthermore, there are qualitative differences as a result of the random connections. In particular, the more realistic model allows a more accurate estimation of connectivity and resilience than the original.

Jorn Dunkel Massachusetts Institute of Technology

Bacterial spin lattices

Despite their non-equilibrium nature, living systems can self-organize in highly ordered collective states that share notable similarities with the thermodynamic equilibrium phases of conventional condensed-matter and fluid systems. Through microfluidic experiments and mathematical modelling, we will demonstrate that lattices of hydrodynamically coupled bacterial vortices can spontaneously organize into distinct patterns characterized by ferro- and antiferromagnetic order. The coupling between adjacent vortices can be controlled by tuning the inter-cavity gap widths. The emergence of opposing order regimes is tightly linked to the existence of geometry-induced bacterial edge currents. Our experimental observations can be rationalized in terms of a generic lattice field theory, suggesting certain analogies with classical spin systems.

Massimiliano Esposito University of Luxembourg

Dynamics and thermodynamics of open chemical networks

Open chemical networks (OCN) are large sets of coupled chemical reactions where some of the species are chemostated (i.e. continuously restored from the environment). Cell metabolism is a notable example of OCN. Two results will be presented. First, dissipation in OCN operating in nonequilibrium steady-states strongly depends on the network topology (algebraic properties of the stoichiometric matrix) [1]. An application to oligosaccharides exchange dynamics performed by so-called D-enzymes will be provided [2]. Second, at low concentration the dissipation of OCN is in general inaccurately predicted by deterministic dynamics (i.e. nonlinear rate equations for the species concentrations). In this case a description in terms of the chemical master equation is necessary. A notable exception is provided by so-called deficiency zero networks, i.e. chemical networks with no hidden cycles present in the graph of reactant complexes [3].

[1] M. Polettini and M. Esposito, J. Chem. Phys. 141, 024117 (2014)
[2] R. Rao, D. Lacoste and M. Esposito, J. Chem. Phys. 143, 244903 (2015)
[3] M. Polettini, A. Wachtel and M. Esposito, J. Chem. Phys. 143, 184103 (2015)

Daniel Fisher Stanford University

Evolutionary Dynamics in High Dimensions

Michael Fisher University of Maryland

TBA

Juan P. Garrahan University of Nottingham

Trajectory vs overlap and pinning transitions in glasses

The central theoretical debate in the glass transition field is whether the slowdown and eventual arrest of glass forming systems is at its origin a purely dynamical phenomenon, as posed for example by dynamical facilitation (DF) theory, or a thermodynamic one, as posed for example by the random first-order transition theory (RFOT). Evidence of the former, as predicted by DF, are a novel class of non-equilibrium transitions in ensembles of trajectories of the dynamics (as revealed by dynamical large-deviation methods), while evidence of the latter, according to RFOT, are static transitions in systems coupled and/or randomly pinned to reference configurations. While these are apparently fundamentally different approaches to metastability, I will discuss possible connections between them, and consider broader implications to the glass transition problem.

William Gelbart UCLA chemistry

What makes RNA genomes special? A search for the "hydrogen atom of viruses

Viruses are the only evolving organisms which have RNA instead of DNA genomes. And the large majority of RNA viruses have single-stranded instead of double-stranded genomes, and experience their full life cycle in the cytoplasm of their host cell, never needing to get in and out of the nucleus. Further, single-stranded RNA behaves effectively as a flexible, branched, polymer and is a much more compact physical object than double-stranded DNA, which is a well-characterized stiff, linear, polymer. Finally, these RNA viruses include the "hydrogen atom of viruses" -- ones involving, in principle, as few as two genes.

Subhro Ghosh Princeton University

Rigidity phenomena in particle systems

In several naturally occurring particle systems, we establish that the number of the particles inside a bounded region is completely determined by the particle configuration outside the region. This includes key examples coming from the one component plasma, random matrices and zeros of random polynomials.

Alex Greer Brooklyn College

Human Rights and Responsibility of Scientists

The talk will be aimed at human rights abuses of scientists around the world. Cases that the Committee of Concerned Scientists (CCS) work on will be discussed, including the deteriorating situation of our colleagues in Turkey.

David Huse Princeton University

The many-body localization phase transition

I will give an overview of our present understanding of the many-body localized phase and of the novel dynamical quantum phase transition between many-body localization and thermalization.

Tuomas Knowles University of Cambridge

Kinetics of protein filament formation

The self-assembly of protein molecules into linear structures is a process that underlies the formation of functional filaments such as actin and tubulin, as well as generally dysfunctional ones such as amyloid aggregates. This talk outlines our efforts to understand the kinetics of such assembly phenomena. We use a master equation formalism to capture the dynamics of a protein system undergoing self-assembly into filaments, and use an array of approaches, including Hamiltonian mechanics and self-consistent field theories to provide closed form integrated rate laws for the overall time evolution. We will discuss the implications of these results for relating experimental measurements of protein aggregation to the underlying microscopic mechanisms.

Halim Kusumaatmaja University of Durham

Analyzing the free energy landscapes of soft matter systems

In this contribution, I will describe a suite of methods designed to efficiently characterize the energy landscapes of continuum, Landau-type free energy models. Using wetting morphologies of liquid droplets on structured surfaces, shapes of lipid membranes and a multistable liquid crystal device as applications, I will show that the methods allow systematic study of not only the most relevant minimum energy configurations, but also the transition pathways between any two minima, as well as their corresponding energy barriers and transition state configurations. Furthermore, a global view of the free energy landscapes can be visualized using either a disconnectivity graph or a network representation. Different forms of functionals and boundary conditions can be readily implemented, thus allowing these tools to be utilized for a broad range of problems.

Albert Libchaber Rockefeller University

Life at low Reynolds number and large Peclet number

Some soil microbes use decomposition to get their energy, oxidizing sulfur. To increase oxygen flow through water, those microbes apply strong hydrodynamic advection of water, a large Peclet number.

The two microbes involved are Eukaryote (a ciliate Uronemella) and a Prokaryote (the bacterium Thiovulum). They both have a fast velocity, close to 0.5 mm/sec, and a comparable size, around 10μm. Their Reynolds number is still low. They both can tether to boundaries and can produce veils on which they attach. They also store sulfur.Their phenotypes are thus surprisingly comparable; in a given environment nature can evolve different organisms with similar phenotypes! The interaction between the microbes is purely hydrodynamic, each acting as a small vortex and pumping water when they are tethered. The forming veils move at constant velocities and are non-linearly unstable (for Uronemella). It also leads to fascinating bacteria crystal formation and various dynamical system modes when in finite size (for Thiovulum).

Those earth microbes shape the world around us, contributing to the soil ecosystem.

David Limmer Princeton University

Phase separation in photo-excited solid state materials

Erik Luijten Northwestern University

Dynamic Collective Behavior and Phase Separation of Active Colloids

Suspensions of active colloidal particles have emerged as prototypical systems for the investigation of collective phenomena that can be either static or dynamic in nature. Here, I will demonstrate how induced many-body interactions result in unexpected and until now unexplored aggregation and phase behavior. These observations, obtained through a combination of experiments and computer simulations, reveal striking connections between colloidal self-assembly and collective dynamics, and between dynamic behavior and classical thermodynamics. Moreover, a remarkable variety of collective dynamics can be realized in a single system merely by variation of the external electric field.

Jonathan Machta University of Massachusetts Amherst

Population Annealing: Theory and Application to Glassy Systems

Population annealing is an efficient sequential Monte Carlo algorithm for simulating equilibrium states of systems with rough free energy landscapes. I will describe the algorithm and discuss its convergence to equilibrium. Results from large-scale simulations of the 3D Edwards-Anderson (Ising) spin glass will be presented and implications for the low temperature spin glass phase will be discussed. I will also present preliminary results from simulations of dense binary mixtures of hard spheres.

Lawrence Pratt Tulane University

Concentration dependence of the Flory-Huggins interaction parameter in aqueous solutions of capped PEO chains

The dependence on volume fraction of the Flory-Huggins interaction parameter describing the free energy of mixing of polymers in water is obtained by exploiting the connection to the chemical potential of the water, for which quasi-chemical theory is satisfactory. We test this theoretical approach with simulation data for aqueous solutions of capped PEO oligomers. Consistent with experiment, this constant is determined to be strongly concentration dependent. These results predict phase separation that is supported by direct observation of the coexistence of the two solutions on simulation time scales. This approach directly provides the osmotic pressures. Reflecting repulsive interactions between the chains in the water, a good solvent for these chains, the osmotic second virial coefficient for the chains is positive.

Sidney Redner Santa Fe Institute

Starvation Dynamics of a Dumb Forager

What is the fate of a forager that depletes its environment as it wanders? We investigate this question within the "starving" random walk model in which a random walk starves when it travels S steps without eating. The forager consumes food whenever it is found and the walk is fully sated. When the walker lands on an empty site, the time until starvation decreases by 1. We determine the lifetime of the walker, analytically in one dimension and numerically in higher dimensions. In two dimensions, long-lived walks explore a highly ramified region so as to remain close to food.

We also investigate the role of intelligence, in which, the walker preferentially moves towards food when the walker is at the interface between food and empty sites. Paradoxically, the average lifetime of the walker can have a non-monotonic dependence on intelligence, with a different sense to the non-monotonicity in one dimension and in higher dimensions.

Yasser Roudi Norwegian University of Science and Technology

Learning and inference when there is little data

When building models for complex systems, in many cases, we face two major problems: (1) how to choose relevant variables amongst many possible degrees of freedom, and (2) once we have chosen the relevant variables, how can we build meaningful statistical models for them? These questions have attracted a lot of attention in recent years in statistical mechanics and machine learning communities and are particularly important in cases where the possible degrees of freedom are much larger than the number of data points available as samples from the system. Examples of such cases include recordings from neuronal networks where only few neurons (compared to the whole network) can be observed for a relatively short period of time (compared to the size of the phase space), financial networks, etc. In this talk, I will discuss some novel approaches to answering these questions. I will first describe a method for selecting relevant variables which are likely to carry meaningful information about what a system is doing, using a small number of observations from the system [1]. I will then describe a Bayesian model selection method for learning a sparse graphical model, namely an Ising model with sparse interactions [2], that differs from existing methods for sparse model selection in several key aspects.

Refs. 1. Marsili, M., Mastromatteo, I., & Roudi, Y. (2013). On sampling and modeling complex systems. Journal of Statistical Mechanics: Theory and Experiment, 2013(09), P09003.

2. Bulso, N., Marsili, M., & Roudi, Y. (2016). Sparse model selection in the highly under-sampled regime. arXiv preprint arXiv:1603.00952.

Eric Siggia Rockefeller University

Geometric models and a phase diagram for developmental biology

Frank Stillinger Princeton University

Molecular Model for Chiral Symmetry Breaking

The basic role of dominant molecular chirality in terrestrial biochemistry invites statistical mechanical modeling of how it could have initially appeared. The specific approach to be described involves a three-dimensional continuum model with flexible tetrameric molecules possessing mirror-image stable geometries. Molecular dynamics results for this model's condensed phases reveal spontaneous chiral symmetry breaking in both liquid and crystalline states.

Julian Talbot Université Paris VI

First passage times in heterogeneous media

Much of the published work on mean first-passage times (MFPTs) neglects the diffusive heterogeneity that is present in fields as diverse as biophysics, ecology and economics. For example tumors are typically heterogeneous and animals forage for food or mates in patchy environments. We present exact analytical expressions for the MFPT and residence times of a point-like particle diffusing in a spherically symmetric d-dimensional heterogeneous system composed of two concentric media with different diffusion coefficients with an absorbing inner boundary (target) and a reflecting outer boundary. By varying the convention, e.g., Itō, Stratonovich, or isothermal, chosen to interpret the overdamped Langevin equation with multiplicative noise describing the diffusion process, we find different predictions and counter-intuitive results for the residence time in the outer region, and hence for the MFPT, while the residence time in the inner region is independent of the convention.

Bruce Turkington University of Massachusetts Amherst

Optimal closure for nonequilibrium statistical models

We propose an optimization-based approach to the general problem of deriving closed reduced equations for macrovariables, or relevant observables, from an underlying microdynamics. The key idea is to view a macroscopic description as a space of trial probability densities on phase space, to evaluate the residual in the Liouville equation of any feasible path of such densities, and to quantify this Liouville residual using the natural metric suggested by information theory. An optimal path is then a macroscopic evolution which best fits the microdynamics. The equations governing optimal paths have the "generic," or "metriplectic," structure of nonequilibrium thermodynamics, with a dissipation potential that solves the Hamilton-Jacobi equation associated with the optimization principle. To illustrate this method we coarse-grain a spectrally-truncated turbulent flow and test the optimal closure against fully-resolved simulations of ensembles.

Suriyanarayanan Vaikuntanathan University of Chicago

Topologically protected modes in biological systems