# CPP 51: Complex Fluids and Soft Matter (joint session DY/CPP)

Time: Friday 9:30–12:15 Location: BH-N 243

CPP 51.1 Fri 9:30 BH-N 243

**Percolation in Suspensions of Rod-like Colloids under Shear Flow** — •Victor Tänzel, Fabian Coupette, and Tanja Schilling — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

Suspensions of electrically conductive fillers are an interesting class of material for applications in energy storage and sensor technology. Their practicality depends on the behavior of the fillers, which is intricate and complex for elongated particles in flow.

We use multi-particle collision dynamics (MPC) to model rod-like particles in shear flow of a hydrodynamic medium. Percolation and conductivity are characterized with regard to the system's properties. MPC also allows us to turn off the hydrodynamic interactions from the solvent, so we can assess their influence.

CPP 51.2 Fri 9:45 BH-N 243

**orientational order and topological defects in a dilute solutions of rodlike polymers at low reynolds number** — •Leonardo Puggioni[1,2], Stefano Musacchio[1], and Guido Boffetta[1] — [1]Dipartimento di Fisica and INFN, Università degli Studi di Torino, via P. Giuria 1, 10125 Torino, Italy — [2]Instituut-Lorentz, Leiden Institute of Physics, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands

The relationship between the polymer orientation and the chaotic flow, in a dilute solution of rigid rodlike polymers at low Reynolds number, is investigated, by means of direct numerical simulations. It is found that the rods tend to align with the velocity field in order to minimize the friction with the solvent fluid, while regions of rotational disorder are related to strong vorticity gradients, and therefore to the chaotic flow. The "turbulent-like" behavior of the system is therefore associated to the emergence and interaction of topological defects of the mean director field, similarly to active nematic turbulence. The analysis has been carried out both in two and three spatial dimensions.

CPP 51.3 Fri 10:00 BH-N 243

**Phase Behaviour of Hard Convex Particles** — •Poshika Gandhi and Anja Kuhnhold — Institute of Physics, University of Freiburg, Germany

The shape of a particle has a significant influence on its phase behaviour. A simple uniaxial particle, like a spherocylinder, produces a larger variety of phases as compared to a sphere. From the existence of the biaxial nematic phase to the search for a polar nematic one, simulations of hard particles of different shapes and symmetries continue to invoke interest.

We used Monte Carlo NVT simulations to produce phase diagrams of convex biaxial particles with both chiral and achiral compositions. The effect of particle shape on the phase behaviour and the effect of initial configurations on particles with $C_{2v}$ symmetry was analysed. The results show generalised behaviour across particles of varying shapes and sizes which betters our understanding of the entropic forces in simulations of hard particles.

CPP 51.4 Fri 10:15 BH-N 243

**Stochastic rotational dynamics of strongly coupled superparamagnetic particles** — •Andrey Kuznetsov[1], Sofia Kantorovich[1], Vladimir Zverev[2], and Ekaterina Elfimova[2] — [1]University of Vienna, Vienna, Austria — [2]Ekaterinburg, Russia

We report a theoretical study of the rotational dynamics of interacting superparamagnetic nanoparticles in time-varying magnetic fields. The research is motivated by an increasing interest in biomedical applications of magnetic nanoparticles (such as cancer hyperthermia or magnetic particle imaging). We consider an ensemble of spherical single-domain particles with a uniaxial crystallographic anisotropy. Particles are uniformly distributed in a 3D space, while their easy axes are either co-aligned or distributed at random. We develop a mean-field approach that allows one to describe the dynamics of the system magnetization under oscillating field of arbitrary frequency and magnitude. To test the validity of the theory, its predictions are compared to Langevin dynamics simulations. It is shown, that if the energy of dipolar interactions is comparable to the energy of thermal fluctuations, the theory works well in wide ranges of particle concentrations and anisotropy constants. However, at lower temperatures the agreement breaks down. In particular, for isotropic nanoparticles our theory predicts a Debye-like susceptibility spectrum with a single relaxation time. In simulations we instead observe an emergence of a uniform band of relaxation times, that broadens with the increase of dipolar coupling parameter.

CPP 51.5 Fri 10:30 BH-N 243

**Nonequilibrium evolution in long-range attractive systems: initial state dependence and averaging in simulations and theory** — •Johannes Bleibel[1] and Martin Oettel[2] — [1]Fachbereich Physik, Universität Tübingen, Tübingen, Germany — [2]Institut für angewandte Physik, Universität Tübingen, Tübingen, Germany

We investigate the dynamics of the so–called capillary collapse of colloidal particles trapped a fluid interface with 1D Brownian Dynamics (BD) simulations and Dynamical Density Functional Theory (DDFT). Interfacially trapped, micrometer–sized colloidal particles interact via long–ranged capillary attraction. The interaction is formally analogous to screened Newtonian gravity with the capillary length $\lambda$ as the tuneable screening length. Within intensive studies of the dynamics in 2D, it turned out that radially averaged DDFT only captures the dynamics at initial times and largely deviates from simulation results later on. This discrepancy has been traced to the role of an initially averaged configuration in DDFT[1].

In order to shed light on the precise role of initial fluctuations in the averaging process and subsequent dynamics both in BD simulations and DDFT, we investigate the dynamics of infinitely long rods trapped at a fluid interface and thus study the dynamics of a long–ranged attractive 1D fluid under a temperature quench. We apply several distinct averaging recipes for initial conditions and noise and discuss possible effects of averaging in an alternative description using Power Functional Theory (PFT).

[1] Bleibel, Domínguez, Oettel, JPCM 28, 244021 (2016)

**15 min. break**

CPP 51.6 Fri 11:00 BH-N 243

**Towards a standard model of liquid matter** — •Alessio Zaccone — University of Milan, Department of Physics, 20133 Milan, Italy — Institute of Theoretical Physics, University of Göttingen, Germany

Our understanding of liquid matter made a leap in 20th century physics thanks to the successful mathematical and numerical development of pair correlation functions, which gave unprecedented insights into the structure of liquids. The same is however not true for the dynamical, mechanical and thermodynamic properties of liquids. The most striking example is the inability of celebrated theories to explain the specific heat of liquids or the propagation of acoustic waves in liquids as they are observed experimentally or in simulations. This of course includes the emergence of rigidity as a function of frequency of mechanical oscillation or as a function of confinement, and the Maxwell interpolation between viscous (Newton) and elastic (Hooke) limits, which has remained largely an empirical assumption in many theories of liquids and supercooled liquids, from generalized hydrodynamics to mode-coupling theory. In my talk I will show that these open issues can be understood mechanistically, and in comparison with experiments, by combining advances from different conceptual frameworks: i) the Instantaneous Normal Modes theory of liquid dynamics, and iii) the nonaffine response theory of liquids and glasses [1-3]. [1] A. Zaccone, "Theory of Disordered Solids", Springer, 2023, [2] A. Zaccone, Phys. Rev. E 108, 044101 (2023), [3] K. Trachenko and A. Zaccone, PNAS 117 (33) 19653-19655 (2020).

CPP 51.7 Fri 11:15 BH-N 243

**Dilute gel networks vs. clumpy gels in colloid-polymer mixtures** — Matthias Gimperlein and •Michael Schmiedeberg — Inst. für Theor. Phys. 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The formation of gels differs from the behavior observed in other slowly relaxing systems [1,2]. A simple system to explore gelation is a colloid-polymer mixture, where there are complex heterogeneous phases due to the competition of short-ranged repulsions, depletion attractions, and longer-ranged screened Coulomb repulsions.

Here we study the differences of dense clumpy gels and dilute gel networks in terms of dynamics and structure formation. For example,

we apply reduction algorithms [3,4] and observe that dilute and dense structures differ in the way structural properties like the typical thickness of the strands emerge. We also analyze the percolation behavior [5] and the formation of pentagonal bipyramids (as in [1]).

Finally we demonstrate that neural networks can be trained to recognize the differences between dilute gel networks and clumpy gels.

[1] H. Tsurusawa and H. Tanaka, Nat. Phys. **19**, 1171 (2023).

[2] M. Schmiedeberg, Nat. Phys. **19**, 1078 (2023).

[3] M. Gimperlein and M. Schmiedeberg, J. Chem. Phys. **154**, 244904 (2021).

[4] J. N. Immink, J. J. Erik Maris, R. F. Capellmann, S. U. Egelhaaf, P. Schurtenberger and J. Stenhammar, Soft Matter **17**, 8354 (2021).

[5] M. Kohl, R.F. Capellmann, M. Laurati, S.U. Egelhaaf, and M. Schmiedeberg, Nat. Comm. **7**, 11817 (2016).

CPP 51.8 Fri 11:30 BH-N 243

**Thermofluidic Non-equilibrium assembly of Functional Structures** — •Desmond Quinn, Diptabrata Paul, and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig

Assembly in equilibrium is dictated by static energy landscapes. Non-equilibrium assembly on the other hand is driven by fluxes that can be controlled by external energy inputs, enabling reconfigurable structures. The non-equilibrium assembly of colloids was explored here, which was mediated by optically driven heat dissipation. The heat dissipated leads to thermofluidic flows and osmotic pressures that drive the colloidal particle towards the heated regions and lead to the formation of ordered structures.

The mechanisms of assembly were disentangled, and the growth dynamics of the structures was modeled. 3D structures were found to assembly in a matter of a few minutes, and the growth dynamics was found to be dependent on the particle fluxes. Analysis of the structure revealed its crystallinity. The emergent photonic properties of such colloidal crystal structures were investigated. A photonic stopband was observed and fit well with theoretical expectations. Furthermore, the photonic property could be modulated by modulating the assembled structure. This shows that non-equilibrium processes could be useful in assembly of reconfigurable functional materials. The manipulation of bacteria was also explored, which is useful to study bacterial interactions.

CPP 51.9 Fri 11:45 BH-N 243

**Analysing seismic waves and velocities including interference effects in granular matter of volcanoes** — •Regine Frank[1,2], Marcel van Laaten[3], Birger Lühr[4], and Ulrich Wegeler[3] — [1]College of Biomedical Sciences, Larkin University, Miami, Florida, USA — [2]Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain — [3]Institut für angewandte Geowissenschaften, Friedrich-Schiller-Universitaet Jena — [4]Deutsches GeoforschungsZentrum GFZ, Helmholtz-Zentrum Potsdam

We present self consistent diagrammatic transport theory and numerical solutions for the analysis of seismic waves and velocities including interference effects in granular matter of volcanoes. We introduce weighted essentially non-oscillatory solvers (WENO) which are suitable to treat extreme non-linear properties and rogue waves. We compare our numerical results to recent experiments and several other theoretical models.

[1] A. Lubatsch, R. Frank, Phys. Rev. Research 2, 013324 (2020) [2] C. Sens-Schönfelder, U. Wegler, Geophys. Res. Lett., v. 33, no. 21, L21302 (2006) [3] U. Wegler, B.-G. Lühr, R. Snieder, A. Ratdomopurbo, Geophys. Res. Lett., v. 33, L09303 (2006) [4] C. Friedrich, U. Wegler, Geophys. Res. Lett., v. 32, L14312, (2005)

CPP 51.10 Fri 12:00 BH-N 243

**Optimal low-resolution representations as a probe of a system's emergent features** — •Raffaello Potestio — University of Trento, Trento, Italy

Gathering data from computer simulations of soft and biological matter systems is becoming increasingly easy as our available computational power keeps growing. While hoarding data is thus "easy", making sense of them is a fully different story. Here, I will illustrate how information can be extracted from data by leveraging reduced representations, that is, by looking at the system under examination in terms of a wisely chosen subset of its constituents - be these atoms, spins, pixels, or else. Taking the moves from the theory of bottom-up coarse-graining in soft matter, it is possible to show that the level of resolution at which a system is described can be leveraged as a magnifying glass to investigate its properties, and that a precise notion of optimal resolution level can be given that is tightly connected with its key emergent features.