DY 28: Poster - Complex Fluids, Granular Matter, Glasses

Time: Tuesday 18:15–21:00 Location: Poster C

DY 28.1 Tue 18:15 Poster C

Simple and efficient implementation of the Hamiltonian Adaptive Resolution Simulation (H-AdResS) scheme in LAMMPS — •Maziar Heidari, Robinson Cortes-Huerto, and Raffaello Potestio — Max Planck Institute for Polymer Research, Mainz, Germany

Computational studies of complex molecular systems often require the usage of multiscale strategies that access simultaneously various time and length scales. The Hamiltonian adaptive resolution simulation scheme (H-AdResS) is a dual-resolution simulation method that joins models with different levels of complexity for the same system within a global Hamiltonian framework. In the past, this method has been implemented in several specific-purpose softwares, in-house modifications of the GROMACS package, and, most notably, the ESPResSo++ platform.

Here we present an efficient implementation of the H-AdResS scheme in the LAMMPS simulation package. The latter is provided with simple extensions of the available potential energy functions and simulation algorithms. Minimal additions in the input files are sufficient to set up a dual-resolution simulation. The algorithmic workflow and the practical usage are explicitly discussed. This implementation is validated by studying thermodynamic properties of prototypical molecular liquids.

DY 28.2 Tue 18:15 Poster C

Thin film model of drops on soft substrates — •Johannes Kemper and Uwe Thiele — Institut für Theoretische Physik, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 9, 48149 Münster

For drops of liquid on a rigid substrate the force balance that gives the contact angle at the three phase contact line is given by the Young condition that only captures forces parallel to the substrate. However, for liquid drops on viscous soft substrates the balance is given by the Neumann condition that has a vertical and a horizontal component. For a soft substrate with elastic properties, elastic stresses (in general, non-local) have to be accounted for. Here, we present a local approximation of elastic influences that can be incorporated in a long-wave evolution equation for thin viscoelastic films and small-contact angle drops when written in gradient dynamics form. First we use the static limit of the model to determine drop profiles and analyse how the equilibrium contact angles depend on the softness of the substrate. Ridge profiles and radially symmetric drops are analysed employing numerical continuation techniques. It is shown that the simplified model reproduces experimentally observed phenomena like the formation of a wedge-shaped protrusion that is drawn out of the elastic substrate at the contact line [1]. Moreover, the dependence of the contact angle on substrate softness reproduces results of the full elastic model in [2]. These static results give a validity range of parameters for which the elastic long-wave model can be employed in time simulations. [1] T. Kajiya et al., Soft Matter, 9:454-461, 2013; [2] L.A. Lubbers et al., J. Fluid Mech., 747:R1, 2014.

DY 28.3 Tue 18:15 Poster C

Long wave modelling of osmotic spreading of biofilms — •Sarah Trinschek[1,2], Uwe Thiele[1,2], and Karin John[3] — [1]Institut für Theoretische Physik, WWU, Münster, Germany — [2]Center of Nonlinear Science (CeNoS), WWU, Münster, Germany — [3]Laboratoire Interdisciplinaire de Physique, CNRS / Université Grenoble-Alpes, Saint-Martin-d'Hères, France

Biofilms are ubiquitous macrocolonies of bacteria that develop at interfaces. Their widespread occurrence and either detrimental or beneficial function implies that it is highly important to understand the principles underlying their development. Biofilm formation starts with the attachment of individual bacteria to a surface, which then proliferate and produce a slimy polymeric matrix - two processes that result in colony growth and spreading.

Our model is based on thermodynamically consitent gradient dynamics developed for passive thin liquid mixtures. We supplement this approach by active processes (i.e. proliferation of bacteria and the secretion of polymeric matrix) that cause volume growth. Osmotic pressure gradients are generated as cells consume water and nutrient to produce biomass. This osmotic imbalance causes swelling and spreading of the biofilm through uptake of water from the moist agar substrate. We treat the system within a coarse-grained long-wave approach assuming that the thickness of the biofilm is small as compared to the typical length scale of lateral variations in film height and composition. This allows us to study the dynamics of swelling droplets with direct time simulations and analyse the front velocity of spreading biofilms.

DY 28.4 Tue 18:15 Poster C

Studying the The dynamics of polymeric liquids under time-delayed feedback — •Peter Kalle and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

Soft materials or complex fluids strongly respond to external fields and thereby show prominent non-equilibrium structure formation. Applying control strategies to shape and engineer the flow of liquids on the micron scale virtually is an unexplored field.

We study the dynamics of the Oldroyd B model, a nonlinear model to treat the dynamics of polymeric liquids, under the influence of time-delayed feedback schemes in the limit of low Reynolds numbers.

Experiments with polymeric liquids in channel flows at low Reynolds numbers have recently demonstrated that a nonlinear bifurcation towards a fluctuating flow field occurs [1]. Hence, we study the impact of time-delayed feedback schemes on a channel flow. Furthermore, as the curvature of a geometry is linked to linear elastic instabilities [2], we present first results for controlling Taylor-Couette flow as in [3] and also address the circular geometry of [4] without inner cylinder.

[1] L. Pan, A. Morozov, C. Wagner, P.E. Arratia, Phys. Rev. Lett. 110, 174502 (2013).
[2] G. H. McKinley, P. Pakdel and A. Öztekin, J. Non-Newt. Fluid Mech. 67, 19 (1996).
[3] R. G. Larson, S. G. Shaqfeh and S. J. Muller, J. Fluid Mech. 218, 573-600 (1990).
[4] M. Zeitz, P. Gurevich and H. Stark, Eur. Phys. J. E 38, 22 (2015).

DY 28.5 Tue 18:15 Poster C

Many-body critical Casimir interactions in colloidal suspensions — Hendrik Hobrecht and •Alfred Hucht — Fakultät für Physik and CENIDE, Universität Duisburg-Essen, 47048 Duisburg

We study the fluctuation-induced Casimir interactions in colloidal suspensions, especially between colloids immersed in a binary liquid close to its critical demixing point. To simulate these systems, we present a highly efficient cluster Monte Carlo algorithm based on geometric symmetries of the Hamiltonian. Utilizing the principle of universality, the medium is represented by an Ising system while the colloids are areas of spins with fixed orientation. Our results for the Casimir interaction potential between two particles at the critical point in two dimensions perfectly agree with the exact predictions. However, we find that in finite systems the behavior strongly depends on whether the Z_2 symmetry of the system is broken by the particles. We present Monte Carlo results for the three-body Casimir interaction potential and take a close look onto the case of one particle in the vicinity of two adjacent particles, which can be calculated from the two-particle interaction by a conformal mapping. These results emphasize the failure of the common decomposition approach for many-particle critical Casimir interactions.

Hendrik Hobrecht and Alfred Hucht, Phys. Rev. E 92, 042315 (2015), http://dx.doi.org/10.1103/PhysRevE.92.042315

DY 28.6 Tue 18:15 Poster C

Dissipation in sheared frictional granular media near the jamming transition — •Florian Spreckelsen, Matthias Grob, Claus Heussinger, and Anette Zippelius — Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Dense assemblies of frictional grains show reentrant flow when sheared, i.e., the system flows for high and low shear stress and jams in between. This behavior is absent in frictionless systems and signals the importance of dissipation mechanisms emerging from frictional particle interaction. We deploy molecular dynamics simulations in order to investigate the dominant contributions to dissipation near the jamming transition in two-dimensional systems.

DY 28.7 Tue 18:15 Poster C

Fracturing of a model cohesive porous medium — •Alexander Schmeink, Arnaud Hemmerle, and Lucas Goehring — Max-Planck-Institiute for Dynamics and Self-Organisation (MPIDS), 37077 Göttingen. Germany

Understanding the way cohesive porous materials fracture is essential in quantifying the mechanical contributions to phenomena like the deterioration of man-made structures, biogenic fracture of rocks, hydraulic fracture, and CO_2-Sequestration. Our goal is to characterize the fracture toughness of a cohesive porous medium in order to analyse the initiation of cracks in such situations. We designed a model porous medium made of glass beads held together by polydimethylsiloxane (PDMS). The cohesion of this medium can be controlled by curing conditions and crosslinking of the PDMS. In addition, the shape of bridges can be tuned by varying the amount of PDMS added to the beads. One advantage of this material is the fact that it can be molded into any desired shape. In order to analyze the initiation and propagation of cracks, we are conducting standard fracture toughness tests which have high requirements on the geometry of a tested specimen. We observe the fracture toughness of our material in dependence of parameters of its composition, such as polymer content, polymer composition, packing fraction, and bead diameter.

DY 28.8 Tue 18:15 Poster C

Measuring the buckling of a chain of permanent magnets under load — •Lucas Bartosch and Reinhard Richter — Experimentalphysik 5, Universität Bayreuth

A one-dimensional chain of spherical neodymium-iron-boron magnets responds to mechanical loadings in a manner reminiscent of an elastic rod, which was recently described by introducing an effective magnetic bending stiffness [1]. We are investigating the deformation of such a chain resting on a plain by means of images recorded by a digital camera. The positions of the magnets are extracted utilizing OpenCV for image processing. The distance between the two endpoints of the chain is manipulated via a computer controlled stepper motor. Moreover, the lateral force is recorded with a magnetic insensitive force gauge. We compare our quantitative results with the model proposed in [1].

[1] D. Vella, E. du Pontavice, C. L. Hall and A. Goriely, *Proc. R. Soc. A* **470**, 20130609 (2013).

DY 28.9 Tue 18:15 Poster C

The densest packing of ellipsoids — Fabian M. Schaller, •Robert F. B. Weigel, and Sebastian C. Kapfer — Theoretische Physik 1, FAU Erlangen, Germany

The relationship between local structure and macroscopic properties is a current research focus in granular matter. We study the distribution of local packing fractions (or Voronoi volumina) as a sensitive observable in order to test theoretical descriptions of such systems. Previously, mainly packings of spherical particles were considered. Here, we focus on packings of uniaxial ellipsoids as an instance of aspherical particles. In particular, we report numerical results on the locally densest packings of ellipsoids with aspect ratio between 0.7 and 1.4, generalizing the famous "kissing problem". Like in the spherical case, these packings locally exceed the density of known crystal structures. In low concentrations, distorted variations of some of these packing motifs can be found embedded in dense random packings of ellipsoids. Moreover, we find that the volume and packing fraction distributions in dense random ellipsoid packings deviate from theoretical predictions in the literature.

DY 28.10 Tue 18:15 Poster C

Flow and clogging of shape-anisotropic grains in a silo — Sandra Wegner[1], •Ahmed Ashour[1], Ralf Stannarius[1], Balázs Szabó[2], and Tamás Börzsönyi[2] — [1]Otto von Guericke University, Magdeburg, Germany — [2]Wigner Research Center for Physics, Hungarian Academy of Sciences, Budapest, Hungary

Storage of granular materials is of considerable importance in many branches of agriculture, pharmaceutics and other industrial branches. It is often realized with silos or hoppers. When grains flow out of a hopper outlet, clogging is a frequently encountered problem. We investigate such clogging events in laboratory experiments by means of 3D imaging and optical characterization techniques, and extract the structure of the dome of grains blocking outflow. Particular emphasize is laid on influences of the geometry of the grains: spherical, prolate and oblate shapes are compared. X-ray computed tomography allows the identification of positions and orientations of all individual particles in the volume. With the complete 3D information of grain positions and orientations, packing fractions and orientational ordering of the systems are calculated and compared.

DY 28.11 Tue 18:15 Poster C

Mechanical properties of sheared wet granular piles — •Anna-Lena Hippler[1], Marc Schaber[1], Somnath Karmakar[1], Mario Scheel[3], Marco DiMichiel[3], Martin Brinkmann[2], and Ralf Seemann[1,2] — [1]Experimental Physics, Saarland University, 66041 Saarbruecken, Germany — [2]MPI for Dynamics and Self-Organization, Am Faßberg 17, 37077 Goettingen, Germany — [3]European Synchrotron Radiation Facility, 6 rue Jules Horowitz, 38000 Grenoble, France

The mechanical properties of dry and wet bead packs are explored when being sheared with a parabolic profile at constant shear volume. The dissipated energy can be determined from the measured differential pressure and increases about linearly with external pressure for both dry and wet bead packs. However, the dissipated energy for wet beads has a finite value for vanishing external pressure and increases slower with external pressure compared to dry beads.

Using a downsized version of the shear cell the reorganization of beads and liquid is imaged using ultrafast x-ray micro-tomography. The movement of each bead can be tracked during the shear process. The relative movement of the beads causes the breakup of liquid capillary bridges and the liquid that was stored in the liquid bridges is redistributing within the bead pack. The contribution of the breaking capillary bridges to the dissipated energy can be quantified by directly detecting individual rupture events and analyzing the corresponding liquid bridge volumes.

DY 28.12 Tue 18:15 Poster C

Thermal conductivity and geometric cohesion in aspherical granular materials — •Katharina Staudt[1] and Thomas Grillenbeck[1,2] — [1]Ignaz-Günther-Gymnasium Rosenheim, Germany — [2]Fachhochschule Rosenheim University of Applied Sciences, Germany

Aspherical granular materials show the phenomenon of geometric cohesion, i.e. cohesion due to particle geometry. Geometric cohesion is influenced by the contacts between particles - as is the thermal conductivity of any granular material. In my study, I examined the thermal conductivity of various package fractions of U-shaped staples as radically aspherical granular material. The experiments showed an increasing thermal conductivity with increasing package fraction, without evidence for an influence of geometric cohesion on thermal conductivity. Therefore, the (trivial) positive correlation between package fraction and thermal conductivity apparently applies also to radically aspherical granular materials like U-shaped staples.

DY 28.13 Tue 18:15 Poster C

Novel readout system and online analysis of dielectric two-pulse echoes — •Andreas Schaller, Sergey Tsurkan, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg

The low temperature properties of glasses are governed by atomic tunneling systems. These tunneling systems can couple resonantly to electric fields and can be studied by phase coherent methods such as two-pulse polarization echo measurements using a reentrant cavity microwave resonator with a resonance frequency of approximately 1 GHz.

We built up a new fully automated data acquisition and analyzing system for the measurement of two-pulse polarization echoes with high accuracy. The new setup allows for measurements at shorter pulse separation-times and for a real-time frequency domain data analysis, which allows us to reject unwanted contributions to the integrated echo amplitude stemming from external disturbances. We will discuss the new setup and data acquisition system. In addition we will show results obtained for BK7 glass.

DY 28.14 Tue 18:15 Poster C

Novel LC-resonator techniques for measurements of MHz dielectric properties of glasses at very low temperatures — •Benedikt Frey, Wiebke Scholz, Guido Homann, Anne Zeissner, Annina Luck, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, 69120 Heidelberg

Many properties of amorphous solids at low temperatures can be ex-

plained with the standard tunneling model, which is based on two level-tunneling systems. Significant deviations from the standard tunneling model were observed in dielectric measurements, both in the kHz and in the GHz regime. Moreover these measurements show a strongly frequency dependent behaviour that indicate a non-phonon based thermal relaxation process.
For further investigations of the crossover into this relaxation process, we have developed novel LC-resonator based measurement setups for the MHz regime. Our current setup operating at 30 MHz allows measurements with both very low field strengths and ultra low input power, while its high quality factor also permits a determination of the dielectric loss factor.
Measurements performed on the samples HY-1, N-BK7, Herasil and PVAc show the influence of nuclear quadrupoles and long range interactions on dielectric properties of glasses in this frequency regime.

DY 28.15 Tue 18:15 Poster C

Confinement effects on binary mixtures of water and glycerol investigated by 1H and 2H NMR — •Max Schaefer, Edda Klotz, and Wida Kohshekan — Institut für Festkörperphysik, Tu Darmstadt, 64289 Darmstadt, Hochschulstraße 6, Germany

Dynamics in binary mixtures of water and glycerol with various concentrations was investigated by NMR. Applying different NMR technics the dynamics was studied in a broad temperature range down to very low temperatures. As a confinement effect the freezing point of water can be suppressed. Using 2H spin-lattice relaxation and stimulated-echo experiments we determined the rotational correlation function. By 1H diffusion measurements in an ultra high static field gradient the confinement effect on the translational motion caused by geometric restrictions as well as by surface interactions was studied. The dynamical properties were investigated within different types of confinement having various solidities. By comparison to the dynamics of their bulk systems, the influence of "soft confinement" (proteins) and "hard confinements" (MCM 41 with various pore diameters) was ascertained. A possible microphase separation of glycerol and water initiated by the confinement, is also of great interest.

DY 28.16 Tue 18:15 Poster C

Molecular dynamcis study of modified SPC/e water in neutral confinements — •Robin Horstmann, Michael Vogel, and Felix Klameth — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt, Germany

Liquids either supercooled close to the glass transition temperature or inside nanoscopic confinements exhibit a slowdown of dynamics of several orders of magnitude. While a full explanation is still missing the ECNLE (elastic collective nonlinear Langevin equation) theory proposed by Mirigian and Schweizer et al. [1] shows promising features explaning the α relaxation as a combination of a local hopping motion and the elastic distortion of the environment.

Recent molecular dynamics simulations [2] showed that the ECNLE theory, proposed for supercooled vdW-like systems, well describes the dynamcis of interfacial water. In this simulation work, neutral pores were used, i.e., a fraction of the bulk water was pinned leaving a nanoscopic pore of selectable geometry. Here, we reduce the partial charges of SPC/e water to systematically study the role of hydrogen bonds and to move in the direction of vdW-like behavior. Using the advantages of trajectories from molecular dynamics simulations we perform spatially resolved calculations of correlations, e.g., of the incoherent scattering functions, near the pore wall.
[1] Mirigan & Schweizer et al., J. Phys. Chem. Lett., 2013, 4 (21), pp 3648-3653
[2] Klameth et al., J. Phys. Chem. Lett., 2015, 6(21), pp 4385-4389

DY 28.17 Tue 18:15 Poster C

Spherical core-shell colloids with multiple cores as probes for rotational dynamics — Stefan Schütter[1], •Nicolai Sänger[1], Jörg Roller[2], and Patrick Pfleiderer[2] — [1]Universität Konstanz Fachbereich Chemie — [2]Universität Konstanz Fachbereich Physik

We introduce two new types of spherical probe particles for investigating rotational dynamics in colloidal fluids and solid states. The particles are tailormade for confocal fluorescence microscopy and coherent anti-Stokes Raman scattering (CARS) microscopy in three dimensions. CARS microscopy is a non-linear technique for tracking non-labeled colloids by generating signal of different polymer materials.[1,2] CARS methods, on the one hand, do not suffer from photobleaching and are attractive alternatives for longterm observations. On the other hand, two-color fluorescence of the cores provides robust access to the rapid determination of the particles* orientation. The two-color labeling strategy is beneficial to be able to observe the full 360 degree rotational movement of single colloidal clusters in contrast to other core-shell geometries where only angles of 180 degrees are accessible. It has already been shown for non-spherical single-color clusters that coupling effects for translational as well as rotational diffusion for different particle volume fractions are of high interest.[3] The choice of materials permits specific experiments for addressing diverse phenomena where rotation plays an important role.

[1] M. Müller and A. Zumbusch, ChemPhysChem, 2007, 8, 2156-2170. [2] M. K. Klein et al., Langmuir, 2014. [3] G. L. Hunter et al. Opt. Express, 2011, 19, 17189-17202.