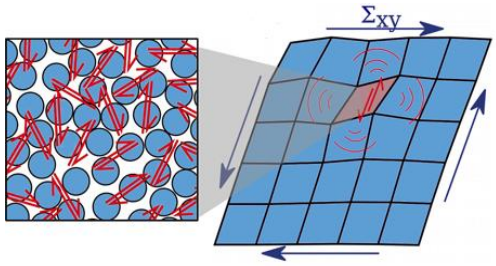
Mesoscale modelling of driven disordered materials: From glasses to active matter



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1. Description

Amorphous materials are ubiquitous around us, encompassing for instance colloids, emulsions, foams, granular matter and metallic glasses, as well as confluent biological tissues. These materials are seemingly very different from each other, as the size of their constituent particles ranges from nanometers (e.g., metallic glasses) to millimeters (e.g., grains) with very dissimilar particle interactions. Nevertheless, they exhibit common features under external forces or self-propulsion, showing universal non-equilibrium behaviors such as localized plastic rearrangements, collective or avalanche-type motion, or the emergence of shear bands. These remarkable observations naturally led researchers to search for a unified description of driven amorphous materials, particularly at a mesoscopic scale where microscopic details become irrelevant [1,2].

It is now well established that the mechanical response of amorphous solids under loading proceeds from local and irreversible rearrangements, resetting disorder locally and generating a highly non-trivial mechanical noise [1,2]. These plastic events were first identified by Argon [3] and later on coined as shear transformation zones (STZs) [4]. They play a central role in mechanical and rheological properties, providing us with the key building blocks for various theoretical descriptions, such as STZ theory [4] and elasto-plastic models (EPMs) [2]. The development of these effective descriptions has been tightly related to advances on other non-equilibrium statistical physics phenomena, such as the depinning transition [5,6] and ferromagnets in random fields [7]. Recent advances in stochastic processes, such as random resetting, could provide useful theoretical tools to refine these descriptions [8]. In this context, understanding the nature of the noise and the characterization of local disorder is becoming one of the forefronts of numerous works, particularly for dense active matter [9] where classical equilibrium concepts are challenged.

On the numerical front, spatio-temporal scales accessible by molecular dynamics are limited. Thus, atomistic simulations have been complemented by discrete mesoscopic approaches, allowing to reproduce the response of driven amorphous materials while considerably reducing the number of degrees of freedom to be processed [2]. EPMs consider a discrete population of STZs triggered in an elastic medium, and can be seen as a mechanical analogue of an Ising model where local plastic deformation and elastic propagator correspond respectively to spin and interaction between the sites. Many versions of coarse-grained, mesoscopic modellings with different ingredients have been devised to investigate the collective organization of STZs, either spatially-resolved [2,10] or effectively mean-field [11], to explore various mechanisms (e.g., avalanches, shear bands [12]) and rheological settings (e.g., stationary, transient regimes, oscillatory protocols [13,14]). Furthermore, recent studies focused on the detailed calibration of these mesoscopic models using microscopic information obtained by molecular simulations [16,17]. This multiscale-modelling approach, mapping from molecular simulations to mesoscopic models, paves the way to construct more realistic modelling, also by applying them to experimental systems such as colloids and granular materials [18,19]. Such mesoscopic modelling is also becoming paramount for dense active matter, by relying on connections with driven yet passive amorphous materials within a unified framework [20].

Key References

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2. Program

Day 1 - Wednesday May 24th 2023

Morning session

- 08:50 to 09:00 - Opening remarks
- 09:00 to 09:30 - **Gilles Tarjus**
  The yielding transition of strained amorphous solids: Nonequilibrium phase transition, finite-size effects and mesoscale modeling
- 09:30 to 10:00 - **Jack Thomas Parley**
  Mean field theory of the brittle yielding transition under uniform shear
- 10:00 to 10:30 - **Suzanne Fielding**
  Shear localization during yielding of amorphous materials
- 10:30 to 11:00 - Coffee break
- 11:00 to 11:30 - **Edan Lerner**
  Strain-stiffening of athermal biopolymer networks
- 11:30 to 12:00 - **Marko Popovic**
  Random traction yielding transition in epithelial tissues
- 12:00 to 12:30 - **Daniel Matoz**
  Active mechanics in thin sheet materials
- 12:30 to 14:00 - Lunch

Afternoon session

- 14:00 to 14:30 - **Silke Henkes**
  The active rheology of gastrulation
- 14:30 to 15:00 - **Carlos Villarroel**
  Critical yielding rheology: From externally deformed glasses to disordered active systems
- 15:00 to 15:30 - **Qinyi Liao**
  Rheology of disordered self-propelled particulate system
- 15:30 to 16:00 - Coffee break
- 16:00 to 16:30 - **David Richard**
  A mapping between the micromechanics of glasses and elasto-plastic models
- 16:30 to 17:00 - **Hongyi Xiao**
  Machine learning-informed structuro-elasto-plastic (step) model for deforming a granular raft
- 17:00 to 17:30 - Open discussion
- 17:30 to 19:00 - Poster session & Aperitif

Day 2 - Thursday May 25th 2023

Morning session

- 09:00 to 09:30 - **Alberto Rosso**
  The fate of shear-oscillated amorphous solids
- 09:30 to 10:00 - **Peter Sollich**
  Mean field theory of yielding under oscillatory shear
- 10:00 to 10:30 - **Damien Vandembroucq**
  Limit cycles and memory effects in mesoscopic elastoplastic models of amorphous solids
- 10:30 to 11:00 - Coffee break
- 11:00 to 11:30 - **Muhittin Mungan**
  Characterizing the irreversibility and yielding transition of a sheared amorphous solid using transition graphs
- 11:30 to 12:00 - **Srikanth Sastry**
  Yielding and fatigue failure in amorphous solids under cyclic shear
- 12:00 to 12:30 - **Debjyoti Majumdar**
  Dynamics of amorphous system subject to time-dependent oscillatory shear at finite temperature and frequencies
- 12:30 to 14:00 - Lunch

Afternoon session

- 14:00 to 14:30 - **Craig Maloney**
  The role of the Eshelby back-stress in amorphous plasticity
- 14:30 to 15:00 - **Alexandre Nicolas**
  Exploring the foundations and the (remote) frontiers of elastoplastic models
- 15:00 to 15:30 - **Daniel Korchinski**
  Temperatures effects on criticality and rheology in a mesoscopic model of amorphous yielding
- 15:30 to 16:00 - Coffee break
- 16:00 to 16:30 - **Yoav Lahini**
  Memory, adaptation and aging in crumpled sheets and networks of instabilities
- 16:30 to 17:00 - **Oguz Umut Salman**
  Pseudoturbulence in crystal plasticity
- 17:00 to 17:30 - Open discussion
- 19:00 to 21:30 - Conference dinner

Day 3 - Friday May 26th 2023

Morning session

- 09:00 to 09:30 - **Camille Scalliet**
  From micro to mesoscale models of viscous liquid dynamics

- 09:30 to 10:00 - **Massimo Pica Ciamarra**
  The energy cost of local rearrangements makes glasses solid

- 10:00 to 10:30 - **Cecilia Herrero**
  Two-step devitrification of ultrastable glasses

- 10:30 to 11:00 - Coffee break

- 11:00 to 11:30 - **Joachim Wittmer**
  Correlations of tensor field components in isotropic systems with applications to stress and strain correlations in equilibrium and driven elastic and viscoelastic bodies

- 11:30 to 12:00 - **Julia Giannini**
  Do nonlinear plastic modes predict the loci of plastic deformation in structural glasses with pressure gradients?

- 12:00 to 12:30 - **Michael Zaiser**
  Deformation and failure of disordered materials: Local and global predictions by machine learning

- 12:30 to 14:00 - Lunch

Afternoon session

- 14:00 to 14:30 - **Kirsten Martens**
  An elasto-plastic approach based on microscopic insights for sheared disordered solids

- 14:30 to 15:00 - **Ylann Rouzaire**
  Defects unbind and superdiffuse in the active XY model

- 15:00 to 16:00 - Closing discussion

3. Abstracts

A mapping between the micromechanics of glasses and elasto-plastic models

David Richard
Université de Grenoble Alpes, France

In contrast to crystalline solids, characterizing glassy amorphous structures remains a challenging task for both condensed matter physicists and material scientists. In recent years, many new computational tools have been developed to this aim, from purely structural descriptions of local motifs, through machine learning based tools, to various analyses of the potential energy landscape. In the context of shear driven amorphous solids, I will present a microscopic method that allows one to estimate local stress activation thresholds from bare static configurations. Obtained local yield rules can serve as inputs for elasto-plastic models to predict stress-strain responses and strain localization. I will illustrate such a mapping for glasses featuring a wide range of mechanical stabilities.

Active mechanics in thin sheet materials

Daniel Matoz
Complutense University of Madrid, Spain

How patterns and body structures are formed in plants and animals is still an active research topic across disciplines. One of the early contributions to explaining how complex shape emerges in life was made by D'Arcy Thompson. By applying methods and principles from the physical sciences to biological problems, Thompson demonstrated how simple mathematical reasoning reveals elegant explanations for complex processes giving the first foundation for describing and classifying the astonishing diversity of shapes and forming the living world.
Morphogenesis processes are regulated by a complex set of chemical and mechanical cues that lead to a dynamic reorganization of cells and their environment. While the importance of biochemistry in morphogenesis, developmental biology and tissue homeostasis has been well appreciated during the last century, only during the last two decades the role of physics and mechanics has started to be uncovered. However, neither biochemistry nor physics alone can individually explain the phenomena of pattern and structure that emerge in plants, animals, and humans.
Despite significant progress in understanding the behavior of active fluids, much less is known about how activity affects the behavior of solid and viscoelastic materials, such as epithelial tissues or biofilms. In this talk, we will show that a viscoelastic thin sheet is driven out of equilibrium by active structural remodeling (e.g., fast growth) develops a wide variety of shapes as a result of a competition between viscous relaxation and activity. In the regime where active processes are faster than viscoelastic relaxation, shapes that are formed due to remodeling are inherently out of equilibrium. The latter regime is of particular interest in developing a physical understanding of morphogenesis, where the embryo has to undergo a series of carefully orchestrated shape changes to establish the functioning organism. Our study suggests that keeping a growing system out of equilibrium increases the range of available morphologies. These observations point to a robust mechanism by which a system that is kept out of equilibrium could be steered toward the desired shape by chemical regulation of remodeling, relaxation, and mechanical parameters.

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An elasto-plastic approach based on microscopic insights for sheared disordered solids

Kirsten Martens[1], Chen Liu[2], Suman Dutta[3], Pinaki Chaudhuri[4]
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[2]Columbia university, United States
[3]ICTS-TIFR, India
[4]Institute of Mathematical Sciences, India

In this presentation I will discuss how we develop a framework to study the mechanical response of athermal amorphous solids via a coupling of mesoscale and microscopic models. Using measurements of coarse-grained quantities from simulations of dense disordered particulate systems, I will present our elasto-plastic model approach for deformation and flow of yield stress materials. For a given set of parameters, this model allows to match consistently transient and steady state features of driven disordered systems with diverse preparation histories under both applied shear-rate and creep protocols.

Characterizing the irreversibility and yielding transition of a sheared amorphous solid using transition graphs

Muhittin Mungan
University of Cologne, Germany

The complex dynamical features such as the irreversibility transition and yielding are already present in a regime where thermal effects are negligible and the system's response to the forcing is largely rate-independent: The athermal and quasi-static (AQS) regime. As we showed recently, the AQS conditions permit a rigorous description of the dynamics of such systems in terms of a directed state-transition graph, the AQS t-graph.
The complex dynamical features are thus encoded in the topology of the AQS t-graph.
Moreover, such AQS transition graphs can be directly extracted from atomistic or mesoscopic simulations of sheared amorphous solids. In this talk I will show how the t-graph permits one to analyze the irreversibility and yielding transition in sheared amorphous solids.

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Correlations of tensor field components in isotropic systems with applications to stress and strain correlations in equilibrium and driven elastic and viscoelastic bodies

Joachim Wittmer
CNRS - Université de Strasbourg, France

Correlation functions of components of second-order tensor fields in isotropic systems can be reduced to an isotropic forth-order tensor field characterized by a few invariant correlation functions (ICFs). The components of this field depend in general on the coordinates of the field vector variable, e.g., the wavevector q in reciprocal space, and thus on the orientation of the coordinate system. Importantly, these angular dependencies should not be confused with those of ordinary anisotropic systems with invariant material functions depending explicitly on the direction of the field vector. The procedure to obtain the ICFs, applicable quite generally also for non-equilibrium driven systems, is discussed for (forth-order tensorial) correlation functions of time-averaged stress fields and instantaneous strain fields in reciprocal space and using "natural rotated coordinates" independent of the coordinate system. (For simplicity, the systems are also assumed to be stationary, achiral and two dimensional.) Since all ICFs must become constant in the large-wavelength limit all correlation functions (in any coordinate system) are known in terms of only three phenomenological parameters. The long-range correlations in real space observed in several recent studies for these fields are thus implied by the known symmetries and the structure of isotropic tensor fields. Moreover, for equilibrium elastic bodies all constants can be traced back to the known elastic moduli. The often-made additional assumption of localized plastic rearrangements ("Eshelbies") is thus not required. For time-dependent correlation functions of tensor fields the phenomenological constants describing the low-q limit depend naturally on time. For equilibrium systems this dependency is completely described in terms of a few invariant

response functions which may be independently measured. The system-dependent microscopic relaxation dynamics, e.g., by means of correlated localized events (“avalanches”), determines these relaxation functions and thus in turn the time-dependence of the q-independent constants. Depending on certain tensorial invariants of response functions strong quadrupolar pattern of time-dependent correlation functions of stress and strain fields are predicted.

Critical yielding rheology: From externally deformed glasses to disordered active systems

Carlos Villarroel, Gustavo Düring
Pontificia Universidad Católica De Chile, Chile

In recent years, active matter systems have exhibited behavior similar to amorphous solids under stress. At large enough density, these materials are mechanically stable. However, it cannot find an equilibrium if sufficiently large self-propulsion is applied. For both drive scenarios, today, it is understood that rheology at low strain rates is controlled by plastic events, which are local, irreversible rearrangements of a few tens or hundreds of particles. However, a detailed study of the critical behavior of yielding phenomenon in the active matter remains unexplored.
We use extensive computer simulations to study the yielding transition under two driving scenarios: standard simple shear dynamics and self-propelled dense active systems. In the active systems, a yielding transition toward an out-of-equilibrium flowing state known as liquid phase is observed when the self-propulsion is increased. The range of self-propulsions in which this pure liquid regime exists appears to vanish upon approaching the so-called "jamming point" at which the solidity of soft-sphere packings is imposed. Such an "active yielding" transition shares similarities with the generic yielding transition for shear flows. A Herschel-Bulkley law is observed in the liquid regime in both loading scenarios, with a clear difference in the critical scaling exponents between the two, suggesting the existence of different critical behavior for the yielding transition under different driving conditions. However, our quasistatic simulations verified that the exponents describing the avalanche distribution had only a slight discrepancy between both driving scenarios. This could indicate that the difference observed in the flow curves may result from a dynamic effect in the avalanche propagation mechanism. To verify this, we present a new simulation protocol that allows the study of the dynamic exponent z, which until today has been challenging to measure.

Defects unbind and superdiffuse in the active XY model

Ylann Rouzaire
University of Barcelona, Spain

We consider a nonequilibrium extension of the 2D XY model, equivalent to the noisy Kuramoto model of synchronization with short-range coupling, where rotors sitting on a square lattice are self-driven by random intrinsic frequencies. We study the static and dynamic properties of topological defects (vortices) and establish how self-spinning affects the Berezenskii-Kosterlitz-Thouless phase transition scenario. The nonequilibrium drive breaks the quasi-long-range ordered phase of the 2D XY model into a mosaic of ordered domains of controllable size and results in self-propelled vortices that generically unbind at any temperature, featuring super diffusion (MSD ~ $t^{3/2}$) with a Gaussian distribution of displacements. We show that the anomalous diffusion is tightly related to self-avoiding random walks, and that this feature can be found in experimental systems.
Our work sheds new light on the problem of synchronization of locally coupled oscillators and provides a simple framework to investigate topological defects in nonequilibrium matter.

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Deformation and failure of disordered materials: Local and global predictions by machine learning

Michael Zaiser
University of Erlangen-Nuremberg, Germany

Machine learning approaches have found a wide range of applications in the field of mechanics of disordered materials. On the one hand, they have been used to identify local 'defects', i.e., local environments with an enhanced propensity to undergo irreversible deformation or failure under load, on the other hand they can serve to make sample specific predictions of global properties such as creep lifetime or failure stress. In this talk we give a critical overview of approaches proposed in the literature, emphasizing the essential importance of domain knowledge in mechanics of materials for the successful implementation of machine learning strategies for both local and global failure prediction. We present own results on failure prediction in glassy solids, and outline future perspectives.

Do nonlinear plastic modes predict the loci of plastic deformation in structural glasses with pressure gradients?

Julia Giannini[1], Edan Lerner[2], Lisa Manning[1]
[1]Syracuse University, United States
[2]University of Amsterdam, Netherlands

When active particles are assembled at high densities, they behave similarly to disordered solids, exhibiting dynamic arrest, resistance to applied deformation, and localized plastic yielding. Thus, several recent studies have drawn connections between the structure and dynamics of dense active matter systems and sheared amorphous solids. In passive structural glasses, it has been shown that populations of microstructural defects forecast plastic rearrangements and explain unique thermal, mechanical, and dynamical properties. A number of structural analyses that successfully locate these defects rely on harmonic and/or higher-order approximations of a system's potential energy and identify modes of localized collective motion, termed 'quasilocalized modes' (QLMs) [1,2]. However, these tools have not been robustly extended to active materials in the solid-like phase. Distinctly from their passive counterparts, active glasses often contain internally generated stresses and global pressure gradients that result from the self-propulsion forces of the constituent particles [3,4]. In a recent study, we reformulated a harmonic/normal mode analysis to predict localized rearrangements in active particle packings that form stable disordered reference configurations with pressure gradients in the limit of persistent self-propulsion. We discovered that global pressure gradients pose a significant challenge to this framework, as the normal mode analysis failed to predict rearrangements in dense regions of these packings [4]. Here, we seek to address this challenge by identifying populations of nonlinear plastic modes (NPMs) in a similar class of models [2]. We will compare the capability of harmonic and anharmonic structural metrics in making spatiotemporal predictions of plastic events in externally driven disordered solids with global pressure gradients.

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Dynamics of amorphous system subject to time-dependent oscillatory shear at finite temperature and frequencies

Debjyoti Majumdar
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We use computer simulations to study the effect of finite temperatures, shearing amplitudes and frequencies on the dynamics of amorphous solids under oscillatory shear. We study the stability of periodic states prepared at zero temperature (limit-cycles) as a function of temperature and frequency as well as the number of forcing cycles needed to reach a periodic state when the temperature and frequency are finite. We observe a cross-over as a function of temperature and frequency between two different scaling regimes. We then show that the length of limit-cycles exhibits power-law statistics close to the crossover point indicating a possible dynamical transition. Our results indicate that below a certain temperature and frequency limit-cycles are very stable and can be used to store memory even in the presence of thermal fluctuations.

Exploring the foundations and the (remote) frontiers of elastoplastic models

Alexandre Nicolas
CNRS, France

Elastoplastic models are extended cellular automata that were designed to mirror the main processes involved in the deformation and flow of disordered solids, namely, elastic deformation under low local shear, swift 'plastic' rearrangements past a stress threshold inducing an elastic deformation of the surrounding medium. At vanishing shear rates, some universality has been unveiled in the response of these systems, notably in the cascading properties of avalanches, and there have been recent successes in tightening the connection between these mesoscopic automata to microscopic systems. At finite shear rates, on the other hand, there is both more freedom in the choice of the 'ingredients' of elastoplastic models and more conspicuous discrepancies in the macroscopic response of actual materials.
In the talk, I will argue that at finite shear rates a gap still needs to be bridged between microscopic systems and mesoscopic automata. This can be achieved by probing the behavior of mesoscopic regions of a microscopic numerical model and simplifying it. Finally, I will turn to recent developments of elastoplastic models to address oscillary shear and the transition to irreversibility and mention the unexpected connections that are thus revealed with widely different complex systems.

From micro to mesoscale models of viscous liquid dynamics

Camille Scalliet
University of Cambridge, United Kingdom

Understanding the mechanism by which liquids transform into glasses is of great experimental and fundamental importance. The goal is to determine the origin of the dynamic slowdown of liquids upon cooling. In this talk, I will present recent numerical developments which allow for the first time to investigate the slow dynamics of supercooled liquids close to the glass transition. I will describe the microscopic picture revealed by our computer simulations [1], and how this feeds recent efforts to develop new mesoscopic models for viscous dynamics. I will discuss the facilitated trap model [2] as a simple mesoscale model and describe how it allows us to rationalize some aspects of slow dynamics.

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Limit cycles and memory effects in mesoscopic elastoplastic models of amorphous solids

Damien Vandembroucq
CNRS, France

When subjected to cyclic loading at a low enough amplitude, complex fluids and amorphous solids can reach limit cycles. Such a reversible plastic behavior disappears beyond a critical value of the loading amplitude. We show that these spectacular effects can be reproduced in the framework of a simple elastoplastic model with quenched disorder. We discuss the effect of glass preparation on the nature of the irreversibility transition and the properties of the limit cycles. We finally present recent results about the encoding and reading of a mechanical memory in amorphous solids.

*[1] D. Kumar, S. Patinet, C. Maloney, I. Regev, D. Vandembroucq, M. Mungan, J. Chem. Phys., **157**, 174504 (2022)*

Machine learning-informed structuro-elasto-plastic (step) model for deforming a granular raft

Hongyi Xiao
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Understanding the role of the disordered structure is important for modeling the deformation of soft amorphous materials. Such structure can be measured experimentally in a model disordered material, a granular raft consisting of polydisperse spheres trapped at an air-oil interface that induces capillary attractions. Under tensile deformation, particle rearrangements gradually localize into an inclined shear band, upon which failure occurs. The ductility of the rafts can be tuned by controlling the ratio of particle size to capillary length. A machine learning method was used to develop a structural descriptor, softness, that predicts the propensity of a particle to rearrange. Microscopic interplay between elasticity, rearrangements and softness were extracted and used to inform a Structro-Elasto-Plastic (StEP) model that can capture the shear band formation and the brittle-to-ductile transition due to the change of capillary interaction. In addition, small amplitude oscillatory deformation was applied to mechanically age the rafts. This induces gradual structural change and leads to brittle behaviors for aged rafts. StEP modeling for incorporating such aging effects will be discussed.

Mean field theory of the brittle yielding transition under uniform shear

Jack Thomas Parley, Peter Sollich
University of Goettingen, Germany

We study the brittle yielding of athermal amorphous solids under uniform shear within the celebrated Hébraud-Lequeux (HL) mean-field elastoplastic model, which incorporates the long-range sign-varying nature of Eshelby interactions as a Gaussian mechanical noise. As in finite-dimensional particle simulations, there is a critical value R_c of the initial disorder, below which yielding becomes a sharp discontinuous transition in the limits of large system size (N going to infinity) and vanishing shear rate . Throughout the analysis, we compare with the corresponding behavior of the random field Ising model (RFIM), which we consider as the paradigmatic description of a slowly driven athermal system with short-range strictly positive interactions. Studying firstly the case of an infinite system for small non-zero shear rates, we show how the susceptibility becomes delta-like at the brittle yield point, as in a first-order transition. We then derive analytically the divergence as the share rate goes to zero of the peak susceptibility, defined as the maximum slope of the stress-strain curve, at the random critical point R_c . Turning secondly to the behavior of finite-size systems in the quasistatic limit, we study the avalanche behavior of the HL model. We show that, provided one accounts for the appearance of a plateau in the local stress distribution, a mapping to a first-passage problem previously introduced by Jagla can indeed be applied to understand the avalanche distribution. Although in principle non-universal, the avalanche exponent is effectively $\tau \approx 1^{+}$ both in steady state and in transient, and avalanches scale with system size; in contrast to the RFIM, where $\tau=3/2$ and avalanches are not extensive.

Mean field theory of yielding under oscillatory shear

Peter Sollich[1], Jack Parley[1], Srikanth Sastry[2]
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We study a mean field elastoplastic model, embedded within a disordered landscape of local yield barriers, to shed light on the non-equilibrium behavior of athermal amorphous solids subject to oscillatory shear. We show that the model presents a genuine dynamical transition between an elastic and a yielded state, and qualitatively reproduces the dependence on the initial degree of annealing found in particle simulations. For initial conditions prepared below the threshold energy, which we derive analytically, we observe a non-trivial, non-monotonic approach to the yielded state. The timescale diverges as one approaches the yielding point from above, which we identify with the fatigue limit. We finally discuss the connections to brittle yielding under uniform shear, and to other systems with a manifold of absorbing states including Kosterlitz-Thouless flows.

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Memory, adaptation and aging in crumpled sheets and networks of instabilities

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A thin sheet that has been crumpled many times exhibits many of the hallmark behaviors of driven and nonequilibrium disordered systems: intermittent global responses, emission of correlated crackling noise, slow relaxations and aging, and a range of mechanical memory effects. Here, through experiments in thin crumpled sheets and simulations of a minimal mechanical model, we reveal a microscopic, real-space, structural mechanism underlying and linking all these behaviors.
Using experiments that combine global mechanical measurements, local probing, acoustic measurements, and 3D imaging of crumpled sheets, we build a mesoscopic description of their mechanics. The global measurements reveal a range of memory effects, including hysteresis, memory of largest strain, and return point memory, as well as clear signatures of underlying intermittent dynamics. Intermittent dynamics are also observed during slow, logarithmic aging of crumpled sheets under load. In this case, however, the intermittent events are grouped into highly correlated, scale-free avalanches. The complimentary local measurements reveal that intermittency, memory, and aging behaviors emerge from the collective dynamics of mesoscopic, bistable elements within the sheet: localized geometric instabilities that act as coupled, hysteretic, two-state degrees of freedom.
Based on this picture, we develop a numerical model of a disordered network of bistable elastic elements that corroborates all our findings: hysteresis, intermittencies, memory formation, return point memory, slow relaxations, aging, and avalanches. The model highlights the role of interactions and frustration between instabilities in driving these behaviors. The emerging picture is of a disordered system with a complex energy landscape, reminiscent of a mechanical spin-glass, that self-organizes to a state which lies on the verge of instability.

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Pseudoturbulence in crystal plasticity

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We will discuss the formation of complex textures in crystals resulting from plastic deformations that cause randomly oriented patches of the unstressed lattice. We use a mesoscopic Landau-type tensorial model of crystal plasticity to demonstrate that such textures can originate from crystallographically exact micro slips, forming laminates of a pseudo twin type. These laminates result from an effective internal "wrinkling" of the crystal lattice that leads to elastically neutral rotations but is inherently dissipative and dislocation-mediated. Numerical experiments reveal that the process of dislocation self-organization is unstable and characterized by pseudo-turbulent effective rotations with power-law distributed spatial correlations, indicating the necessity of a probabilistic description of crystal plasticity.

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Random traction yielding transition in epithelial tissues

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We investigate how randomly oriented cell traction forces lead to fluidization in a vertex model of epithelial tissues. We find that the fluidization occurs at a critical value of the traction force magnitude F_c. We show that this transition exhibits critical behavior, similar to the yielding transition of sheared amorphous solids. However, we find that it belongs to a different universality class, even though it satisfies the same scaling relations between critical exponents established in the yielding transition of sheared amorphous solids. Our work provides a fluidization mechanism through active force generation that could be relevant in biological tissues.

Rheology of disordered self-propelled particulate system

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[2]University of Science and Technology of China, China

We numerically investigate the active rheology of the two-dimensional self-propelled particulate system in the athermal limit. We find that the self-propulsion and the active velocity can be qualitatively mapped to the shear stress and inverse shear rate. We reveal a jamming transition under self-propulsion with critical exponents different from the counterparts under shear. To further investigate the rheology of self-propulsion, we invent a simulation method to mimic constant active velocity driving as the analogue of applying a constant shear rate. We thereby extensively compare the self-propelled and shear systems and reveal propulsion force overshoot, propulsion force overshoot, reversible-irreversible transition under cyclic propulsion, and propulsion bands in plastic flows.

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Shear localization during yielding of amorphous materials

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Amorphous materials include soft solids such as emulsions, colloids, gels and granular matter, as well as harder molecular and metallic glasses. In contrast to conventional crystalline solids, the internal arrangement of their constituent microstructures (emulsion droplets, sand grains, etc.) lacks long ranged order. Understanding the rheology (deformation and flow properties) of these materials thus poses a difficult challenge. Typically, they behave in an elastic way at low loads then yield plastically at larger loads. This talk will summarize recent progress in understanding the yielding transition between an initially solid-like state and a finally fluidized one, as a function of time since the imposition of a strain or load. A particular focus will be on the phenomenon of strain localization during this dynamical process of yielding.

Strain-stiffening of athermal biopolymer networks

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Athermal biopolymer networks are disordered fibrous biomaterials abundant in living cells and tissues that feature strong rigidity scale separation between the bending and stretching response of the constituent fibers. Such networks - that are generically underconstrained in terms of their degree of connectivity - undergo a dramatic macroscopic stiffening transition when subjected to sufficiently large external strains. In my talk I will present a complete scaling theory of the critical strain-stiffened state in terms of the small ratio between fiber bending and stretching/compression rigidities. I will show that the small bending forces may be viewed as an isotropic singular perturbation applied to the stiff anisotropic backbone corresponding to fibers' stretching/compression. The critical state features quartic anharmonicity, from which a set of nonlinear scaling relations for key observables are derived. These results, which are validated by numerical simulations, are then used to derive scaling predictions for the macroscopic elastic modulus beyond the critical state, revealing a previously unidentified characteristic strain scale. I will end by discussing a few open problems and the challenges they pose.

Temperatures effects on criticality and rheology in a mesoscopic model of amorphous yielding

Daniel Korchinski
University of British Columbia, Canada

Amorphous solids are a disparate class of materials, including glasses, foams, emulsions and granular packings. Surprisingly, they exhibit some shared universal behavior in their mechanical response to load, with an initially elastic regime giving way to a jerkily flowing state characterized by intermittent bursts of activity dubbed “avalanches”. This driven state is a dynamical phase transition, exhibiting avalanches and rheological behavior characterized by nontrivial critical exponents. This yielding transition has been extensively studied in the zero-temperature limit, where the presence of long-range elasticity and an anisotropic stress propagator leads to an intriguing universality class distinct from many other examples of self-organized criticality. Comparatively little work studies the effects of temperature on the self-organized criticality of this system. In this talk, I will discuss how temperature, driving rate, and finite-size effects compete to truncate avalanches and tune the system away from criticality. Using an elastoplastic model of amorphous plasticity equipped with a temperature dependent activation of weak-sites, along with various scaling arguments, we derive a nonequilibrium phase diagram that captures onset of avalanche overlap, when temperature effects are prevalent, and when finite-size effects dominate the critical behavior [1]. In the continuously flowing state, when avalanches overlap, we also find a change in the flow exponents at high temperature, which we will compare to data obtained at other scales.

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The active rheology of gastrulation

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In the early embryo, tissue layers deform, flow, and exert forces in a tightly coordinated sequence to build the developing body. During convergence-extension flows, which occur in gastrulation and germ band extension, tissues contract and then elongate perpendicular to the tissue stress, i.e., with an apparent negative shear modulus. This rheology emerges through active T1 transitions, where quartets of cells rearrange against the stress, in addition to normal passive T1 transitions that yield along the principal stress direction.
I will present a vertex model formulation of such a tissue [1], where the activity enters through a catch-bond mechanism feedback loop with stress of the actomyosin on individual junctions. We reliably find and characterize active T1 transitions in an optimal stress range, and compute flow curves for this material. We match T1 orientational distributions and flows with experimental data from chick embryo gastrulation. I will complement this result with a continuum model of the process [2] that highlights how the fixed points of the myosin feedback dynamics, together with boundary stresses, are responsible for this striking rheology.

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The energy cost of local rearrangements makes glasses solid

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Which phenomenon confers rigidity to glasses is a long-standing question of condensed-matter. In most popular theories, liquids rigidify into glasses as their relaxation becomes more cooperative under cooling. Instead, other approaches consider that local barriers associated with the elementary rearrangement of a few particles or “excitations” govern the dynamics. Here we resolve this conundrum by introducing a new algorithm, SEER, to extract hundreds of excitations from any given configuration systematically. From the excitations' density of states, one can directly predict how local barriers slow down the dynamics, assuming no cooperative effects. We find this prediction to be quantitative in liquid models that can be simulated up to time scales of milliseconds, revealing that cooperativity is uninfluential and leading to new perspectives on the glass transition.

The fate of shear-oscillated amorphous solids

Alberto Rosso
CNRS - Université de Paris Saclay, France

The behavior of shear-oscillated amorphous materials is studied using a coarse-grained model. Samples are prepared at different degrees of annealing and then subject to athermal and quasistatic oscillatory deformations at various fixed amplitudes. The steady-state reached after several oscillations is fully determined by the initial preparation and the oscillation amplitude, as seen from stroboscopic stress and energy measurements. Under small oscillations, poorly annealed materials display shear-annealing, while ultra-stabilized materials are insensitive to them. Yet, beyond a critical oscillation amplitude, both kinds of materials display a discontinuous transition to the same mixed state composed by a fluid shear-band embedded in a marginal solid. Quantitative relations between uniform shear and the steady-state reached with this protocol are established. The transient regime characterizing the growth and the motion of the shear band is also studied.

The role of the Eshelby back-stress in amorphous plasticity

Craig Maloney
Northeastern University, United States

We study an elasto-plastic automaton model of an amorphous solid subject to athermal quasi-static shearing. Most contemporary approaches in the statistical physics community to elasto-plastic modeling of amorphous matter assume that after a region in the material yields the region will find itself in a state of zero stress. However, in the Eshelby problem, an inclusion, after it undergoes a plastic transformation, will find itself under a non-negligible negative stress, σ_c.
The magnitude of σ_c depends on the Poisson ratio and the shape of the inclusion, but for a disk-shaped inclusion in two dimensions in an incompressible material, the inclusion will be under a stress of (-1/2) times the shear modulus; clearly a non-negligible amount. The magnitude of σ_c monotonically decreases as the material becomes more compressible. We show that σ_c has a profound impact on yielding both in cyclic and steady shear. In both cases, the probability distribution of local stresses, $P(\sigma)$, shows a pronounced signature of σ_c. For the cyclic shear case, we show that it determines the critical cycling amplitude below which the final steady states are trivially elastic. For the steady shear case, we show that it determines the value of the flow stress for varying Poisson ratio.

The yielding transition of strained amorphous solids: Nonequilibrium phase transition, finite-size effects and mesoscale modeling

Gilles Tarjus
CNRS - Université de Sorbonne, France

The yielding transition of amorphous solids under very slow strain deformation may occur discontinuously with a jump in the stress or continuously as a function of the preparation of the material. From analytical mean-field arguments and molecular simulations we have argued that the passage from discontinuous to continuous yielding is controlled by a nonequilibrium critical point akin to that of the driven random-field Ising model. Finite-size effects are however very strong in these nonequilibrium phase transitions in the presence of quenched disorder, both in the discontinuous region and at the critical point. This has led to debates on the most appropriate theoretical description of yielding. Mesoscale modeling and effective theories are therefore needed to sort out the issues and will be discussed in this presentation.

Two-step devitrification of ultrastable glasses

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The discovery of ultrastable glasses has raised novel challenges about glassy systems. Recent experiments studied the macroscopic devitrification of ultrastable glasses into liquids upon heating but lacked microscopic resolution. We use molecular dynamics simulations to analyze the kinetics of this transformation. In the most stable systems, devitrification occurs after a very large time, but the liquid emerges in two steps. At short times, we observe the rare nucleation and slow growth of isolated droplets containing a liquid maintained under pressure by the rigidity of the surrounding glass. At large times, pressure is released after the droplets coalesce into large domains, which accelerates devitrification. This two-step process produces pronounced deviations from the classical Avrami kinetics and explains the emergence of a giant length scale characterizing the devitrification of bulk ultrastable glasses. Our study elucidates the nonequilibrium kinetics of glasses following a large temperature jump, with similarities between devitrification and crystal melting that point towards a thermodynamic interpretation of the glass transition as a first order phase transition. We also aim at guiding future experimental studies, where one should consider the existence of three different states: glass and two liquids at two different pressures.

Yielding and fatigue failure in amorphous solids under cyclic shear

Srikanth Sastry
JNCASR, India

The yielding behavior of amorphous solids under cyclic shear deformation has been investigated extensively in computer simulations, and more recently, through a variety of modeling approaches including mesoscale models. Some of these investigations have also addressed fatigue failure, an important aspect of the phenomenology for cyclic loading. Here I present results from a finite element based elastoplastic modeling of cyclic shear yielding, and compare with earlier approaches. Our results highlight the important role of the distribution of local stabilities, a feature that has been incorporated in recent modeling efforts but not systematically explored. Results concerning fatigue failure from simulations and model calculations will also be presented, focusing on the dependence of the time to failure on the amplitude of applied shear strain.

4. Posters

Active fluid-induced dynamics of passive polymers

Zahra Valei
The University of Edinburgh, United Kingdom

The presence of both active and passive components is a hallmark of many biomaterials. Many of these composite materials are composed of large biomolecular polymers suspended in rheologically complex active backgrounds. Passive polymers embedded in active liquid crystalline solvents are particularly interesting because of the interplay of the broken symmetry of the background medium, nonequilibrium activity and the conformational degrees of freedom of the macromolecules. We study the structural and dynamical features of individual polymers in active nematic liquid crystals, employing a hybrid Multi-Particle Collision and Molecular Dynamics simulation. The intimate coupling of thermal noise, hydrodynamic interactions, orientational ordering, polymer entropy and activity leads to complex dynamics. We qualify polymer conformations through shape descriptors, including the radius of gyration and asphericity as a function of activity and nematic coupling. Surprisingly, we find that these conformational states contribute to dynamics that are reminiscent of bacterial run-and-tumble behavior. The polymers “run” when they are stretched by the extensile activity, then fold causing a “tumbling” event that suddenly changes the direction of motion. These dynamics are strikingly different from those observed in previous simulations of intrinsically active polymers and of polymers suspended in out-of-equilibrium heat baths. This suggests that the nature of the activity is crucial to the actuation of the polymers, and so suggests pathways for tuning and designing active and adaptive biomimetic materials.

Breaking the size constraint for nano cages using annular patchy particles

Vikki Varma, Sujin B. Babu
IIT Dehli, India

Engineering nano structures like cages, containers through self-assembly of nano particles have been very challenging. One of the challenges is to control the radius of the closed shell structures.
In this work, we have proposed a model of nano particle which consist of a hard core having the shape of a sphere, oblate or prolate, with an annular patch through which bonds are formed. By self-assembly the nano particles will lead to the formation of monodispersed spherical cages (closed shell) or containers (curved clusters). The curvature of the shell is analytically related to the patch angle of the nano particle, there by engineering cages with a desired radius. The formation of nano cages is similar to nucleation and growth kinetics and is the key factor in determining the yield of closed shells.

Cavitation instabilities in amorphous solids

Umang Dattani
The Institute of Mathematical Sciences, Chennai, India

Amorphous solids have diverse applications. But they are also known to fail catastrophically. As evidenced in experiments [1,2], cavitation instabilities are known to play a role in the fracture of amorphous solids. These instabilities are known to stem from gas+glass coexistence region in the temperature-density phase diagram of these solids [3]. Using numerical simulations, we investigate the occurrence of such instabilities via an athermal quasistatic expansion process, starting from a dense spatially homogeneous amorphous solid [4]. We find many interesting similarities with the well-studied athermal quasistatic shear response of amorphous solids, viz. saddle-node bifurcation, scale-free avalanche size distributions, quadrupolar displacement fields in the homogeneous regime etc. Further, we demonstrate that via a combination of expansion with a secondary deformation, in the form of cyclic shear or local random deformation via activity, it is possible to induce cavitation at higher densities and lower energy thresholds [5].

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*[4] U. Dattani, S. Karmakar, P. Chaudhuri, Phys. Rev. E, **106**, 055004 (2022)*
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Compositional disorder induces quasi-localized modes in high entropy alloys

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We investigate the low-frequency vibrational properties of High Entropy Alloys (HEAs), an emergent class of materials with exceptional mechanical performance. HEAs are designed by mixing several metallic species in nearly the same amount. They can exist in either a glassy state, characterized by positional disorder, or a crystal state, which displays distinctive compositional disorder. Compositional disorder in HEA-crystals arises due to the random distribution of atomic species on the lattice sites. Previous studies have shown that the low frequency density of states in glassy systems exceeds Debye's contribution typical of crystalline counterparts and is proportional to the fourth power of the frequency due to positional disorder. However, not much is known about the density of states of HEAs and its relationship with the compositional disorder that distinguishes HEA crystals from conventional crystals. To address this topic, here we analyze a realistic model of HEA in amorphous, partially crystallized, and crystal states. We show that the quartic laws hold across all levels of positional disorder and remarkably in HEA-crystals. The associated quasi-localized vibrations, however are highly suppressed compared to the glassy counterpart. Our work offers a uni ed perspective on the vibrational properties of high entropy alloys, providing insight into the behavior of these promising materials.

Correlations of plastic events in a 2d glassy system after yielding

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Université de Montpellier, France

Correlations between the occurrence of shock sequences in natural phenomenon such as earthquakes are well studied in seismology and found to follow the scale-free empirical laws. Recent granular experiments revealed the same behaviors for the slip events in the shear band. Scale-free statistics are also observed for the plastic behaviors in glassy systems. Here we study the correlation of plastic events in a 2d glassy system under simple shear in the athermal quasistatic limit. Previous studies have shown that well annealed glassy systems display a brittle yielding in this limit after which a clear shear band is formed. The system relaxes via a succession of scale-free elastic events and plastic events in the band. The spatial and temporal correlations between the plastic events are investigated. We finally compare with poorly annealed glassy systems where the plastic events happen in the bulk.

Fragile to strong crossover as general glassy feature

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WWU, Germany

As a liquid is cooled below the melting temperature, the dynamics become increasingly sluggish with the degree of supercooling, known as fragility. The fundamental question is whether the liquid ceases to flow at some finite temperature, the material undergoing the glass transition, or dynamics diverge smoothly to zero temperature. This is a central question of pivotal importance for unraveling the nature of glass and theoretical understanding, concealing with astronomical long observation times. We circumvent this infeasibility by taking advantage of swap Monte Carlo with multi-billion speedups for equilibration well beyond the glass transition. Our investigation of a wide range of system sizes and temperatures across the experimental glass transition unveils the nature of the energy landscape. We observe a notable deviation from the Gaussian nature of the potential-energy landscape. Rapid depletion of states is associated with the glassy bottom of the landscape, unveiling the fragile to strong crossover is the general glassy behavior. Our result ultimately rules out the finite-temperature divergence and establishes the conceptualized Arrhenius description of the dynamics at low temperatures. Our findings are critical in advancing the investigation of glass in an experimental and theoretical framework.

Plasticity in amorphous carbon as a stress-assisted chemical reaction

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Amorphous carbon (a-C) films, due to their high wear resistance and excellent tribological properties, offer a remarkable solid lubricant for applications involving extreme mechanical conditions [1]. Since the lubrication process relies on the plastic flow of a-C films, it becomes essential to understand their plastic properties. We study the plasticity of a-C networks within the framework of shear transformation zones which are believed to be the fundamental carriers of plasticity in amorphous solids [2]. We use atomic-scale simulations to show that for amorphous carbon, a shear-transformation can be reduced to a simple chemical reaction: the stress-induced breaking or forming of a single covalent bond. By forcing the breaking/forming of individual bonds in auxiliary calculations, we extract the potential energy landscapes of single bonds as a function of bond length. We find a good correlation between the energy barriers associated with a bond, the energy dissipated when the bond undergoes a plastic event, and the bond jump distance identified as the change in bond length due to the plastic event. Additionally, we apply a simple shear to an ensemble of a-C networks, all prepared by the same liquid-quench protocols, in the athermal quasistatic limit. By identifying plastic events that occur and using the correlation previously derived, we were able to calculate the average dissipated energy as a function of the applied strain. We use this to predict the yield stress of the carbon systems at hand. Our results help in interpreting some of the plastic properties of a-C networks and allow the parametrization of mesoscopic models of their plastic flow.

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Spectral properties of jammed packings recovered from (marginal) random matrices

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The density of states (DOS) captures very important features of a material (e.g., its heat capacity and transport properties) and, in the case of crystalline solids, the Debye theory provides a well-established description of it. In contrast, no such description exists for amorphous solids despite their ubiquity in nature: glasses, polymers, granular matter, etc. Possibly, the most salient difference between the DOS of crystalline and amorphous solids is their behavior at low frequencies. While Debye theory predicts that the former exhibits a power-law whose exponent depends on the dimensionality, numerical simulations consistently show that, near the jamming transition, amorphous solids display a quadratic behavior across dimensions d=3-9. Fully explaining this discrepancy is a far from solved problem since the basic ingredients responsible for the "anomalous" DOS of amorphous solids remain unknown. This has led to consider more abstract models with the aim of reproducing the main features of such DOS, with significant progress in recent years, mainly by adopting a mean field (MF) approach. Indeed, MF allows to recover the quadratic power-law in a variety of models, but only in the fully connected regime, which amounts to considering systems in very high dimensions. In turn, when sparsity is introduced along with a finite d, current models fail to reproduce the features observed numerically in particles-based simulations. In this talk I will introduce a random matrix model that, by mimicking the structure of particles-based interactions, faithfully reproduces the expected quadratic behavior at low frequencies as well as the localization properties of these low frequency modes. From our results, we provide a tentative explanation of the universal quadratic DOS observed in sphere packings, namely, that it is caused mainly by their topology.

Speed-up sampling with nonequilibrium drives: A theoretical, quantitative evaluation

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We consider a class of nonequilibrium dynamics that nevertheless sample the Boltzmann distribution in their steady state. For these dynamics, it is known that the relaxation time is shorter than the one of their equilibrium counterparts, though a quantitative understanding of the acceleration in systems with many interacting degrees of freedom is lacking. We contribute to this framework with theoretical computation of the speed-up in a mean field spin glass and in structural glasses. Our analysis focuses on temperature dependence, optimality and saturation of the acceleration. The appearance of odd transport coefficients is also discussed. We complement our findings with numerical simulations.

Study of hessian matrix eigenvalues of the glassy system before and after yield stress and its prediction using random matrix theory

Vijay Yadav
IIT Jodhpur, India

We study the plastic response of amorphous solids subjected to simple shear in the athermal and quasistatic limit (AQS). Athermal quasistatic trajectories have smooth, reversible elastic branches intermittently broken by discrete catastrophic plastic events [1]. We use molecular dynamics simulations to prepare an ensemble of two-dimensional Kob-Andersen binary Lennard-Jones glasses with a 65:35 ratio [2]. The glass is quenched to a very low temperature (T≈0), and simple shear in the AQS limit is applied. We then determine the yield stress and calculate the eigenvalues of the hessian matrix (second derivative of free energy) at different plastic events before and after the yield stress [3, 4]. We are currently investigating the distribution of these eigenvalues and trying to predict it using random matrix theory.

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Towards many-body nonequilibrium calorimetry: Specific heat of a driven fermionic array

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Calorimetry for equilibrium systems reveals the parameter-dependent occupation statistics of energy levels by measuring thermal response. Nonequilibrium versions are expected to add information on their dynamical accessibility. Calculations on a driven many-body system confirm that expectation. Modeling electrons hopping between quantum dots, the asymmetric exclusion process provides a Fermi Golden Rule approximation upon adding births and deaths at each dot. This yields a fermionic nonequilibrium steady state where the heat capacity is computed exactly by evaluating the heat fluxes entirely due to the changing of the ambient temperature. In particular, the heat capacity depends on the symmetric kinetic barrier for loading and emptying the quantum dot, invisible at equilibrium. Moreover, we find a zero-temperature dynamical phase transition, shown by the sudden divergence of the heat capacity when the Fermi energy and the kinetic barrier become approximately equal. The nonvanishing heat capacity at absolute zero, violating an extended Third Law, is caused by the relaxation times exceeding the dissipation time. Finally, when the kinetic barrier is density-dependent, a low-temperature regime of negative heat capacity appears, indicating an anti-correlation between the temperature dependence of the stationary occupation and the excess heat.

Yielding via asymmetric cyclic shear protocol

Pushkar Khandare
JNCASR, India

We implement an elastoplastic model of an amorphous solid based on the model presented in a previous publication [1] to investigate the plasticity and yielding behavior under symmetric and asymmetric cyclic shear. Under cyclic shear deformation of glasses, yielding is observed to be accompanied by shear band formation, with significant dependence on the degree of annealing of the glasses. Under asymmetric shear, the yielding behavior has characteristics that are different in some ways from the case of symmetric cyclic shear and exhibit pronounced finite size dependence. These cases are thus investigated with respect to annealing, strain amplitude and system size.

*[1] S. Sastry, Phys. Rev. Lett., **126**, 255501 (2021)*

5. Participant list

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