# Workshop: Machine Learning Glassy Dynamics

**Date:** 7-8 November 2022

**Venue:** Collège de France - site Ulm (3 rue d'Ulm - 75005) Paris

## Schedule

### Monday

- 9:00 - 10:30 **Olivier Dauchot** (Tutorial)
  *Open questions in glass physics : a naive perspective*
- 10:30 - 11:00 Coffee break
- 11:00 - 12:30 **Laura Filion** (Tutorial)
  *Investigating supercooled liquids with machine learning*
- 12:30 - 14:00 Lunch break
- 14:00 - 14:30 **David Richard**
  *Non-linear micromechanics of simple structural glasses*
- 14:45 - 15:15 **Camille Scalliet**
  *Equilibrium dynamics close to the glass transition: what is there to be learned?*
- 15:30 - 16:00 Coffee break
- 16:00 - 16:30 **Daniele Coslovich**
  *Dimensionality reduction of structure in glassy liquids*
- 16:45 - 17:15 **Joerg Rottler**
  *Exploring the Slow Dynamics of Grain Boundaries and Glasses With Markov State Models Constructed from Graph Dynamical Networks*

**Tuesday**

- 9:00 - 9:30 **Andrea Liu**
  *A softness-based model of glassy dynamics*
- 9:45 - 10:15 **Victor Bapst**
  *Unveiling the predictive power of static structure in glassy systems*
- 10:30 - 11:00 Coffee break
- 11:00 - 11:30 **Francesco Zamponi**
  *Where the really hard sampling problems are*
- 11:45 - 12:15 **Giovanni Volpe**
  *Quantitative Microscopy with Deep Learning*
- 12:30 - 14:00 Lunch break
- 14:00 - 14:30 **Gerhard Jung**
  *Predicting Dynamic Heterogeneity in Glass-Forming Liquids*
- 14:45 - 15:15 **Sylvain Patinet**
  *Relaxations in supercooled liquids: Connection between thermal excitations and local yield stresses of their inherent states*
- 15:30 - 16:00 Coffee break
- 16:00 - 16:30 **Miguel Ruiz Garcia**
  *Discovering dynamic laws from observations: the case of self-propelled, interacting colloids*
- 16:45 - 17:15 **Francois Landes**
  *Learning representations of glasses with roto-translational equivariant Graph Neural Networks*

## Abstracts

**Olivier Dauchot**: *Open questions in glass physics : a naive perspective*

When a molecular liquid is cooled below its melting point sufficiently fast that crystallization is avoided, it enters the meta-stable supercooled regime. Further decreasing the temperature, one observes a dramatic increase of the structural relaxation time over many orders of magnitude. Eventually, the system is presumed to fall out of equilibrium and to become an amorphous solid, a glass. The past 30 years have seen a surge of results which have significantly deepened our understanding of the physics of glass forming systems, including several breakthroughs: the emergence of a number of theoretical approaches, advanced computer simulations, and the quantitative experimental study of glassy phenomena in very different systems, extending the field of research from molecular liquids to colloidal suspensions and granular assemblies amongst a range of other materials. In this lecture, after a review of the key phenomenological facts associated with the glass transition, I will superficially describe what has been successfully achieved on the theoretical side in order to highlight the core questions that remain open, at least to my naive understanding. In particular I will focus on the gap that remains to be bridged between the mean field theoretical description and the activated dynamics that takes place in real glasses.

**Laura Filion**: *Investigating supercooled liquids with machine learning*

Over the last few years, machine learning has been shown to be a powerful tool in trying to unravel the structural and dynamics of supercooled liquids. In this talk, I will briefly describe the basics behind both supervised and unsupervised machine learning, including support vector machines, artificial neural networks, autoencoders, and graph neural networks. Using a few illustrations, I will then show how machine learning has been used to shed light on new features of supercooled liquids and the interplay between their local structure and dynamics.

**David Richard**: *Non-linear micromechanics of simple structural glasses*

We present a formalism to characterize elastic heterogeneities in amorphous solids. In particular, we derive high-order strain-energy expansions for pairwise energies under athermal quasistatic dynamics. We then use the presented formalism to study the statistical properties of pairwise expansion coefficients and their link with the statistics of soft, quasilocalized modes, for a wide range of glass stabilities in both two- and three-dimensional systems. We further exploit the presented framework to construct a structural field with predictive power of the loci of plastic events and of the formation of shear bands upon glass deformation. Finally, we discuss the tensorial properties of the proposed structural field and its connection with the micromechanics of non-linear plastic modes and of the local yield stress measured using the so-called cavity method.

**Camille Scalliet**: *Equilibrium dynamics close to the glass transition: what is there to be learned?*

Our understanding of the mechanism by which liquids transform into glasses is often described as a major open problem in condensed matter physics. In this talk, I will present very recent numerical developments which allow for the first time to investigate the slow dynamics of supercooled liquids close to the glass transition. I will discuss the microscopic picture revealed by our computer simulations, how it helps us both to rationalize key experimental signatures of glassy dynamics and guide theoretical developments. I will discuss how these recent results provide exciting opportunities to shift machine-learning studies closer to the glass transition.

**Daniele Coslovich**: *Dimensionality reduction of structure in glassy liquids*

I will assess the ability of dimensionality reduction techniques to identify collective variables that capture structural heterogeneity in several glassy models. These structural variables can be used to provide a coarse-grained definition of locally favored structures, as well as for fitting the fluctuations of the particles' mobility. I will compare the results obtained with such

an unsupervised approach to those of simple regression models and discuss outstanding issues in data-driven and theoretical modelling of structure-dynamics relationships.

**Joerg Rottler**: *Exploring the Slow Dynamics of Grain Boundaries and Glasses With Markov State Models Constructed from Graph Dynamical Networks*

A persistent challenge for molecular simulations is to assess slow processes efficiently from short trajectories. Important examples of slow phenomena in materials are the motion of interfaces (grain boundaries) in crystals or the structural relaxation in glass forming liquids. Markov State Models (MSM) are an attractive tool to unveil the slowest processes of a complex atomistic system in a low dimensional space of feature variables. This talk describes the predictions and insights gained from such MSMs constructed using machine learning techniques. In the context of high-symmetry grain boundaries (GB) in a bcc crystal, the model learns a hierarchy of timescales that can be associated with transformations between geometrically distinct motifs. While the slowest timescale always determines the bulk mobility of the GB, faster processes provide further insight into the local atomistic migration mechanisms inside the GB. When applied to a standard binary glass former, our model finds a transition timescale between states that is larger than the conventional structural alpha-relaxation time. Here, the learned map of states assigned to the particles corresponds to local excess Voronoi volume. These results resonate with classic free volume theories of the glass transition, singling out local packing fluctuations as one of the dominant slowly relaxing features. In both systems, the MSMs are able to simultaneously identify slow (hydrodynamic) variables, their associated relaxation time scales and spatial features. Moreover, they provide access to kinetics at temperatures where brute force calculations become computationally expensive or impossible.

Reference: Phys Rev E 106, 025308 (2022)

**Andrea Liu**: *A softness-based model of glassy dynamics*

I will describe how we construct a model for dynamics based on softness, a machine-learned particle-level quantity that quantifies the strength of a particle's cage. The model treats the interplay between softness and rearrangements—softness determines the energy barrier that must be overcome in order for the particle to participate in a rearrangement, while a rearrangement scrambles local structure and thereby changes the softness of the rearranging particle as well as the softnesses of particles nearby. These changes of softness must obey the constraint of detailed balance. I will describe how we incorporate this constraint in the model and show that the model captures dynamics reasonably well.

**Victor Bapst**: *Unveiling the predictive power of static structure in glassy systems*

Despite decades of theoretical studies, the nature of the glass transition remains elusive and debated, while the existence of structural predictors of its dynamics is a major open question. Recent approaches propose inferring predictors from a variety of human-defined features using machine learning. Here we determine the long-time evolution of a glassy system solely from the initial particle positions and without any handcrafted features, using graph neural networks as a powerful model. We show that this method outperforms current state-of-the-art methods, generalizing over a wide range of temperatures, pressures and densities. In shear experiments, it predicts the locations of rearranging particles. The structural predictors learned by our network exhibit a correlation length that increases with larger timescales to reach the size of our system. Beyond glasses, our method could apply to many other physical systems that map to a graph of local interaction.

**Francesco Zamponi**: *Where the really hard sampling problems are*

I will discuss a class of glassy problems that are exponentially hard to sample using conventional local Monte Carlo at low enough temperatures, and in particular the antiferromagnetic Potts model on a random graph, which reduces to the coloring of random graphs at zero temperature. We tested

several strategies that were proposed in order to improve sampling efficiency using machine learning, and found that they all fail. We conclude that these problems are good benchmarks for smart sampling algorithms.

**Giovanni Volpe**: *Quantitative Microscopy with Deep Learning*

Video microscopy has a long history of providing insights and breakthroughs for a broad range of disciplines, from physics to biology. Image analysis to extract quantitative information from video microscopy data has traditionally relied on algorithmic approaches, which are often difficult to implement, time consuming, and computationally expensive. Recently, alternative data-driven approaches using deep learning have greatly improved quantitative digital microscopy, potentially offering automatized, accurate, and fast image analysis. However, the combination of deep learning and video microscopy remains underutilized primarily due to the steep learning curve involved in developing custom deep-learning solutions. To overcome this issue, we have introduced a software, currently at version DeepTrack 2.1, to design, train and validate deep-learning solutions for digital microscopy. We use it to exemplify how deep learning can be employed for a broad range of applications, from particle localization, tracking and characterization to cell counting and classification.

**Gerhard Jung**: *Predicting Dynamic Heterogeneity in Glass-Forming Liquids*

Dynamic heterogeneity has been identified as one of the key features of glassy dynamics. Studying dynamic heterogeneity, in particular at low temperatures, could thus give deep insights into the glass transition itself. In this talk we propose a physics-informed supervised machine learning technique to predict dynamic heterogeneity in glass-forming liquids. Different from previous approaches our goal is to go beyond predicting single-particle propensity and rather focus on their spatial correlations.

We present results for several dynamic quantities used to characterize dynamic heterogeneity in glasses such as susceptibilities, four-point dynamic structure factors and four-point correlation functions. We show that the learned machine is indeed able to predict the intricate spatial correlations in

deeply supercooled liquids. Using these predictions we will discuss the novel observation that geometric changes of the rearranging clusters strongly impact growing heterogeneity at low temperatures.

**Sylvain Patinet**: *Relaxations in supercooled liquids: Connection between thermal excitations and local yield stresses of their inherent states*

While deeply supercooled liquids exhibit divergent viscosity and increasingly heterogeneous dynamics as the temperature drops, their structure shows only seemingly marginal changes. Understanding the relaxation processes involved in this dramatic slowdown is a key question for understanding the glass transition. Here, we study a binary Lennard-Jones mixture in the supercooled regime using molecular dynamic simulations. At low temperatures, thermal relaxation proceeds in a series of activated jumps between inherent structures, i.e. local minima of the potential energy landscape. From these inherent dynamics, we recover information about the location and kinetics of thermally activated rearrangements. By employing a local shear test method that gives access to the shear stress thresholds, we observe a strong connection between the local rate of thermal relaxations and their residual plastic strengths. The correlation is dominated by the softest shear orientations and increases with decreasing temperature, the underlying potential energy landscape playing an increasing role in the dynamics. For the lowest temperature investigated, the maximum correlation is comparable with the best values of literature dealing with the structure-property mapping, but here providing a real-space picture of relaxation processes. Our detection method of thermal rearrangements allows us to investigate the first passage time statistics and to study the scaling between the activation energy barriers and the residual plastic strengths. It further provides a way to study the back and forth, reversible thermal rearrangements whose relative rates increase as the temperature is lowered. By emphasizing the analogy in real space between thermal relaxations in supercooled liquids and plastic shear transformation of amorphous solids, these results shed new light on the nature of relaxations of glassy systems.
In relation to our previous works, the local yield stress method employed here has been shown to be highly helpful to capture the barrier dependencies to glass preparation [1], shear banding [2], plastically induced anisotropy [3] and has been found to be one of the best structural indicators to predict plastic activity in athermal amorphous solids [4]. It is, therefore, an ideal

tool for documenting, in a very rich way, what happens "inside" an amorphous solid and better characterizing the relationship between structure and plasticity. From a practical point of view, it makes it possible to envision a more quantitative multi-scale modeling strategy as demonstrated in [5].

[1] A. Barbot, M. Lerbinger, A. Hernandez-Garcia, R. García-García, M. L. Falk, D. Vandembroucq and S. Patinet, Local yield stress statistics in model amorphous solids, Phys. Rev. E 97, 033001 (2018). (pdf)
[2] A. Barbot, M. Lerbinger, A. Lemaître, D. Vandembroucq, S. Patinet, Rejuvenation and Shear-Banding in model amorphous solids, Phys. Rev. E 101, 033001 (2020) (pdf)
[3] S. Patinet, A. Barbot, M. Lerbinger, D. Vandembroucq, A. Lemaître, On the Origin of the Bauschinger Effect in Amorphous Solids, Accepted in Phys. Rev. Lett. 124, 205503 (2020) (pdf)
[4] D. Richard, M. Ozawa, S. Patinet, E. Stanifer, B. Shang, S. A. Ridout, B. Xu, G. Zhang, P. K. Morse, J.-L. Barrat, L. Berthier, M. L. Falk, P. Guan, A. J. Liu, K. Martens, S. Sastry, D. Vandembroucq, E. Lerner, M. L. Manning, Predicting plasticity in disordered solids from structural indicators, Physical Review Materials 4, 113609 (2020) (pdf)
[5] D. Fernández Castellanos, S. Roux, S. Patinet, Insights from the quantitative calibration of an elasto-plastic model from a Lennard-Jones atomic glass, Comptes Rendus Physique, Académie des sciences (2021) (pdf)

**Miguel Ruiz Garcia**: *Discovering dynamic laws from observations: the case of self-propelled, interacting colloids*

Active matter spans a wide range of time and length scales, from groups of cells and synthetic self-propelled particles to schools of fish, flocks of birds, or even human crowds. The theoretical framework describing these systems has shown tremendous success at finding universal phenomenology. However, further progress is often burdened by the difficulty of determining the forces that control the dynamics of the individual elements within each system. Accessing this local information is key to understanding the physics dominating the system and to create the models that can explain the observed collective phenomena. In this talk, we present a machine-learning model, a graph neural network, that uses the collective movement of the system to learn the active and two-body forces controlling the individual dynamics of the particles. We verify our approach using numerical simulations of active brownian particles, considering different interaction potentials

and levels of activity. Finally, we apply our model to experiments of electrophoretic Janus particles, extracting the active and two-body forces that control the dynamics of the colloids. Due to this, we can uncover the physics dominating the behavior of the system.

**Francois Landes**: *Learning representations of glasses with roto-translational equivariant Graph Neural Networks*

In this pedagogical talk, I will start by explaining the most common strategy for learning a representation of a glassy liquid, i.e. the supervised learning setup, applied to glasses. I will then sketch out the key features of Graph Neural Networks, motivating their use for the Glass problem. Indeed, the state of the art was surpassed by Graph Neural Networks (GNNs) [Bapst 2020], which however are heavy models (numerous parameters) and are not interpretable at all. I will then explain the notion of group-equivariance with respect to group-invariance, and motivate the use of roto-translational equivariant features (representations) for glasses. Following recent advances [Thomas 2018 and more recent], we propose using roto-translational equivariant Graph Neural Networks for the glass problem, showing it significantly improves the predictive power but also significantly reduces the number of parameters, while increasing the interpretability of the architecture. In particular, if time allows, I will show how the first layer of this kind of network can compute the expert features shown to perform very well [Boattini 2021].

[Bapst 2020: Unveiling the predictive power of static structure in glassy systems, Nature Physics]
[Thomas 2018: Tensor field networks: Rotation- and translation-equivariant neural networks for 3D point clouds, Google Research]
[Boattini 2021: Averaging local structure to predict the dynamic propensity in supercooled liquids, Physical Review Letters]