PhD subject

Smart disorder: linking structure to flow events with machine learning in amorphous solids

Profile

Master of Science — excellent level in science and general culture. A good level of English is required. The essential skills sought for this doctorate are: human qualities, communication, creativity, autonomy and adaptation, pedagogy and a strong motivation for research. A good level of programming, data analysis, physics and mechanics of materials is particularly appreciated.

Application

The doctoral contract is scheduled for three years, starting in the fall. Please send your application to sylvain.patinet@espci.fr : a detailed CV, cover letter, detailed exam results, master's notes, names and contact details of professors and supervisors who have followed your work, letters of recommendation, master's thesis, journal and conference articles or any other document establishing your skills for this doctorate.

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Doctoral school : ED 391, Sciences mécaniques, acoustique, électronique et robotique de Paris

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Websites : PMMH, Sylvain Patinet's web pages.

Keywords : Machine learning, Amorphous solids, Atomistics, Plasticity and Damage

Description of the thesis

Amorphous solids, unlike crystals, lack long-range structural order and exhibit universal yet complex mechanical properties. Their deformation involves localized, irreversible rearrangements, leading to strain softening and flow localization. However, understanding their mechanical behavior is challenging due to their out-of-equilibrium nature and the absence of identifiable topological defects. This project aims to quantitatively characterize plastic rearrangements in amorphous solids, linking structure to mechanics through atomistic simulations. Leveraging a novel numerical method for measuring local yield stresses into machine learning frameworks, we will address existing biases and inefficiencies in predicting flow defects.

Additionally, we will develop structural descriptors to enhance interpretability and establish robust flow defect classifications. This approach will provide a solid foundation for deriving physically justified constitutive laws, bridging the gap between crystalline and amorphous solid mechanics. The results will advance fundamental understanding while guiding the rational design of tough, durable materials with tailored mechanical properties.

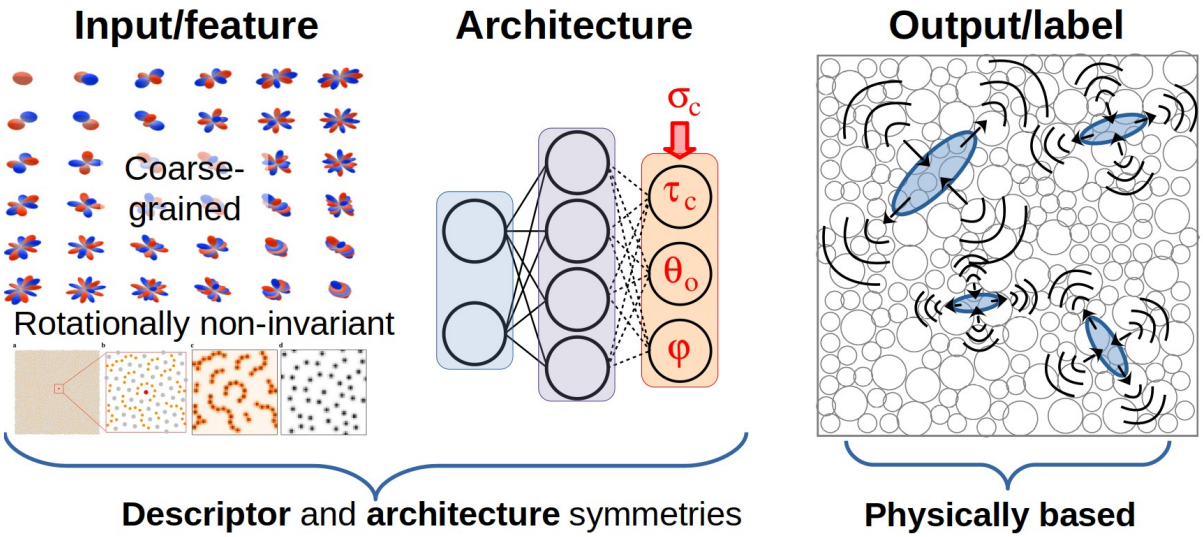

Figure 1: Quantitative framework for linking structure to mechanics, ensuring efficient, unbiased, and interpretable learning.

Scientific Problems and Objectives

Amorphous solids, such as glasses, colloids, and granular materials, lack long-range structural order yet exhibit universal mechanical behaviors. Their deformation is governed by localized, irreversible particle rearrangements, leading to strain softening and flow localization. However, their mechanical properties remain poorly understood due to their disordered nature, which prevents the identification of topological defects like dislocations in crystals. This challenge is underscored by the absence of dedicated sections on amorphous solid mechanics in classical physics textbooks. A deeper understanding of elementary flow events is essential for fundamental research and designing tougher, more durable materials. This project aims to systematically quantify plastic rearrangements in amorphous solids through innovative numerical simulations based on a new machine-learning approach.

Methods and Novelty

Our research group has recently developed a numerical technique to measure local yield systematically stresses in amorphous solids, providing a complete spatial field of plastic susceptibility [1-3]. This method is versatile, non-perturbative, and tensorial, making it an ideal tool for linking structure to mechanical properties. It has already been successfully applied to study shear banding, plastically induced anisotropy, and multiscale modeling. Leveraging this novel numerical method for measuring local yield stresses into machine learning frameworks, we will address existing biases and inefficiencies in predicting flow defects. In addition, this project will extend these approaches to more realistic systems, including granular media and cavitation phenomenon.

While machine learning has been widely used to predict amorphous solid dynamics, existing approaches rely so far on arbitrary binarization and fail to account for nonlocal effects, limiting their predictive accuracy. We propose integrating our quantitative yield stress measurements into machine learning models, offering a physically meaningful input that eliminates biases and captures the full threshold distribution of structural rearrangements. Such a strategy will enhance learning efficiency and require fewer training samples.

To improve interpretability, we will develop structural descriptors based on physical properties, such as stress and instability criteria, ensuring a clearer connection between structure and flow defects. These descriptors will include both anisotropic and isotropic features, enabling a comprehensive understanding of deformation mechanisms. Additionally, we will classify flow defects using a robust identification method based on multimodal Gaussian decomposition, mapping structural classes to specific mechanical instabilities.

Expected Results

This project will provide a fundamental understanding of amorphous solid mechanics, bridging the gap between crystalline and disordered materials. Linking micromechanics to macroscopic behavior will offer new ways to interpret experiments and develop physically justified constitutive laws. The findings will also contribute to the rational design of new materials with tailored mechanical properties. Beyond mechanics, this approach could help identify a relevant order parameter for glassy systems, addressing a long-standing question in the field.

References

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[2] 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*, PRE **97**, 033001 (2018)

[3] D. Ruan, S. Patinet, and M. L. Falk, *Predicting plastic events and quantifying the local yield surface in 3D model glasses*, J. Mech. Phys. Solids **158**, 104671 (2022)