Machine learning prediction of dynamics in amorphous materials

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Amorphous materials, such as supercooled liquids, glasses, colloids, foams, and granular materials under external loading, display rich and highly heterogeneous dynamics. For example, particle rearrangements, relaxation events, or plastic deformation often occur only in localized regions, giving rise to what is known as dynamical heterogeneity. Yet, despite this complex behavior, static snapshots of these systems often look nearly homogeneous, with few obvious visual features that would allow one to predict where or when motion will occur. This situation is in sharp contrast to crystalline materials, where dynamics and deformation are often associated with identifiable defects such as dislocations.

In recent years, developments in machine learning have opened a new route to this problem. A growing body of work has shown that future dynamics in amorphous materials can be predicted, at least to some extent, from static configurations alone. This raises fundamental questions: what structural information is encoded in a snapshot, how machine learning extracts it, and to what extent prediction leads to physical understanding. In this talk, I will review these recent advances, discuss their physical interpretation, and highlight methodological connections with the community working on machine-learning interatomic potentials and data-driven modeling of materials.