DY 14: Invited Talk: Machine Learning and Complex Fluids

Time: Tuesday 9:30–10:00   Location: MOL 213

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Unraveling structural and dynamical features in glassy fluids using machine learning — •Laura Filion[1], Frank Smallenburg[2], and Rinske Alkemade[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, Netherlands — [2]Laboratoire de physique des Solides, Université Paris-Saclay, France

Developments in machine learning (ML) have opened the door to fully new methods for studying phase transitions due to their ability to extremely efficiently identify complex patterns in systems of many particles. Applications of machine learning techniques vary from the use of developing new ML-based order parameters for complex crystal structures, to locating phase transitions, to speeding up simulations.

The rapid emergence of multiple applications of machine learning to statistical mechanics and materials science demonstrates that these techniques are destined to become an important tool for soft matter physics. In this talk, I will briefly present an overview of the work my group is doing on using ML to study soft matter systems, with a focus on how ML can be used to explore new connections between structure and dynamics in supercooled liquids. In particular, I will present a strategy to fit the dynamics in glassy systems using advanced hierarchical order parameters combined with simple linear regression. Additionally, I will present a method for extracting the cage structure of a glassy configuration, and demonstrate that this information significantly improves our ability to predict glassy dynamics over a broad range of time scales.