Molecular Dynamics and explainable Machine Learning methods to extract material properties

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Abstract

In recent years, the integration of machine learning (ML) into material science has brought transformative advancements, from computational methods to experimental analysis and prediction. Machine learning stands as a potent tool for predicting material properties from historical data, particularly beneficial when further experiments or simulations are difficult, expensive, or timely to perform. The data pool comes from accurate molecular dynamics (MD) simulations, which have been traditionally employed to extract properties at the atomic scale, providing valuable insights into dynamic material behavior. Here, MD simulations are exploited to extract the transport properties of fluids, such as the diffusion coefficient, shear viscosity and thermal conductivity, which, most of the time, involve timely, computationally intensive calculations. Towards accelerating this procedure, an explainable ML method, symbolic regression (SR), is employed to bypass MD simulations and suggest an intermediate mechanism of upscaling the simulations to higher scales, in a hybrid approach. Trained by MD data, new symbolic expressions of low complexity and error are derived without violating physical laws, achieving comparable (or, better) results to well-known microscopic and empirical expressions.

In this lecture, basic concepts of MD will be presented, along with an introduction to SR methods for explainable, symbolic expression extraction. Practical applications of synergistic MD/SR will be shown, and current research output will be highlighted.