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Rapid Prediction of Liquid Properties from Molecular Dynamics Simulations using Deep Learning

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Molecular dynamics simulations are indispensable tools in understanding collective in nature atom/molecule behavior in gas, solid and liquid phases on the molecular level if the quantum effects can be neglected. In order to accurately predict the structural and dynamic properties of complex solutions, tens of nanosecond-long simulation trajectories have to be analyzed.

In this work, we show that we can circumvent a need for computationally expensive simulations by using a point cloud-based deep learning strategy. As a result, rapid and accurate insight into the liquid structure can be achieved from much shorter trajectories. We implemented neural-network architectures to estimate structural property predictions of molecularly diverse systems composed of monatomic, diatomic, or triatomic entities at varying pressure and temperature.

A deep learning network based on PointNet is trained to extract atomic positions from a single MD snapshot and compute a temporal-averaged structural property, illustrated by the radial distribution function. We demonstrated that a well-trained deep learning architecture could rapidly predict the local structure of simple (Lennard-Jones particles) and complex (NO, H_2O) fluids. Next, we extended our approach to the fluid properties at the fluid/solid interfaces – and illustrated for water/calcite interface. The latter is important for a broad range of geochemical interfaces and offers a first step in a paradigm shift in the fast analysis of interfacial properties using molecular geochemical simulations.