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Scale-bridging using machine-learning: nanoconfinement effects in porous media

HARI VISWANATHAN, JAVIER SANTOS, ALEKSANDRA PACHALIEVA, QINJUN KANG AND TIM GERMANN

Los Alamos National Laboratory

Presenting Author: viswana@lanl.gov

Predicting the spatial configuration of gas molecules in nanopores geochemistry and flow through these connected nanopores is crucial for predicting the performance applications such as hydrocarbon recovery, CO_2 sequestration and fuel cells. All of these applications must rigorously account for nanoscale effects while simultaneously simulating much larger domains to predict overall system behavior. These applications have suffered from a computationally intractable multi-scale problem since fluid properties such as viscosity, density and adsorption must be calculated at the using expensive molecular simulation within a nanopore whereas flow through these connected nanopores must be simulated at the micron scale. We utilize machine techniques to bridge the nano- and micron- scales. We present a method for building and training physics-based deep learning surrogate models to carry out fast and accurate predictions of the molecular configuration of gas inside nanopores. Since training deep learning models requires extensive databases that are computationally expensive to create, we employ active learning (AL). AL reduces the overhead of creating comprehensive sets of high-fidelity data by determining where the model uncertainty is greatest, and running simulations on the fly to minimize it. Another outstanding issue in ML modeling is the untractable memory requirements needed to train with 3D domains. We will present our novel multiscale workflow that enables training models with large 3D array in a hierarchical, efficient manner. Our workflow enables nanoconfinement effects to be rigorously considered at the mesoscale where complex connected sets of nanopores affect flow.