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Physics-based machine learning framework for extracting multiphase pore-scale dynamics: Capturing phase distribution

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Incorporating pore-scale dynamics into reactive transport models is essential for enhancing their predictive capabilities, especially under multiphase conditions. Accurate reactive transport simulations are required for operational design and decision-making in various subsurface energy and storage applications, such as geothermal energy extraction, nuclear waste disposal, and carbon sequestration. Pore-scale dynamics are often derived using direct numerical simulations, such as the Lattice-Boltzmann method, on pore-network structures obtained from core samples or drill cuttings. These simulations are typically performed in two steps: phase distribution and transport. The phase distribution step initializes the phase distribution within the pore-network structures, accounting for capillary pressure, while the transport step calculates the effective properties of the multiphase-saturated structure. However, this two-step numerical simulation is computationally expensive due to the need for fine discretizations to resolve complex pore geometries and phase distributions, while also ensuring numerical stability. One strategy to reduce computational costs is the use of surrogate modeling.

We propose a physics-based machine learning approach to construct a surrogate model for addressing the first step of numerical simulation. Specifically, we use the saturation-conditioned U-Net method, where water saturation is incorporated into the U-Net architecture. This is achieved by modifying the skip connections in the U-Net, employing a Neural Network model that takes water saturation as input. This method enables the surrogate model to efficiently and accurately handle the high-dimensional variability of complex pore-network structures.

We demonstrate our approach by predicting phase distributions in two 3D porous media structures at multiple water saturations. To generate training and test datasets, we employ Lattice-Boltzmann simulations using the Shan-Chen model. We design the saturation-conditioned U-Net architecture to accept 2D images as input, rather than 3D images, to reduce the computational cost of model construction. Our results show that the proposed approach provides accurate 2D predictions and 3D reconstructions in a short time. It is also computationally efficient, as it does not require large training samples to achieve high accuracy. Furthermore, this framework is promising for robustly estimating effective properties from real core samples or drill cuttings, enabling their efficient integration into reactive transport solvers to enhance simulation accuracy.