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Fast evaluation of effective properties of partially saturated media using a derivative-based multiscale operator

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Effective properties, such as effective diffusivity, describe the movement of fluids, solutes, and charges in porous media and are strongly controlled by pore geometry and phase configuration. Evaluation of effective properties is the critical first step in understanding subsurface processes and is central to predictive modeling in subsurface energy and storage systems, including geothermal energy extraction, carbon sequestration, and nuclear waste disposal. Yet, the evaluation of effective properties remains a bottleneck from both numerical simulation and experimental perspectives.

Direct measurement of effective properties is labor-intensive due to long experimental times and the need to consider multiple saturation states. Consequently, direct numerical simulations are often employed to evaluate effective properties using microtomography reconstructions. However, these simulations are computationally expensive because fine discretizations are required to resolve complex pore geometries. Machine learning models have been proposed to address these challenges by mapping microtomography-reconstructed images to effective properties. The primary motivation for deploying machine learning here is to reduce computational cost and experimental effort in evaluating effective properties from given microtomography reconstructions.

However, because many machine learning models operate in a data-driven manner, they typically require large training samples and often lack physical interpretability due to their black-box nature. This contrasts with practical situations, where experimental data is limited, generating training samples via direct numerical simulations remains expensive, and physical consistency must be guaranteed.

We propose an approach to overcome these limitations by combining a derivative-based operator, formulated through a Taylor expansion, with K-means clustering. Effective properties are approximated using a Taylor expansion with respect to key geometrical parameters and saturation states within clustered regions sharing similar pore structures and phase configurations. This approach significantly reduces the number of required training samples while maintaining physical interpretability. Validation against experimental datasets demonstrates reliable predictions with more than three orders of magnitude computational speedup compared to full direct numerical simulations. This approach will reduce computational cost and experimental effort for accurate predictive modeling of transport in porous media.