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## Bridging Microscale Physics to Macroscale Models in Confined Porous Media

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Tight subsurface formations and shales often act as seals for subsurface systems that are envisioned to store fluids such as CO<sub>2</sub> and H<sub>2</sub> as part of a transition to low-carbon economies of the future. These seals often comprise complex nano-confined systems with heterogeneous physical and chemical features. The extreme confinement and heterogeneity in such systems present difficulties in terms of scale separation in modeling efforts. We aim to address this challenge by developing a scale translation framework that bridges the dominant physics at the microscale to model systems with complex geometries featuring a host of flow regimes. The scale-translation framework uses an optimized implementation of a multi-grid lattice Boltzmann method (MG-LB), capable of simulating complex pore networks that feature wide ranges of Knudsen numbers. The simulator is optimized using hash tables, indirect addressing, and parallelization techniques, extending the reach of the simulator to large and complex domains. The modeling tool generates a dataset of flow behavior in complex porous media, which is used to train a Machine Learning model, specifically, a deep neural network (DNN). Features of the pore networks, such as connectivity of the pore structures and pore size distributions, serve as input and the resulting DNNs estimate the transport properties in computational domains beyond the reach of the MG-LB models. The estimates will inform the macroscale properties of large-scale and heterogeneous, confined porous media.

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### Porous Media & Biology Focused Abstracts

### References

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