TAXILA LBM: A LATTICE-BOLTZMANN SIMULATOR FOR SINGLE- AND MULTI-PHASE FLOW IN COMPLEX POROUS MEDIA

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It has been recognized that many of the assumptions underlying conventional continuum models for flow and transport in porous media are not always met for engineering problems of practical interest. Thus, modeling efforts that couple the pore-scale to the continuum (Darcy) scale through upscaling or hybrid modeling have recently gained interest. Such problems are inherently computationally expensive, as resolving micro-scale features within a continuum-scale domain, even in relatively localized regions, requires signicant resources. In this work, we introduce the Los Alamos National Laboratory, open source simulator Taxila LBM - a parallel, lattice-Boltzmann simulator for single-, multi-phase and multi-component flow through complex porous media. First, we discuss the implementation of the LB method and some of the more advanced features including multiple relaxation time, higher order isotropy in the fluid-fluid interaction potential, mixed wettability, and the various equations of state available. Next we demonstrate the capabilities of Taxila LBM with some examples. In the first example, we highlight simulations for immiscible displacement in a micromodel porous medium. We specically focus on the comparison of specific fluid-fluid interfacial length between the experiments and the LB simulations. In the next example, we discuss simulations of CO2 and H2O in porous media. In these simulations we quantify trapped CO2 and estimate relative permeability curves. In addition, Taxila LBM has been coupled to PFLOTRAN (a continuum scale multi-phase flow and reactive transport simulator), where the transport equations in PFLOTRAN have been modied to work at the pore-scale. In this coupling, flow is simulated using Taxila LBM, while multi-mineralic and many-species reactions are simulated using PFLOTRAN. We present examples of reacting flows that are not well-mixed at the pore-scale, and discuss implications for common assumptions at the continuum scale.