COUPLING LATTICE BOLTZMANN AND CONTINUUM EQUATIONS FOR THE SOLUTION OF MULTISCALE FLOW AND REACTIVE TRANSPORT IN POROUS MEDIA.

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In reservoir simulations including complex geometries and/or multiphase, reactive flows, continuum equations based upon Darcy's law may break down in specific spatial and temporal regimes. In these cases, hybrid methods solving strongly coupled systems of Darcy's law and some form of Navier-Stokes on the physical geometry may be necessary.
Here we demonstrate an overlapping-Schwartz domain decomposition strategy for hybrid simulations combining lattice Boltzmann simulations of flow at the micro-scale with continuum-scale simulations of Darcy's law. Lattice Boltzmann methods (LBM) have the advantage of converging to the Navier-Stokes equations on the pore-scale geometry, which can then be upscaled to the continuum scale. By using a Finite Volume Element Method for the continuum regime, interpolations implied by the finite elements impose a choice for removing non-uniqueness in downscaling from the continuum scale to the micro-scale. We implement the coupling within the Taxila LBM and PFLOTRAN frameworks, resulting in a massively parallel hybrid simulator for flow and reactive transport in fractured porous media.
We demonstrate the method with a few examples. A fracture is included within a porous medium; within the fracture, Darcy's law is not valid, and Navier-Stokes equations are solved using the LBM. Away from the fracture, continuum equations are solved, and the regions are coupled through flow. In another example, simulations including reactive transport are shown, in which heterogeneous multi-mineralic structures are resolved at the pore-scale, enabling reactions to include this heterogeneity, while homogenous structures are resolved at the continuum scale.