

# An Adaptive Embedded Boundary Method for Pore Scale Reactive Transport

Advanced Simulation of Subsurface Flow and Transport at the Pore Scale

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## *Abstract*

Precipitation (or dissolution) of mineral grains modifies the geometry of the pore space in subsurface sediment with evolving solid-liquid boundaries. In turn, changes in the pore space alter the groundwater flow through the sediment, which ultimately affects the continuum scale reaction rates that are relevant for field applications such as carbon sequestration. Modeling provides a unique tool to understand and quantify the feedback processes between mineral precipitation (or dissolution) and flow at the pore scale. However, for modeling to accurately resolve the flow and reactive transport dynamics at microscopic length scales in real porous media sediments, a method capable of representing complex solid-fluid and fluid-fluid boundaries in a high performance simulation framework is necessary.

We present a simulation capability that models flow and transport at the pore scale with multicomponent geochemistry. The equations for flow and conservative transport (scalar advection-diffusion) are modeled using embedded boundary finite volume methods and high performance simulation tools developed in the Chombo framework; reactive transport is included by interfacing the flow and transport solver with the geochemical module in the CrunchFlow package. Reactions are advanced explicitly using operator splitting. The embedded boundary method is a natural choice to characterize fluid-solid interfaces—the reactive surface area used in CrunchFlow is the area of the embedded boundary of a cut cell on a Cartesian grid. This approach is also compatible with adaptive mesh refinement for tracking sharp gradients in concentration that typically drive precipitation and dissolution reactions. Furthermore, embedded boundary finite volume discretizations are the basis of algorithms used for moving fluid-solid and fluid-fluid interfaces, providing a robust and consistent methodology that we will apply to multiphase, reactive transport problems (ongoing work with G. Miller, UC Davis). We show simulation results for calcite dissolution in complex pore structures that are reconstructed from synchrotron-based X-ray computed microtomography images. In this example, the geometry of the pore space is not affected by the mineral reactions. Also, toward the ultimate goal of upscaling better parameterizations to the field scale, we use the model to examine the inter-dependence between continuum-scale dissolution/precipitation rates and flow patterns at the pore scale in different porous media geometries by using volume averaging methods.