Code interoperability in reactive transport modeling: The adaptive mesh refinement example

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The fate of reactive solutes in the subsurface is the result of the coupling between physical processes and complex reaction networks. Capabilities available in geochemical codes reflect this complexity, typically including a wide range of homogeneous and heterogeneous reactions, under kinetic and equilibrium assumptions. For convenience, implementation of new geochemical capabilities into flow and transport codes is often circumvented by coupling them to existing reaction codes. While these couplings have been successfully accomplished on a case by case basis, a systematic way to carry them out may improve efficiency and facilitate code maintenance. Further, interoperability can make it possible to access a range of capabilities not available in legacy codes.

Adaptive mesh refinenment (AMR) is a numerical technique for locally adjusting the resolution of computational grids. AMR makes it possible to superimpose levels of finer grids on the global computational grid in an adaptive manner allowing for more accurate calculations locally. In reactive transport problems, AMR may be particularly useful in accurately capturing concentration gradients (hence, reaction rates) that develop in localized areas of the simulation domain, while using a coarser grid elsewhere, thus without need of trading off resolution for simulation domain size.

Here, we have used Alquimia, a biogeochemistry API and wrapper library that provides a unified interface to the biogeochemistry routines from geochemical codes, to couple the existing codes CrunchFlow and PFlotran to Amanzi, a flow and transport simulator built with AMR capabilities. Both Alquimia and Amanzi have been developed as part of Advanced Simulation Capability for Environmental Management (ASCEM), a software project that aims at developing next-generation, science-based reactive flow and transport simulation capabilities to address DOE-EM’s waste storage and environmental cleanup challenges.

In this presentation, we will describe the challenges associated with the development of such interfaces. Further, we will present applications of the resulting coupled simulation with an emphasis on highlighting the use of adaptive mesh refinement in reactive transport modeling.