ACCELERATING REACTIVE TRANSPORT SIMULATIONS WITH AN ON-DEMAND LEARNING STRATEGY FOR CHEMICAL EQUILIBRIUM AND KINETICS CALCULATIONS

Allan Leal

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Geochemical reaction calculations in reactive transport simulations are extremely costly. These are chemical equilibrium and/or kinetics computations involving many fluid species and rock minerals, which are needed (at least once) in every mesh cell, at every time step of the simulation. As a result, they can account for over 99% of all computing costs in the simulation when realistic chemical descriptions of fluids and rocks are considered in the model. It turns out, however, that many such geochemical calculations, during the course of a reactive transport simulation, have similar (*not identical*) input conditions. As such, by solving key chemical equilibrium and kinetics problems (*determined on-demand during the simulation*), and computing the derivatives of their output with respect to their inputs (*sensitivity derivatives*), we are able to quickly and accurately estimate the majority of subsequent geochemical reaction calculations in the simulation. This is done by applying a first-order Taylor approximation using the currently recorded input/output conditions and their associated sensitivity derivatives. This on-demand learning strategy effectively allows us to **entirely bypass** *(i)* Newton iterations when solving the equations that govern chemical equilibrium (using either Gibbs energy minimization or law of mass action formulations) as well as *(ii)* the integration time steps when solving the ordinary differential equations that govern chemical kinetics. This on-demand learning algorithm can also be used to speed up other costly computations, such as evaluations of fluid properties, equations of state, reaction rates, and so forth. Some reactive transport simulation examples are shown, which demonstrate speedups of several orders of magnitude when solving chemical equilibrium and kinetics calculations with the on-demand learning strategy.

A. Leal
ETH Zurich
allan.leal@erdw.ethz.ch