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Physics-based machine learning for reactive transport simulations

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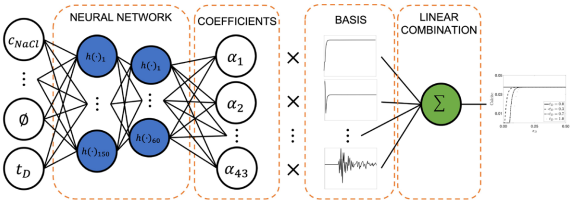

Reactive transport simulations are essential to understand the impact of fluid flow and chemical reactions on subsurface reservoir properties and processes, such as reduced permeability due to mineral precipitation. Reactive transport simulations are numerically expensive (especially for large-scale simulations) since they often require fine numerical meshes to achieve numerical stability, while solving non-linear algebraic and differential equations to account for chemical equilibrium and kinetic processes in each grid element at each time step. Performing uncertainty quantification for reactive transport simulations can therefore be prohibitive, given the large number of simulations required to characterize uncertain physical and chemical aspects of the subsurface. In this work, we present a novel surrogate modeling approach to enable efficient uncertainty quantification studies involving reactive transport processes.

The novel approach we present, based on physics-based machine learning, is compared to a pure data-driven machine learning approach. For the physics-based machine learning approach, we use the *non-intrusive reduced-basis* (NI-RB) method, which has so far not been applied to reactive transport simulations. The NI-RB expresses the state of a reactive transport simulation at each time step as a linear combination among basis functions and coefficients. This construction guarantees preserving the structure of reactive transport problems. The data-driven machine learning approach utilizes a Neural Network model to capture the solutions from given inputs and outputs, generated from a reactive transport model. We provide comparisons based on accuracy and efficiency at the training stage, as well as acceleration at the prediction stage.

We use a reactive-transport-with-dolomitization case for our comparisons. It is a non-linear system which has “shock” features in its solutions. For the generation of a training and test dataset, we use Reaktoro, an open-source framework for simulating chemically reactive systems. We show that the NI-RB surrogate model can accurately capture sharp transitions in mineralogy transformations during reactive transport simulation, whereas the data-driven surrogate model cannot, even with a much larger number of training samples.