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Accelerating Micro-Macro Models for Two-Mineral Reactive Systems with Machine Learning

Monday, May 31, 2021 10:40 AM (15 minutes)

In this talk, we present an effective micro-macro model for reactive flow and transport in evolving porous media exhibiting two competing mineral phases. As such, our approach comprises flow and transport equations on the macroscopic scale including effective hydrodynamic parameters calculated from representative unit cells. Conversely, the macroscopic solutes'concentrations alter the unit cells' geometrical structure by triggering dissolution or precipitation processes on the distinct mineral surfaces. Gradually, such processes result in complex and hardly predictable geometries. Therefore, these do not allow for low dimensional parameter representations. Accordingly, associate effective parameters cannot be covered by simple heuristic laws. Hence, we derive hydrological parameters directly from the full geometry represented by level-set methods. The numerical realization of such micro-macro models poses several challenges, especially in terms of computational complexity due to the increased dimensionality of the problem. Costly computations of effective parameters directly from the representative geometry often constitute a bottleneck in the simulation of highly heterogeneous media. In this talk, the significant performance enhancements arising from machine learning techniques are evaluated. To this end, convolutional neural networks (CNNs) are trained on geometries derived from geological microCT scans to predict hydrodynamic parameters such as permeability and diffusivity. The pretrained networks are subsequently deployed in a micro-macro simulation. We investigated the results in terms of computation time reduction and maintenance of high predictive quality.

Time Block Preference

Time Block B (14:00-17:00 CET)

References

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