Contribution ID: **470** Type: **Oral Presentation**

Improving the Performance of Reactive Transport Simulations using Artificial Neural Networks

Thursday, 2 June 2022 14:30 (15 minutes)

Reactive transport models (RTM), which couple geochemical reactions with solute, water and heat transport, are extensively used in a broad range of geoscientific applications related to e.g. Oil & Gas, Carbon Capture & Storage, Mining and Nuclear Waste Management. Despite being powerful tools, RTM often require significantly large computational times, which means that massively parallel high-performance computing equipment and codes are needed for direct numerical solutions in realistic applications. Thus, increasing efforts are currently being made to improve the computational performance of available reactive transport codes. In this contribution, we present a modelling framework using Artificial Neural Networks (ANN) that provides a substantial reduction of the computational burden of reactive transport simulations.
Typical reactive transport simulations involve recursive calculations of chemical reactions at each element and time step of the spatio-temporal discretization of the model domain. These calculations, which might be considerably slow, are sometimes redundant as they might be based on a very similar set of input values. In this work, an ANN is trained to calculate calcite replacement by dolomite with data obtained with PhreeqC, a widely used geochemical simulator. Several training strategies are tested to obtain the best trained ANN. It is shown that the ANN, if trained correctly, can provide considerable accuracy, typically in the range of tolerances required by RTM, and dramatically improves the performance of chemical calculations.
Subsequently, we use the trained ANN in conjunction with Comsol Multiphysics to carry out reactive transport simulations in a three-dimensional highly coupled system: the hydrothermal dolomitization of a fractured carbonate reservoir [1]. This realistic test case is used to evaluate the performance of the proposed modelling tool in comparison with that of a more traditional reactive transport code. The overall conclusion of this study is that the Machine Learning approach presented here results in a speed up of one order of magnitude as compared to traditional reactive transport, while providing accurate results. This makes the proposed algorithm potentially appealing for the simulation of large-scale complex geochemical systems.

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References

[1] Abarca, E., Idiart, A., Grandia, F., Rodríguez-Morillas, N., Pellan, C., Zen, M., Aït-Ettajer, T., & Fontanelli, L. (2019). 3D reactive transport modeling of porosity evolution in a carbonate reservoir through dolomitization. Chemical Geology 513, 184–199.

Time Block Preference

Time Block A (09:00-12:00 CET)

Participation

Online

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