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Surrogate Models for Reactive Transport

ANGUS FOTHERBY[1], HAROLD J BRADBURY[1], JENNIFER L DRUHAN[2] AND ALEXANDRA (SASHA) TURCHYN[1]

[1]University of Cambridge

[2]University of Illinois at Urbana-Champaign

Presenting Author: af606@cam.ac.uk

Reactive transport modelling is a widely used approach in Earth sciences for process-based, quantitative descriptions of a variety of environments. The development of high-fidelity reactive transport models (RTMs) requires both accurate parameterization and validation using real-world data. To date, these simulations are commonly developed in application to a specific field site or dataset, and their use to infer basic balances between various effects of transport and reactivity is relatively limited. One cause for this scarcity is the time necessary to run many realizations of computationally costly algorithms across a representative range of parameter space, such as may be needed to optimise a particular process or chemical reaction for a given criteria.

We present a new approach for interrogating and analysing RTMs. By choosing a subset of the boundary and initial conditions for an RTM and drawing values for each condition from a uniform distribution we build a data set that describes the behaviour of the model over a wide range of parameter values. Using this synthetic dataset as training data for a gradient boosted trees (GBT) model, we can create a surrogate model of the underlying reactive transport simulation that can be interrogated in the parameters that were varied in the original dataset. The time for a single query to the surrogate model is on the order of milliseconds rather than the seconds/minutes/hours for a single forward RTM simulation, so we can examine the geochemical space at a much higher resolution, much faster than we can by directed iteration of the RTM boundary/initial conditions. In this study, we demonstrate the utility of these surrogate models in optimising reactive transport boundary/initial conditions for maximising mineral precipitation by finding local maxima in the parameter space.

We also present a tool for creating the synthetic datasets in an automated fashion in the form of a Python wrapper around the open-source reactive transport modelling software CrunchTope. Our results have implications for bioremediation, carbon capture and storage, and other areas where optimisation of chemical reaction in the subsurface is of interest.