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Surrogate model approach for improving the performance of reactive transport simulations

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Reactive transport models can serve a large number of important geoscientific applications involving underground resources in industry and scientific research. It is common for simulation of reactive transport to consist of at least two coupled simulation models.

First is a hydrodynamics simulator that is responsible for simulating the flow of groundwaters and transport of solutes. Hydrodynamics simulators are well established technology and can be very efficient. When hydrodynamics simulations are performed without coupled geochemistry, their spatial geometries can span millions of elements even when running on desktop workstations.

Second is a geochemical simulation model that is coupled to the hydrodynamics simulator. Geochemical simulation models are much more computationally costly. This is a problem that makes reactive transport simulations spanning millions of spatial elements very difficult to achieve.

To address this problem we propose to replace the coupled geochemical simulation model with a surrogate model. A surrogate is a statistical model created to include only the necessary subset of simulator complexity for a particular scenario.

To demonstrate the viability of such an approach we tested it on a popular reactive transport benchmark problem that involves 1D Calcite transport. This is a published benchmark problem (Kolditz, 2012) for simulation models and for this reason we use it to test the surrogate model approach. To do this we tried a number of statistical models available through the caret and DiceEval packages for R, to be used as surrogate models. These were trained on randomly sampled subset of the input-output data from the geochemical simulation model used in the original reactive transport simulation. For validation we use the surrogate model to predict the simulator output using the part of sampled input data that was not used for training the statistical model. For this scenario we find that the multivariate adaptive regression splines (MARS) method provides the best trade-off between speed and accuracy.

This proof-of-concept forms an essential step towards building an interactive visual analytics system to enable user-driven systematic creation of geochemical surrogate models. Such a system shall enable reactive transport simulations with unprecedented spatial and temporal detail to become possible.

References:

Kolditz, O., Görke, U.J., Shao, H. and Wang, W., 2012. Thermo-hydro-mechanical-chemical processes in porous media: benchmarks and examples (Vol. 86). Springer Science & Business Media.