



Charge and mass-balance as accuracy control of data-driven geochemical surrogates

Marco De Lucia, Janis Jatnieks, Mike Sips, and Michael Kühn

GFZ German Research Centre for Geosciences, Potsdam, Germany (delucia@gfz-potsdam.de)

A promising way to speedup coupled reactive transport simulations is offered by the use of statistical surrogates instead of the "full-physics" geochemical submodels, which usually represent the computational bottleneck of such simulations. Data-driven surrogates are simplified statistical models obtained by fitting on an ensemble of precalculated full-physics simulations, capturing their behaviour while being fast to compute. Our previous work demonstrates the achievable speedups on a benchmark scenario [1]. However, more complex models require exponentially larger computational resources for surrogate fitting and tuning.

For application in coupled reactive transport, it is required that the geochemical surrogates honour the charge and mass balance of chemical elements and species across the fluid and mineral phases, a feature which is not guaranteed by regressors. We evaluate the balance equations themselves as criteria for accuracy of surrogates. This allows the use of simple but fast surrogates in the parameter space regions where they are most accurate. The correctness of balance, evaluated at runtime during coupled simulations, can discriminate whether a surrogate response can be accepted or a costly full-physics geochemical simulation is needed.

We present the performance evaluation of different surrogate models on reactive transport examples of increasing complexity, with geochemistry both at local thermodynamic equilibrium and kinetically controlled.

[1] Jatnieks, J., De Lucia, M., Dransch, D., Sips, M.: "Data-driven surrogate model approach for improving the performance of reactive transport simulations.", *Energy Procedia* 97, 2016, p. 447-453.