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Integrating surrogate models into subsurface simulation framework allows computation of complex reactive transport scenarios

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Reactive transport simulations - where geochemical reactions are coupled with hydrodynamic transport of reactants - are extremely time consuming and suffer from significant numerical issues. Given the high uncertainties inherently associated with the geochemical models, which also constitute the major computational bottleneck, such requirements may seem inappropriate and probably constitute the main limitation for their wide application.

A promising way to ease and speed-up such coupled simulations is achievable employing statistical surrogates instead of "full-physics" geochemical models [1]. Data-driven surrogates are reduced models obtained on a set of pre-calculated "full physics" simulations, capturing their principal features while being extremely fast to compute. Model reduction of course comes at price of a precision loss; however, this appears justified in presence of large uncertainties regarding the parametrization of geochemical processes.

This contribution illustrates the integration of surrogates into the flexible simulation framework currently being developed by the authors' research group [2]. The high level language of choice for obtaining and dealing with surrogate models is R, which profits from state-of-the-art methods for statistical analysis of large simulations ensembles. A stand-alone advective mass transport module was furthermore developed in order to add such capability to any multiphase finite volume hydrodynamic simulator within the simulation framework.

We present 2D and 3D case studies benchmarking the performance of surrogates and "full physics" chemistry in scenarios pertaining the assessment of geological subsurface utilization.

[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.

[2] Kempka, T., Nakaten, B., De Lucia, M., Nakaten, N., Otto, C., Pohl, M., Chabab [Tillner], E., Kühn, M.: "Flexible Simulation Framework to Couple Processes in Complex 3D Models for Subsurface Utilization Assessment.", Energy Procedia, 97, 2016 p. 494-501.