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

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Abstract

We showcase a flexible, extensible yet efficient framework for reactive transport modelling, including the ability to replace “full physics” geochemical simulations with surrogate models for speedup. Surrogates are data-driven models trained on a set of pre-calculated simulations by means of machine-learning methods. We offer also an input-output-error visualization component for interactive assessment and tuning of their accuracy. Our framework, based on open source or freely available software, makes possible complex reactive transport simulations and ease further research on optimized algorithms to tackle many geoscientific problems.

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1. Introduction

Numerical simulations of subsurface processes are required to assess feasibility of, e.g., CO₂ or hydrogen storage projects, recovery scenario optimization, geothermal projects, estimation of long-term environmental impacts, nuclear waste disposal as well as forecasting energy or petroleum production. The complexity and the diversity of hydrodynamical, geochemical, geomechanical and thermal processes requires highly specialised software for each subprocess in order to profit from state-of-the-art methods and numerical algorithms. The coupling of these processes - i.e., the simultaneous simulation of concurrent and interacting physical phenomena - can be achieved with “software bridges” which make the specialized subprocess simulators communicate to each other. To this specific end the authors developed a flexible simulation framework [1,2] providing an efficient workflow for integrating diverse data sources and diverse software packages to perform coupled process simulations.

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In the case of coupled reactive transport modelling [3], which considers subsurface geochemical interactions between migrating fluids and rocks, hydrodynamic simulations are complicated by the transport of an arbitrary number of solute species and the chemical reactions occurring between those solutes and the rock-forming minerals. The phenomenological model used to simulate chemical reactions, either based on the Law of Mass Action or Gibbs Energy Minimization, relies upon a large number of thermodynamic and kinetic parameters and its solution is hampered by non-linearity and stiffness of the resulting differential-algebraic system of equations, often generating numerical instabilities and convergence failures. For this reason, massive parallelization of reactive transport simulators is necessary for speed, but still does not guarantee successful simulations. In general terms, the total computational cost of reactive transport simulations is governed by geochemistry, which can account for up to 90% of CPU time [4]. This is an important limiting factor for their wide application. As result, only relatively simple geochemical systems at significantly lower spatial resolution and timescales than pure hydrodynamics simulations are achievable, mainly on 2D or coarse 3D models, and many relevant geological features such as spatial heterogeneity, are often completely disregarded [5].

However, geochemical reactions are affected by extremely large uncertainties both in the characterization of the subsurface and in the parametrization of the phenomenological model itself. Typically, the kinetic constants and the measurements of reactive surfaces of minerals display an uncertainty which may span across several orders of magnitude [6,7]. Also the thermodynamic parameters associated to geochemical reactions are affected by large uncertainties, especially for high salinity, high temperature fluids [8,9]. Thus, expensive and unstable reactive transport simulations in presence of such large uncertainties appear unjustified.

A promising way to enhance calculation speed is represented by the substitution of the “full physics” complex geochemical simulations by statistical surrogate models trained by machine-learning algorithms on a large set of pre-calculated simulations of the specialised software, as was demonstrated by a proof-of-concept implementation [10]. The surrogates are efficient to compute and smooth, which is a decisive advantage for coupled simulations. The price to pay for such an increase in computational efficiency is a loss of accuracy, which is however justified by the large uncertainties associated with the geochemical processes as discussed above.

This contribution shows recent enhancements in our simulation framework concerning reactive transport modelling, specifically aimed at the inclusion of surrogates instead of standard geochemical models for coupled simulations. Starting point and building blocks of the framework are the MUFITS reservoir simulator [11,12]. It is a freely available research code, based on finite volumes, able to efficiently simulate multiphase flow problems. In order to employ MUFITS as hydrodynamical engine for reactive transport, we implemented a multispecies mass transport module, which is at the moment limited to pure advection, intended for file-based coupling with MUFITS. The open source “full physics” simulator PHREEQC [13] has been extensively used in our research group for geochemical modelling. In particular, we developed the Rphree¹ [8] interface to the high-level language and environment R [14]. This interface served as foundation for the development of the infrastructure for surrogate training as exposed in [10]. The R environment is particularly suited for machine-learning, given its status as leading platform in this domain and the plethora of extension packages implementing state-of-the-art data science algorithms. We therefore decided to use R as the main programming language for this reactive transport infrastructure and implemented the coupling with MUFITS, the transport module, the reactive transport algorithms and some visualization functions in form of R extension packages. For better performance, the most computationally intensive algorithms are written in C++ using the Rcpp interface [15].

Furthermore, we recognised the need for a Visual Analytics tool in order to interactively explore the accuracy of surrogate models. The next section illustrates our approach in this matter. In the following sections, we illustrate with more detail the implemented transport module. Finally, a few test cases of reactive transport simulations calculated with the newly developed framework are given.

2. An interactive visualization component to explore and tune surrogate models

The creation of data-driven surrogates for geochemical models is a challenging task and a fertile research area with many open questions [10]. Namely, geochemical models involve many input-output parameters, thus requiring

¹ Rphree is open source software downloadable at: rphree.r-forge.r-project.org

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