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Enhancing Reactive Transport Simulations with Machine Learning, Adaptive Algorithms, and High-Performance Computing

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Abstract

Reactive transport simulations in porous media are used to investigate the temporal and spatial evolution of the system of interest in various scientific and industrial applications such as geothermal energy, CO_2 sequestration and deep geological disposal of nuclear waste. For such systems the interplay between flow and chemical reactions plays an important role while the evolving solid structure may give rise to strong non-linearities. For the case of geological disposal very long periods of geochemical interactions have to be considered which may span up to 1 million years while the involved processes are of multiscale nature. High-resolution simulations have the potential to provide crucial information regarding the understanding of the underlying mechanisms, as well as the design of engineered systems.

Over the last years the efficiency of such algorithms has been significantly improved, in some cases by several orders of magnitude by advancements on several key areas: (a) by resorting to machine learning techniques, such as neural network models, to develop surrogate models for the (geo)chemical solver, which can be integrated during simulations [1]; (b) by implementing adaptive algorithms capable of dynamically adjusting time steps based on the identification of stationary system states; and (c) by optimizing code parallelization for hybrid CPU/GPU supercomputing architectures, significantly enhancing resolution and reducing time to solution.

The gains in efficiency for the geochemical solvers have been recently studied in a benchmark exercise within the EURAD-DONUT project [2]. Such a scheme along with a smart time-stepping algorithm have been implemented to a Lattice Boltzmann simulator which is used to study the microstructural evolution of cement-clay interfaces, central to several applications. The model considers dissolution and precipitation reactions which are driven by the geochemical contrast of the two materials. Such reactions alter the microstructure of the pore-space and in turn impact the mass transport properties. By combining all algorithmic and hardware capabilities the simulations are completed several orders of magnitude faster, paving the way for digital twins of experiments [3] as well as of subsurface engineered systems for sustainable resource management.

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