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Accelerating reactive transport simulations by combining machine learning, smart algorithms and high performance computing

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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. Realistic high resolution simulations are computationally challenging, especially when long periods of geochemical interactions, or multiple temporal and spatial scales have to be considered. A considerable boost in efficiency may be achieved by improving algorithms in three directions: a) machine learning techniques, e.g. neural networks can be used to create surrogate models of the geochemical solver to be used during the simulation, b) smart algorithms can adapt the time step by identifying stationary system states on-the-fly, and c) parallelization of code for hybrid CPU/GPU supercomputing architectures can dramatically increase the resolution of the simulation and the time to solution. The efficiency gains will be demonstrated by several examples such as the cement-clay interaction which is of great relevance for underground constructions. The pore-level simulator is based on the lattice Boltzmann method and can describe the microstructural evolution (dissolution and precipitation), which is driven by the geochemical contrast of the involved materials, in two and three dimensions. The numerical model allows to follow the induced microstructural evolution, which in tunr significantly alter 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 as well as of subsurface engineered systems for sustainable resource management.