Accelerating chemical kinetics for geochemical modeling

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Chemical kinetics is essential for the understanding of geochemical processes that occur at a wide range of time scales. In geochemical modelling, it is primarily used for simulating the dissolution and precipitation of minerals under a variety of fluid composition and temperature conditions. In contrast to chemical equilibrium, chemical kinetics requires the solution of a time-dependent problem, governed by a system of ordinary differential equations. Thus, calculating the evolution of fluid and rock compositions, altered as a result of geochemical reactions, is a more challenging and computationally expensive operation.

We present the use of an on-demand machine learning strategy that enables predicting entirely new chemical kinetics paths from previously calculated ones. This approach is then able to bypass all expensive computations that would have been performed from scratch otherwise, and thus resulting in large speed-ups. More specifically, fully computed chemical kinetics paths are used to estimate new ones that start from similar initial conditions. The learning nature of the proposed algorithm is dynamic, i.e., it is performed only when it is needed as the simulation proceeds.