The future of reactive transport modeling: using on-demand machine learning for its massive acceleration

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Reactive transport simulations have historically endured a difficult computational challenge: how can we drastically accelerate them in a way that is accessible to anyone, and not to only those with access to state-of-the-art supercomputers? Performing these simulations dozens to hundreds of times faster, for example, has the benefit of allowing us to properly study subsurface systems under a variety of conditions, and also to conduct sensitivity analyses that will indicate how each of the various parameters in the model affect the behavior of the system under investigation. Thus, to solve that challenge, the future of reactive transport modeling has to rely not only on the use of massively parallel computing, but also on smart and high performance algorithms.

In this presentation, an unconventional machine learning method is proposed to speed up the most expensive computations in reactive transport modeling: *chemical equilibrium* and *chemical kinetics*. Since these chemical reaction calculations can easily account for over 90% of the overall simulation costs, substantially accelerating them will also strongly reduce reactive transport simulation times. The machine learning strategy proposed here requires no a priori training with statistical methods. Instead, it uses an *on-demand training scheme* in which previously solved equilibrium and kinetics problems are used to rapidily and accurately predict the solution of subsequent similar problems, requiring for this no iterative computations and/or time stepping.