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Inverse modeling in vadose zone geochemistry using differentiable modeling in JAX

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Recently significant progress has been made in differentiable modeling in various fields, such as fluid mechanics and vadose zone hydrology. In differentiable modeling frameworks physics-based numerical models (i.e., ODE and/or PDE solvers) are implemented on machine learning platforms such as JAX and PyTorch. The use of the machine learning platforms eliminates the need to code derivatives directly to solve the nonlinear set of equations, and thus drastically reduces the development time. In addition, differentiable numerical solvers provide accurate derivatives that can be used to estimate unknown functions or parameters in physical models using gradient-based optimization methods. We have developed fully differentiable numerical solvers for saturated-unsaturated flow, coupled water and heat transport, and chemical reaction networks in JAX. Such differentiable models in JAX can be used to solve various inverse problems in geochemistry. As examples, we estimate ion exchange parameters (i.e., selectivity coefficients and exchange site concentrations) from batch and column transport experiments. Furthermore, we discuss the choice of optimization methods (e.g., quasi-Newton method and Newton-CG method) to speed up the solution of inverse problems and share practical experience with their implementation.