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LINEAR AND NONLINEAR PRECONDITIONING FOR REACTIVE TRANSPORT

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Summary. Reactive transport in porous media leads to a large nonlinear system of equations, coupling one advection-dispersion type partial differential for each species, to algebraic (if local equilibrium is assumed) or ordinary differential (if a kinetic model is chosen) equations for each grid point. The coupled problem is formulated as a fixed point problem, by using local inverses for each of the subproblems. By applying the Newton-Krylov framework on the resulting non-linear system, a globally coupled method is obtained with the complexity of a xed point method, making it possible to keep the transport and chemistry codes separated. At each time step, the linear system for Newton's method is solved by an iterative method of Krylov type, requiring only the computation of the Jacobian of the system with a given vector, but not the computation of the Jacobian matrix itself.

A critical aspect of the method is an efficient matrix-free preconditioner. Preconditioning techniques that respect the block structure of the system are introduced,a and several block preconditioners are compared. As the transport problem is solved as part of the nonlinear preconditioning, a convergence rate independent of the mesh size is expected. Indeed, an analysis of a simplfiied chemical system for a single species with sorption shows that the eigenvalues of the preconditioned Jacobian matrices are bounded independently of the mesh size, so that the number of outer Newton iterations, as well as the number of inner GMRES iterations, are independent of the mesh. The resulting preconditioner can be extended to the case with multi-species chemistry. These results are illustrated by numerical experiments comparing the performance of the methods on a synthetic example related to CO2 sequestration.