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Parallel Newton-Krylov Methods for Ultrascale Subsurface Reactive Multiphase Flow

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Reactive multiphase flow and transport codes play a vital role in predicting the migration of subsurface contaminants and evaluating the viability of alternatives for mitigating global climate change (e.g. geologic sequestration of anthropogenic carbon). To perform such analyses, scientists incorporate sophisticated physical and chemical process models within their simulators to assess the impact of reactive fluids on subsurface porous media. For large 3D field-scale models, these simulators employ preconditioned Newton-Krylov methods to solve the tightly-coupled systems of equations governing multiscale physical and chemical processes in the subsurface.

Due to the extreme stiffness of the systems arising from the strong feedback mechanisms between processes and the wide range of timescales involved, significant challenges exist in the development of scalable solver/preconditioner algorithms for these coupled process models. In the case of carbon sequestration, simulation requires at a minimum the coupling of multiphase fluid flow (i.e. supercritical CO_2 and water), energy, and salt (solute transport), which results in large and complex Jacobian matrices with irregular blocks of coefficients representing the coupling between processes within a grid cell or matrix element. For conventional multilevel algorithms, this unpredictable coupling of system PDEs presents new challenges, especially at the extreme scale (i.e. 10,000+ processor cores).

This presentation focuses on research in the development of multilevel preconditioners for ultrascale subsurface problems. In particular, results are presented on the performance of parallel Newton-Krylov solvers employed within codes executed on leadership class computing platforms such as Oak Ridge National Laboratorys Jaguar for simulation of variably-saturated, single phase flow with reactive transport and multiphase carbon sequestration.