PFLOTRAN: NEXT-GENERATION PETASCALE SUBSURFACE REACTIVE FLOW AND TRANSPORT CODE

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PFLOTRAN, a next-generation reactive flow and transport code for modeling subsurface processes, has been designed from the ground up to run efficiently on machines ranging from leadership-class supercomputers to laptops. Based on an object-oriented design, the code is easily extensible to incorporate additional processes. It can interface seamlessly with Fortran 9X, C and C++ codes. Domain decomposition parallelism is employed, with the PETSc parallel framework used to manage parallel solvers, data structures and communication. Features of the code include a modular input file, implementation of high-performance I/O using parallel HDF5, ability to perform multiple realization simulations with multiple processors per realization in a seamless manner, and multiple modes for multiphase flow and multicomponent geochemical transport. Chemical reactions currently implemented in the code include homogeneous aqueous complexing reactions and heterogeneous mineral precipitation/dissolution, ion exchange, surface complexation and a multirate kinetic sorption model. P FLOTRAN is currently being enhanced to incorporate high-order Mimetic Finite Differences and adaptive mesh refinement through SAMRAI. Linkages are also being developed to couple PFLOTRAN to models at other scales (i.e. regional/climate, pore scale). PFLOTRAN has run at the petascale (i.e. employed up to 204,000 processor cores on problems composed of over 2 billion degrees of freedom). The code is currently being applied to simulate uranium transport at the Hanford 300 Area, uranium and nitrate plumes from S-3 waste disposal ponds at Oak Ridge and CO2 sequestration in deep geologic formations.

This presentation delivers an overview of PFLOTRAN capability within the context of current research in radionuclide transport and CO2 sequestration with discussion of numerical methods employed to efficiently solve the equations governing the physicochemical process models in parallel.