SOLVER STRATEGIES TO AMELIORATE BARRIERS TO SCALABLE PERFORMANCE FOR SUBSURFACE REACTING FLOW SIMULATIONS ON LEADERSHIP-CLASS SUPERCOMPUTERS USING PFLOTRAN

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Current generation leadership-class supercomputers possess hundreds of thousands of processor cores, and next-generation supercomputers will push this number above one million. Accompanying this trend to such high levels of concurrency is a trend towards "many-core" CPU and GPU architectures in which processors have very high theoretical peak FLOP rates but relatively poor per-core memory bandwidth. These architectural trends pose some distinct challenges for sparse algebraic solvers: 1) Latency of the global reduction operations (``{\tt MPI_Allreduce()}'') required to compute vector inner products and norms becomes extremely high when spanning such large core counts and 2) Relatively low memory bandwidths for manycore processors allow only a small fraction
of theoretical peak performance to be achieved for sparse matrix operations. We discuss some approaches we have employed to ameliorate these barriers in PFLOTRAN, a computer code that simulates coupled thermal-hydrologic-chemical processes in variably saturated, nonisothermal, porous media, when running on extremely large scale supercomputers such as Jaguar, the Cray XT5 system at Oak Ridge National Laboratory. PFLOTRAN employs implicit time stepping, and uses the inexact Newton-Krylov solver framework of the Portable, Extensible Toolkit for Scientific Computation (PETSc) to solve the sparse Jacobian sytems that arise. For large PFLOTRAN simulations spanning a significant fraction of a machine like Jaguar, the aforementioned challenges are pronounced. We will describe our experiments with addressing the high cost of global reductions in the sparse solves by using reformulated Krylov-solver algorithms that reduce the number of global reductions required at the cost of some additional local work. Furthermore, we will also describe experiments with two level overlapping Schwarz preconditioners with non-standard coarse grid spaces. Finally, we will present preliminary results from experiments with full approximation scheme (FAS) nonlinear multigrid solvers to solve reactive transport problems. Such schemes have the potential to greatly increase the percent of theoretical peak processor performance achieved due to vastly reduced memory bandwidth requirements compared to standard Newton-multigrid approaches.