Office of Science
U.S. DEPARTMENT OF ENERGY

Advanced Scientific Computing Research
Applied Mathematics
FY 2007 Accomplishment

Robust and Scalable Solution Methods for Strongly-Coupled Multi-physics Systems

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Summary

An important goal of our research is to develop new robust, efficient and scalable parallel solution methods for multi-physics systems modeled by PDEs. Our work includes basic algorithm research, software development and comprehensive numerical experimentation in critical scientific applications of interest to DOE. FY2007 accomplishments centered on the continued development and comprehensive evaluation of Newton-Krylov solution algorithms with multilevel preconditioners and the development of new challenging scientific applications in resistive magnetohydrodynamics (MHD).

Strongly coupled nonlinear PDE systems are common mathematical models of the natural physical world and are highly important for simulating advanced technology applications of importance to DOE. The predictive computational simulation of these systems requires the solution of strongly-coupled interacting physics on high resolution unstructured meshes. The discretization of the governing PDE equations produces large non-linear systems of equations, for which robust and efficient parallel iterative solution methods are required. Our work focuses on basic algorithm research, development, and the comprehensive evaluation of robust Newton-Krylov (NK) based solution methods with scalable parallel algebraic multilevel preconditioners. The numerical methods are then delivered to the computational science community by a collaborative software development effort in the Trilinos solver framework in three specific software packages. These are the NOX nonlinear solver, the ML multi-level, and the Meros approximate block factorization preconditioner packages.
In FY2007 we have had a number of significant accomplishments that have enabled, and demonstrated, the robust and scalable parallel solution of complex multi-physics systems. We recently developed a new fully-implicit and direct-to-steady-state low Mach number resistive MHD capability for large-scale parallel simulations. The method is based on an unstructured stabilized finite element (FE) method. This capability will drive algorithm development in multi-level and physics-based preconditioners that will have potentially significant impacts on the MHD simulation community. Employing our fully-coupled NK solution technology we have demonstrated bifurcation studies for thermal buoyancy driven flows with interacting magnetic fields (Hydro-magnetic Rayliegh-Bernard type instabilities). These coupled mechanisms are, for example, critical components of large-scale geo-dynamo simulations that model the time dependent behavior of the Earth's magnetic field (see Fig. 1). Initial results applying our algebraic multi-level methods (AMG) to resistive MHD formulation are very promising.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

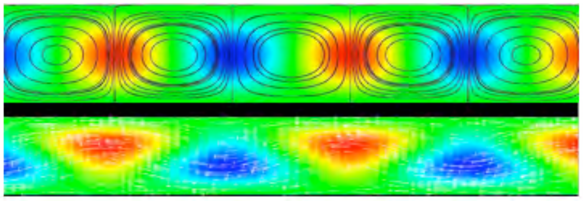

Fig 1. Stable hydro-magnetic Rayleigh-Bernard flow (Vy velocity/streamlines above; current Jz / magnetic field vectors ,B, below). Direct to steady-state solution and bifurcation studies are enabled by NK methods with multi-level preconditioners.

We have also made significant contributions to algorithm development and evaluation this year. This includes the appearance of a significant journal article on globalization techniques for fully-coupled NK methods in SIAM Review[1]. While these methods were demonstrated on fluid flow and transport type systems, the techniques are routinely applied (with NOX) to a variety of coupled nonlinear PDE systems. A partial list includes Navier-Stokes, transport / reaction, combustion, semi-conductor device simulations and resistive MHD systems.

Finally, we have continued collaboration on the development and comprehensive evaluation of new preconditioners for fully-coupled NK methods based on block AMG methods and physics based preconditioners [2,3]. In our work we recently demonstrated the superior scalability, and CPU solution times of these methods on problems as large as 200+ million unknowns on up to 8000+ processors. These studies have been carried out for low Mach number fluid flow with transport, and semi-conductor device simulation with drift-diffusion models. In Fig. 2 we demonstrate a factor of 10x improvement in the solution time for a semi-conductor device simulation problem. The improved 3 level block AMG preconditioner shows a very significant CPU time scalability advantage, over the more standard parallel domain decomposition methods. This improved scalability will allow larger simulations to be carried out more efficiently on the next generation PetaFlop machines. Current work includes a detailed study of the parallel NK multi-level methods on challenging resistive MHD applications and the development of physics-based preconditioners for implicit extended MHD.

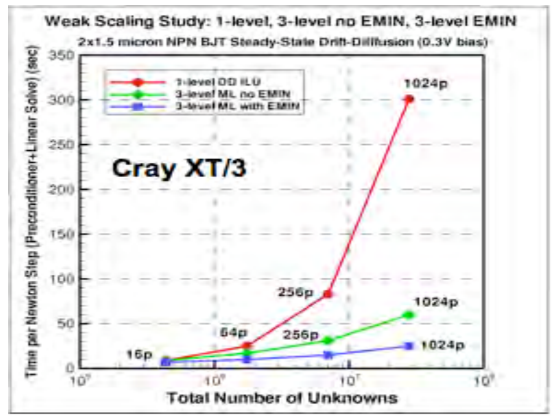

Fig 2. Scaling of CPU time for solution of drift-diffusion problem by fully-coupled NK method with multi-level preconditioner

[1] Pawlowski, Shadid, Simonis, Walker, "Globalization Techniques for Newton-Krylov methods and applications to the fully-coupled solution of the Navier-Stokes equations", SIAM Review; 2006, 48, 4, p.700-721

[2] Lin, Sala, Shadid, Tuminaro, "Performance of Fully-Coupled Algebraic Multilevel Domain Decomposition Preconditioners for Incompressible Flow and Transport", IJNME 2006; 67, 2, p.208-25

[3] Elman, Howle, Shadid, Shuttleworth, Tuminaro, "A Taxonomy of Parallel Block Preconditioners for the Incompressible Navier-Stokes Equations", in revision for J. Comp. Physics.

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