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SEMINAR

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3 Shaffer Hall
Refreshments: 3:30 p.m.
Seminar: 4:00 p.m.

SCALABLE SOLVERS AND SOFTWARE FOR PDE-BASED APPLICATIONS

Abstract

Like the theoretical peak performance of a computer system, theoretical efficiency for algorithms is rarely closely approached for real applications. While the quest for the "textbook efficiency" continues on many fronts, applications scientists need to have their solver capabilities upgraded today to exploit the platform potential to run more highly resolved computations. The Terascale Optimal PDE Simulations (TOPS) project is working on both fronts—attempting to make fundamental advances in numerical algorithms that will be integrated into tomorrow's scalable solver software while achieving gains for application developers at the outset of the initiative.

This talk dwells on some practical aspects of migrating from a legacy (usually operator-split) nonlinear solver for evolutionary or equilibrium systems of PDEs to a Jacobian-free Newton–Krylov framework that provides strong controls on splitting error while still incorporating physically-based operator-split methodology (and even legacy subroutines) where possible. It is emphasized that to support even a single application from development through production use on various platforms, contemporary solver libraries must offer a menu of flexibly combinable and tunable components to allow application-specific and architecture-specific trade-offs (e.g., memory versus flops, synchronization frequency versus stability, robustness versus efficiency). We discuss some experiences with magnetohydrodynamics codes to underscore the desirability of being able to draw from a broad family of solvers within a single application.

More information about the above project can be found at

http://www-unix.mcs.anl.gov/scidac-tops/ .

Please see the next page for a biographical sketch of the speaker.

David E. Keyes

David E. Keyes is the Fu Foundation Professor of Applied Mathematics in the Department of Applied Physics and Applied Mathematics at Columbia University, an affiliate of the Center for Data Intensive Computing (CDIC) at Brookhaven National Laboratory, and Acting Director of the Institute for Scientific Computing Research (ISCR) at the Lawrence Livermore National Laboratory.

Keyes graduated *summa cum laude* with a B.S.E. in Aerospace and Mechanical Sciences and a Certificate in Engineering Physics from Princeton University in 1978. He received his Ph.D. in Applied Mathematics from Harvard University in 1984. He was then a postdoctoral fellow in the Computer Science Department at Yale University and taught there for eight years, as Assistant and then Associate Professor of Mechanical Engineering, prior to joining Old Dominion University and the Institute for Computer Applications in Science & Engineering (ICASE) at the NASA Langley Research Center in 1993. At Old Dominion, Keyes was the Richard F. Barry Professor of Mathematics & Statistics and Director of the Center for Computational Science.

Keyes is the author or coauthor of over 100 publications in computational science and engineering, numerical analysis, and computer science. He has co-edited eight conference proceedings concerned with parallel algorithms and has delivered over 200 invited presentations at universities, laboratories, and industrial research centers in over 20 countries and 35 states of the U.S. With backgrounds in engineering, applied mathematics, and computer science, and consulting experience with industry and national laboratories, Keyes works at the algorithmic interface between parallel computing and the numerical analysis of partial differential equations, across a spectrum of aerodynamic, geophysical, and chemically reacting flows. Newton–Krylov–Schwarz parallel implicit methods, introduced in a 1993 paper he coauthored at ICASE, are now widely used throughout engineering and computational physics, and have been scaled to thousands of processors on the ASCI platforms.

Keyes has co-organized and lectured in numerous conferences and short courses on high-performance computing for systems modeled by PDEs for NASA Langley, LLNL, SIAM, the DoD Modernization Centers, the domain decomposition and parallel CFD communities, and university departments. He is currently a member of the editorial boards of *Parallel and Distributed Computing Practices*, *International Journal of High Performance Computing Applications*, *Journal of Multiscale Computational Engineering*, and Springer's *Lecture Notes in Computational Science & Engineering* and has served as an editor of *SIAM Journal on Scientific Computing*.

Among Keyes's awards are the Gordon Bell Prize for High Performance Computing, Special Category (shared), 1999; a National Science Foundation Presidential Young Investigator Award, 1989; the Yale College Prize for Teaching Excellence in the Natural Sciences, 1991; a Yale University Junior Faculty Fellowship, 1990–1991; a Harvard–Danforth Certificate for Excellence in Teaching, 1982; and the Hayes–Palmer Prize in Engineering at Princeton (shared with Tom Leighton and Chris Milly), 1978. Keyes has led one of the 37 NSF "Grand, National, and Multidisciplinary Challenges" centers and one of the 14 DOE ASCI "Level 2" centers. He currently directs a nine-institution Integrated Software Infrastructure Center (ISIC) for the Office of Advanced Scientific Computing Research of the DOE, one of seven such centers nationally under the Scientific Discovery through Advanced Computing (SciDAC) initiative.

Keyes served as the Chairman of the Connecticut Section of the American Institute of Aeronautics and Astronautics from 1991 to 1993. He has been a SIAM Visiting Lecturer since 1992 and a member of the SIAM Council since 2000. Keyes also serves on the Advisory Board of the DOE Computational Science Graduate Fellowships.