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Frontiers of Scientific Computing Lecture Series

A Nonlinearly Implicit Manifesto

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Abstract:
Many simulations must be followed over time intervals that are long compared to the shortest timescales in the system, e.g., convective versus acoustic timescales in aerodynamics, ocean turnover versus gravity wave timescales in climate, plasma discharge versus Alfven timescales in tokamaks, piston travel versus fast reaction timescales in internal combustion. Often, the phenomena associated with the shortest timescales may be assumed to be in equilibrium relative to dynamics of interest; however, they control the computational timestep if an explicit method is used, with the result that even weak scaling cannot be achieved. Often, as well, one would ideally employ a high-order timestepping scheme and take relatively large timesteps for computational economy; however, if operator splitting techniques are used the lower order splitting error thwarts this objective. For these and other reasons, fully implicit methods are increasingly important for the nonlinear multiscale applications that pace large-scale simulations in energy, environment, and other complex systems. The good news is that advances in solution algorithms, globalization algorithms, and software that implements them (without necessarily demanding that the user constructs a full Jacobian) make implicit methods more inviting than ever. Moreover, we argue that computational challenges on the immediate horizonÂ uncertainty quantification, inverse problems, multiphysics coupling, etc. Â are most naturally tackled with fully nonlinearly implicit formulations well in hand. This talk illustrates the case for implicit methods with model problems and challenge problems arising from systems governed by partial differential equations.

Speaker's Bio:
David E. Keyes is the Fu Foundation Professor of Applied Mathematics in the Department of Applied Physics and Applied Mathematics at Columbia University, and Acting Director of Institute for Scientific Computing Research (ISCR) at Lawrence Livermore National Laboratory. With backgrounds in engineering, applied mathematics, and computer science, Keyes works at the algorithmic interface between parallel computing and the numerical analysis of partial differential equations, across a variety of applications. Newton-Krylov-Schwarz parallel implicit methods, introduced in a 1993 paper, are now widely used throughout computational physics and engineering and scale to many thousands of processors. Keyes is currently the Vice President-at-Large of SIAM, a member of the Presidential Council of Advisors in Science & Technology (PCAST, Networking and Information Technology Committee) and of the Advisory Committees of the Mathematics and Physical Sciences Directorate and the Office of Cyberinfrastructure of the National Science Foundation.

This lecture has a reception.