Terascale Optimal PDE Simulations (TOPS)

Building a Holistic Approach to PDE-based Modeling

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Vision

Multicomponent nonlinear partial differential equations (PDEs) give mathematical expression to many DOE applications. PDE simulation codes require implicit solvers for multiscale, multiphase, multiphysics phenomena from hydrodynamics, electromagnetism, radiation transport, chemical kinetics, and quantum chemistry. Problem sizes are typically now in the millions of unknowns; and with emerging large-scale computing systems and inexpensive clusters, this size is expected to increase by a factor of a thousand over the next five years. Moreover, these simulations are increasingly used in design optimization, parameter identification, and process control contexts, which require many repeated, related PDE analyses.

Fortunately, the continuous origin of these problems provides a natural way to generate a hierarchy of approximate models, through which the required solution may be obtained efficiently by various forms of "bootstrapping." The most famous examples are multigrid methods, but other types of hierarchical representations are also exploitable, making user of lower fidelity models, lower order discretizations, inexact linearizations, and even lower precisions. The philosophy that underlies optimality is to make the majority of progress towards a high quality result through less expensive intermediates.

The Terascale Optimal PDE Simulations (TOPS) Center is researching and developing and will deploy a toolkit of open source solvers for the nonlinear partial differential equations that arise in many application areas, including fusion, accelerator design, and the collapse of supernovae. These algorithms — primarily multilevel methods — aim to reduce computational bottlenecks by one or more orders of magnitude on terascale computers, enabling scientific simulation on a scale heretofore impossible.

Along with usability, robustness, and algorithmic efficiency, an important goal of this DOE Integrated Software Infrastructure Center (ISIC) is to attain the highest possible computational performance in its implementations by accommodating to the memory bandwidth limitations of hierarchical memory architectures and to distributed memory.

Major Goals and Technical Challenges

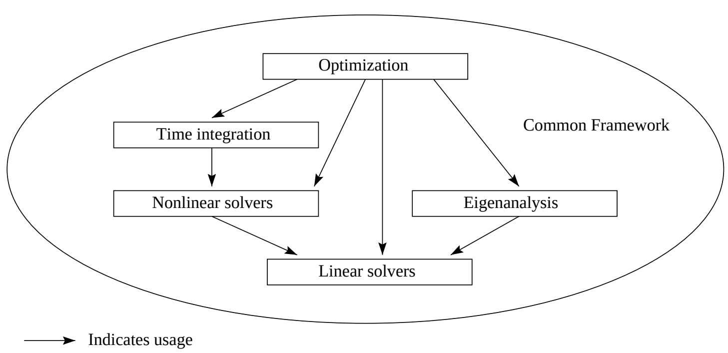

Figure 1: *The five classes of solver software to be developed as part of TOPS. All five, in a PDE context, share grid-based data structures and considerable parallel software infrastructure.*

The efforts defined for TOPS, the co-PIs joining to undertake them, and the collaborations proposed have been chosen to exploit the present opportunity to revolutionize large-scale solver infrastructure through incorporation of new optimal algorithms and through interoperability. The co-PIs' current software (including hypre, PETSc, ScaLAPACK, and SuperLU), though not algorithmically optimal in some cases, and not yet as interoperable as ultimately required, is in the hands of thousands of users, and has created a valuable experience base on which to build.

Most PDE simulation is ultimately a part of some larger scientific process that can be hosted by the same data structures and carried out with many of the same optimized kernels as the simulation, itself. Adding a convenient software path from PDE analysis to eigenanalysis will impact the scientific approach of users with complex applications. For instance, a PDE analysis can be pipelined into the scientific added-value tasks of stability analysis for small perturbations about a solution and reduced dimension representations (model reduction), with reuse of distributed data structures and solver components. Similarly, we expect to significantly impact the scientific priorities of target users by emphasizing optimization (parameter identification, optimal control, optimal design, and data assimilation) as part of our solver toolkit. Of course, (predominantly sparse) linear solvers, nonlinear solvers, and adaptive time-integrators constitute core, inner loop technologies for these respectively higher tasks.

Major Milestones and Activities

- Year 1: Assist collaborators with existing implicit solver technology, concentrating on functionality over performance. Deliver reference application/solver implementations to CTTSS and PERC ISICs to influence and help direct their research, and to adaptive discretization and applications partners to serve as templates for their use of current and future TOPS solvers. Lay foundations for interoperability and higher performance in key kernels through close CTTSS and PERC collaborations. Study characteristics of next generation applications.
- Year 2: Migrate new high-performance solver implementations into collaborator codes. Research more optimal, robust algorithmic successors.
- Years 3, 4 & 5: Migrate more optimal algorithms into new solver code releases. Continually improve and "harden" TOPS solver toolkits. Educate users community in TOPS toolkits and in "holistic PDE simulation" through their natural combinations.

Key Connections with Other SciDAC Projects

- **Component Technology for Terascale Simulation Software.** Collaborate on creating suites of interoperable solver components and on defining standard interfaces for these components.
- **Performance Science and Engineering.** Provide testbed of optimal solver codes for performance evaluation and collaborate to implement cache- and network-aware versions.
- **Terascale Simulation Tools and Technology.** Adapt optimal iterative solvers to dynamically evolving data structures and to novel complex discretizations.
- **Framework for Applied Partial Differential Equations.** Provide AMR-based multilevel solvers that are robust with respect to anisotropy and in homogeneity.
- **Extended Magnetohydrodynamic Modeling.** Improve performance of currently dominating implicit algorithmic stages and evaluate novel fully nonlinearly implicit methods.
- **21^{st} Century Accelerator Science & Technology.** Extend modal analysis techniques into complex and nonsymmetric regimes and apply formal optimization methods to large-scale parameter identification and design issues.
- **Terascale Supernovae Initiative.** Jointly develop implicit solver technology for severe multiscale multiphysics phenomena in core collapse supernovae.

Project Personnel

The TOPS project involves over two dozen senior personnel at nine institutions, plus associated post-doctoral and graduate student members. In the following list (accurate as of September 2001), the names of lead PIs at each institution are italicized.

Argonne National Laboratory Steve Benson, Matt Knepley, Mike Minkoff, *Jorge Moré*, Todd Munson, *Barry Smith*, Hong Zhang

Carnegie Mellon University *Omar Ghattas*

Lawrence Berkeley National Laboratory Parry Husbands, Sherry Li, Osni Marques, *Esmond Ng*, Chao Yang

Lawrence Livermore National Laboratory Edmond Chow, Miguel Dumett, *Rob Falgout*, Radu Serban, Panayot Vassilevski, Carol Woodward

New York University George Biros, Bernhard Hientzsch, *Olof Widlund*

Old Dominion University Florin Dobrian, *David Keyes*, Alex Pothen

University of California *Jim Demmel*

University of Colorado Xiao-Chuan Cai, Tom Manteuffel, *Steve McCormick*

University of Tennessee *Jack Dongarra*, Victor Eijkhout

The project webpage is `http://www.math.odu.edu/~keyes/scidac`.

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