TOPS Software for Optimization of Simulated Systems

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Summary

In support of known and anticipated application requirements for parameter identification, design optimization, optimal control, and data assimilation in complex systems, the Terascale Optimal PDE Simulations (TOPS) project is creating optimization packages that leverage and integrate its scalable solvers.

One of the outstanding challenges of computational science is nonlinear parameter estimation of partial differential equation (PDE) systems. Such inverse problems are significantly more difficult to solve than the associated forward problems, due to ill-posedness, large dense ill-conditioned inversion operators, multiple minima, space-time coupling, the possibility of discontinuous inversion fields, and the need to solve the forward problem repeatedly. TOPS has developed a nonlinear parameter estimation code for a large class of time-dependent PDEs. This code is based on the parallel PDE solver software PETSc and uses preconditioners from the PDE-constrained optimization library Veltisto (which, in turn, is built from PETSc components).

Figure 1 illustrates the application of the parameter estimation code to reconstructing the shape of a pelvic bone geometry. The inverse problem involves 2.1 million inversion parameters, and was solved in 3 hours on 256 processors of a Compaq AlphaServer system. The underlying parallel algorithm scales well: the number of outer and inner iterations is insensitive to problem size. This work represents one of the largest inverse problems ever solved, and won "Best Paper Award" at SC2002.

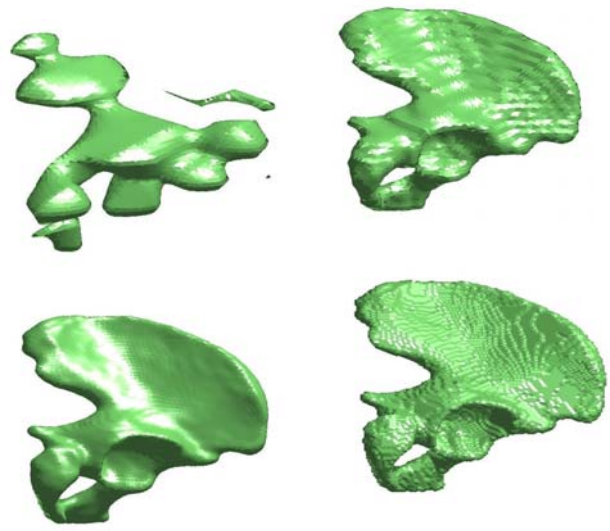

Figure 1. *Reconstruction of pelvic bone geometry via solution of a synthetic inverse wave propagation problem using the TOPS-developed parallel multiscale Gauss-Newton-Krylov code. The first three images show multiscale progression of algorithm, from coarse to fine grid optimal reconstruction. The fourth image shows the target shape.*

The parameter estimation code integrates total variation regularization (addressing the ill-posedness of high frequency components and the discontinuity of the inversion field), matrix-free Gauss-Newton-Krylov iteration, algorithmic checkpointing (addressing the forward-backward time coupling), multiscale continuation (addressing multiple min-

ima), and a modified limited-memory preconditioner.

TOPS is also developing optimization tools for molecular geometry optimization, and related computational chemistry problems. In this effort we are working in collaboration with the Center for Component Technology for Terascale Simulation Software (CCTTSS), and the developers of two high-performance packages for chemical simulations, NWChem from Pacific Northwest National Laboratories and MPQC from Sandia National Laboratories. The aim of this work is to join, with component software interfaces, the optimization algorithms in TAO (Toolkit for Advanced Optimization) with the simulations of NWChem and MPQC.

As part of this work we have developed a new limited-memory algorithm for large, bound-constrained optimization problems. This algorithm has remarkable efficiency on large-scale applications where only function values (evaluation of the potential) and gradient (evaluation of the forces) values are available. The TAO algorithm outperforms the competition on single-processor architectures. In addition, results for a benchmark obstacle problem on the Cray T3E at NERSC, show that with 10,000 variables per processor, the flop rate per processor remains nearly constant as the problem size grows to 2.5 million variables.

We highlighted this work in a demonstration at SC2002, which featured interactions between electronic structure components based on NWChem and MPQC for energy, gradient, and Hessian computations; optimization components based on TAO; and linear algebra components based on Global Arrays (developed at PNNL) and PETSc. These components now work together to enable molecular geometry optimizations (for example, those in Figure 2), and provide the foundation for investigations of new algorithms and parallel performance issues.

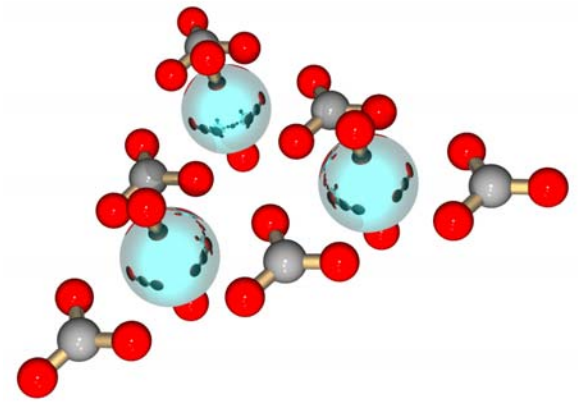

Figure 2. Relativistic quantum chemistry calculation of $(UO_2)_3$ $(CO_3)_6$ using NWChem. Image courtesy of Wilbe deJong, PNNL.

Motivated by our collaborations with computational chemists, we are also developing new algorithms for studying how systems transition between stable states. Determining these transition states is a fundamental problem in computational chemistry. However, all current algorithms are based on an intuitive notion of how the system changes, and lack a convergence proof. We have proposed the elastic-string algorithm for the computation of transition states based on the mountain-pass theorem, a fundamental mathematical result. This work is significant because the elastic string algorithm is the first algorithm with a rigorous convergence proof for general problems.

The TOPS project webpage may be found at http://www.tops-scidac.org.

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