From *SIAM News*, Volume 38, Number 6, July/August 2005

PDE-Constrained Optimization at the 2005 SIAM Conferences on CS&E and Optimization

By Omar Ghattas

Many computational science and engineering problems can be formulated as optimization problems that are governed by partial differential equations. Solution of such optimization problems is known as "PDE-constrained optimization" or, more generally, "simulation-based optimization." Because of their size, complexity, and infinite-dimensional nature, the PDE constraints often present significant challenges for general-purpose optimization algorithms.

Recent years have seen sustained progress in PDE solvers and large-scale optimization algorithms, along with a rapid rise in computing capability. Accompanying these advances has been a growing interest in simulation-based optimization in such diverse areas as aerodynamics, atmospheric and geosciences, the chemical process industry, the environment, homeland security, infrastructure, manufacturing, medicine, and physics. Simulation-based optimization arises in the form of inverse problems (in which estimates of model parameters characterizing a simulation are sought from observations) and control and design problems (in which optimal control strategies and optimal designs are sought based on desired goals). Specialized optimization methods that are tailored to the structure of the PDE constraints in these problem classes are being developed to address the need for PDE-constrained optimization across many of the active application areas.

PDE-constrained optimization has been a focus of a number of workshops in recent years, both in the U.S. (hosted by Sandia National Labs and the Institute for Mathematics and its Applications) and in Europe (held in Graz, Heidelberg, Oberwolfach, and Trier). Two recent SIAM conferences featured a number of talks on PDE-constrained optimization. CS&E 2005 in Orlando included the three-part minisymposium "Large-Scale PDE-Con-strained Optimization" and the two-part minisymposium "Optimiztion and Applications." In addition, a short course on PDE-constrained optimization was offered the day before the conference began. At Optimization 2005 in Stockholm, several minisymposia featured the theme of simulation-based optimization, including "Simulation-Based Design Optimization, I and II," "Optimization of Complex Systems, I and II," "Numerical Methods for PDE-Constrained Optimization," and "Multi-scale Optimization." In addition, one of the plenary talks dealt with PDE-constrained optimization in the context of inverse earthquake modeling (see Figure 1).

Speakers in these sessions presented results of research in four broad areas: faster solvers, improved algorithms for state and control inequalities, advanced discretization methods, and complex applications. Discretization of infinite-dimensional PDE-constrained optimization problems introduces a number of issues beyond those encountered in solving the PDEs alone. Several speakers addressed such advanced discretization techniques as discontinuous Galerkin, higher-order approximations, and mesh adaptivity. A continuing challenge for PDE-constrained optimization problems is that discretization leads to very large-dimensional

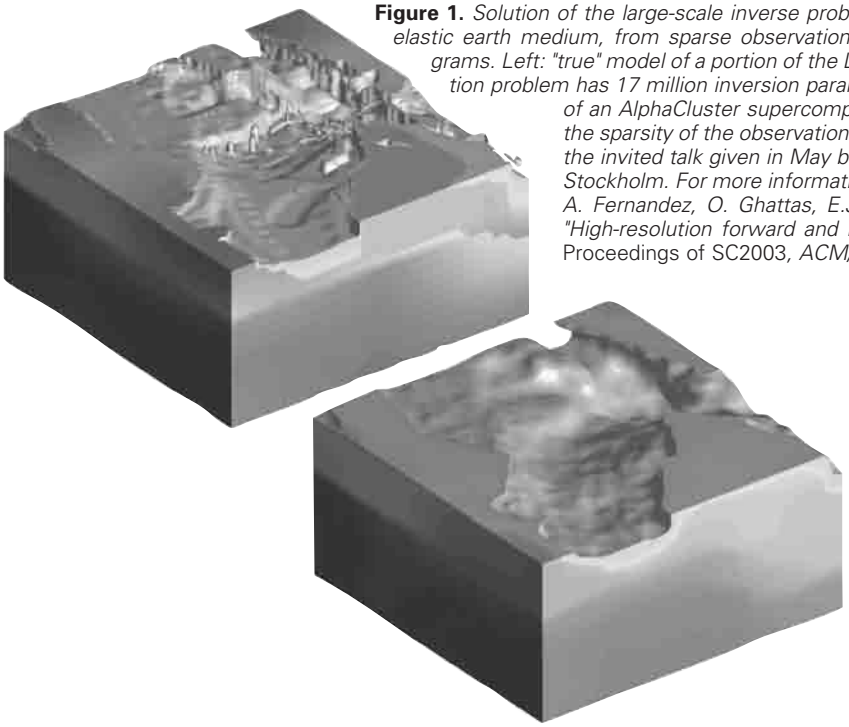

Figure 1. *Solution of the large-scale inverse problem of estimating the distribution of wave speed of an elastic earth medium, from sparse observations of (synthetic) earthquake-generated surface seismograms. Left: "true" model of a portion of the Los Angeles Basin; below: inverted model. The optimization problem has 17 million inversion parameters and was solved in 24 hours on 2048 processors of an AlphaCluster supercomputer at the Pittsburgh Supercomputing Center. Despite the sparsity of the observations, the reconstruction is quite good. The images are from the invited talk given in May by Omar Ghattas at the SIAM optimization conference in Stockholm. For more information, see V. Akcelik, J. Bielak, G. Biros, I. Epanomeritakis, A. Fernandez, O. Ghattas, E.J. Kim, J. Lopez, D. O'Hallaron, T. Tu, and J. Urbanic, "High-resolution forward and inverse earthquake modeling on terascale computers,"* Proceedings of SC2003*, ACM/IEEE, Phoenix, Arizona, 2003.*

algebraic optimization problems, particularly for 3D spatial problems. This provided the motivation for several talks on multigrid/multilevel/multifidelity methods, preconditioning, and (space/time) domain decomposition for the optimality systems associated with the optimization problem. Indeed, efforts to extend these successful PDE solver methods to corresponding optimization problems account for much current activity.

Another significant challenge for PDE-constrained optimization is addressing state and control inequality constraints, which is made more difficult by their infinite dimensional nature. Speakers described recent work on interior point methods and primal-dual active set methods that target such inequality constraints. Finally, demonstrating the breadth and complexity of applications of PDE-constrained optimization, speakers addressed applications problems involving electromagnetics, acoustics, aerodynamics, compressible and incompressible flows, cardiac electrophysiology, atmospheric transport, earthquake modeling, electrorheological fluids, elastic contact, composite design, image processing, water networks, and reservoir simulation, among others.

Omar Ghattas, a professor of biomedical engineering and of civil and environmental engineering at Carnegie Mellon University, is the program director of the SIAM Activity Group on CS&E and an organizer of SIAM's 2005 Conference on CS&E. In May, he gave an invited talk, "Large-Scale Earth-quake Inversion," at the 8th SIAM Conference on Optimization.