Advanced Scientific Computing Research
FY 2006 Accomplishment

Large-Scale Optimization Algorithms

David Womble[*], Sandia National Laboratories

Summary

The Large-Scale Optimization Algorithms project built optimization capabilities for otherwise-intractable OSC and NNSA problems. In the years ahead, weapons problems will continue to focus more heavily on uncertainty, as evidenced by QMU (quantitative margins and uncertainty) NNSA milestones. Tools are deployed through DAKOTA and Trilinos. In delivering these capabilities, the MICS program has benefited the NNSA engineering analysis and design programs. Highlights include surrogate-based optimization (SBO) for expensive (and uncertain) engineering simulations; and SAND without model modification, coupling and redesigning optimization (MOOCHO) and solvers (Trilinos) to obtain some of the efficiency gains of intrusive-optimization with little modification to the simulation code.

Introduction

Rarely does one run a simulation once, and say, “Aha, that is the number I was looking for.” Nearly all formal or informal design and assessment studies, such as sensitivity analysis, uncertainty quantification, and optimization, require multiple simulations. When each simulation is a massively-parallel large-scale ASC engineering simulations taking hundreds of hours on DoE’s biggest supercomputers, finesse is required.

Surrogate Based Optimization

Using a surrogate model judiciously vetted against full-fidelity simulations boasts two great advantages. First, it can significantly reduce computational expense, by replacing many of the full simulations with their surrogate equivalents. Second, it tames artificial non-smoothness (numerical and mesh issues often cause simulations at nearby domain points to return non-nearby values) that can cause standard algorithms to fail. In this way, many previously intractable studies are suddenly possible.

Most realistic design problems involve nonlinear constraints, say on required performance or reliability (due to uncertainty). Intelligent constraint management is essential to algorithm efficiency because it allows surrogate-based approaches to balance feasibility and optimality and converge more rapidly and reliably. Alternative approaches require the user to experiment with problem-specific guesses.

Mike Eldred (DAKOTA PI) and Danny Dunlavy (2006 MICS von Neumann Fellow) produced general facilities for constraint management. Techniques include constraint relaxation (e.g., homotopy) for handling infeasible iterates, merit function selections (e.g., augmented Lagrangian), and iterate acceptance logic selections (e.g., filter methods).

Surrogate-based optimization (SBO), and surrogate-based optimization under uncertainty (SBOUU), are workhorses of the DAKOTA toolkit. This project leveraged a decade of ASC-investment in DAKOTA.

---

[*] (505) 845-7471, dewombl@sandia.gov

These capabilities were published in the open literature and deployed as part of the DAKOTA 4.0 release in June 2006. DAKOTA is open-source with over 3300 registered participants across DoE/OSC labs, industry partners, and university collaborators. DAKOTA is the tool of choice for UQ in the V&V program across the NNSA Trilabs: LANL, LLNL, and SNL.

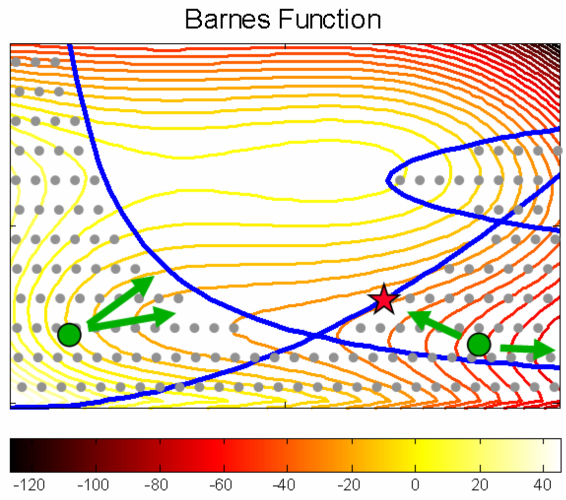

Figure 1. Constraint management on the well-known Barnes test function. Star is a local optimum. Blue shows constraints. At the leftmost green circle, the new algorithm balances optimality and feasibility and proceeds directly to the constrained minimizer. At the rightmost green circle, these directions are nearly opposed and the strategy must adapt to strictly enforce the constraints.

SAND without Model Modification

A complementary approach to these nearly-intractable problems is to form one coupled problem and converge the simulation and optimization problem simultaneously: SAND, Simultaneous Analysis and Design. The downside is the massive per-code customization required. This project found a way to gain many of the benefits of SAND with as little modification to the simulation code as possible. Roscoe Bartlett developed a minimally invasive, reduced-space SQP SAND solver. This solver requires only objective and constraint values and can use finite-difference approximations, which greatly reduces the need for customization. The approach is still efficient: the number of finite-differences required scales independent of the global dimension of the simulation problem. A major benefit of the coupled approach is it exploits efficient block linear solvers. The optimization package MOOCHO implements the new approach. It interfaces through Thyra and will be deployed in Trilinos 7.0 in fall 2006. An important SNL parameter estimation problem in Charon further demonstrates the capability.**Error! Not a valid link.***Figure 2. Reduction in solver time for a large example. The minimally invasive coupled approach (lowest line) is significantly faster than the decoupled finite-difference approach and achieved a better solution.*

For further information on this subject contact:
Dr. Anil Deane, Program Manager
Mathematical, Information, and Computational
Sciences Division
Office of Advanced Scientific Computing Research
Phone: 301-903-1465
deane@mics.doe.gov