



The University of Chicago
Departments of Computer Science,
Mathematics, and Statistics

Scientific and Statistical Computing Seminar

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The TAO Linearly-Constrained Augmented Lagrangian Method for PDE-Constrained Optimization

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ABSTRACT

Parameter estimation, inverse problems, and optimal control problems frequently appear in physical applications and can be cast as constrained optimization problems with partial differential equation constraints. In particular, we are interested in solving discretized optimization problems of the form

$$\begin{aligned} \min_{u,v} \quad & f(u, v) \\ \text{subject to} \quad & g(u, v) = 0, \end{aligned}$$

where the state variable u is the solution to the discretized partial differential equation defined by g and parametrized by the design variable v , and f is the discretized objective function, whose form depends on the application. Examples include estimating the porosity and permeability parameters from observables such as the piezometric head at monitoring wells for reactive flows, to applications in optical tomography and electromagnetic imaging.

In this talk, we will discuss the linearly-constrained augmented Lagrangian method available in the Toolkit for Advanced Optimization (TAO) for solving PDE-constrained optimization problems. This method computes two directions, a Newton direction to reduce the constraint violation and a reduced-space direction to improve the augmented Lagrangian merit function. The reduced-space direction is computed from a limited-memory quasi-Newton approximation to the reduced Hessian matrix. This method requires a minimal amount of information from the user to solve the optimization problem. The computational time for the method is dominated by computing the necessary directions using iterative methods and preconditioners supplied by the user for solving the linearized forward and adjoint problems. The parallel performance is strongly influenced by the parallel performance of these solves.

To evaluate the performance of our linearly-constrained augmented Lagrangian method, we use the Haber-Hansen test problems, which include elliptic, parabolic, and hyperbolic partial differential equations, and their corresponding discretizations so that we can compare methods. We implemented parallel versions of these applications in the Toolkit for Advanced Optimization to investigate the scalability of the method on high-performance architectures. Results from these studies will be presented.

Our algorithms and test problems are available in the latest release of the Toolkit for Advanced Optimization, which also includes methods for derivative-free optimization, unconstrained and bound-constrained optimization problems using derivative information, and complementarity problems and variational inequalities on high-performance architectures.

Joint work with Evan Gawlik, Jason Sarich, and Stefan Wild.

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