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"Controlling Numerical Uncertainty in PDE-Constrained Optimization"

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Summary

Numerical solution of optimization problems governed by large-scale PDE models is evolving into a critical enabling technology within the DOE complex. Example applications include optimal design of semiconductor devices, optimal control of turbulent flows, and optimization-based solution of a variety of coupled-physics problems. Regardless of the application, the solution of the governing PDEs introduces uncertainty, which comes in three basic flavors: model uncertainty, data uncertainty, and numerical uncertainty. The latter, defined as the combination of (1) the loss of information involved in translating the infinite-dimensional problem formulation into its algebraic form and (2) the inexactness in the iterative solution of the corresponding large-scale linear systems, significantly reduces the predictive capability of numerical techniques used in PDE-constrained optimization. Our goal is to develop advanced solution methods that will enable efficient control of both sources of numerical uncertainty.

During this fiscal year we pursued two research directions. The first involved a study of the loss of information involved in the process of translating the infinite-dimensional formulation of a PDE-constrained optimization problem into its algebraic form. Our study was motivated by optimal design and parameter estimation problems arising in the modeling of semiconductor devices.

We studied the impact of different state equation discretizations on optimization problems whose objective functionals involve flux terms. Galerkin methods, in which the flux is a derived quantity, were compared with mixed Galerkin methods, which approximate the flux directly. Our results show that the latter approach leads to more robust and accurate solutions of the optimization problem, especially for highly heterogeneous materials with large jumps in material properties. At the same time, both approaches yield equally good numerical solutions of the governing PDEs.

Figure 1 shows that the two discretizations, each of which is well suited for the solution of the governing PDE, can give rise to entirely different solutions of the optimization problem. In this example,

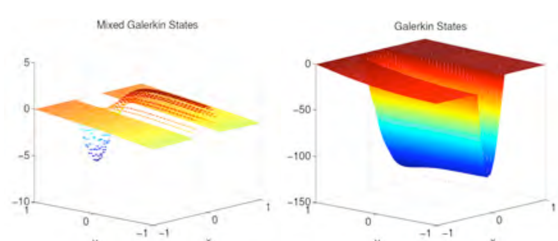

Figure 1. State solution of a flux-control optimization problem obtained using the mixed Galerkin discretization (left) and the standard Galerkin method (right).

a close inspection of the final value of the objective functional reveals that the standard

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Galerkin approach generates solutions that are grossly inaccurate. Generally speaking, our study indicates that the compatibility of a discretization scheme with respect to a PDE need not imply its compatibility with respect to an optimization problem governed by that PDE. This is a first-of-its-kind numerical result; a detailed theoretical study is in progress.

The second research direction focused on the control of inexactness due to the iterative solution of large-scale linear systems arising from the linearized constraint equations. In this context, we examined the global convergence of second-order schemes for nonlinear constrained optimization, in particular sequential quadratic programming (SQP).

Each iteration within an SQP algorithm requires the solution of several linear systems involving the linearized constraints. For problems governed by PDEs, these systems are solved using iterative solvers, which are inherently inexact. In this case, the optimization algorithm must be responsible for dynamically managing the stopping tolerances for linear solvers, based on its progress toward a solution. This is a significant departure from the traditional viewpoint, in which the end user selects fixed linear solver tolerances in an ad-hoc manner, often resulting in either failing or very inefficient optimization runs.

To this effect, we have extended the global convergence theory of composite-step trust-region SQP methods to efficiently control inexactness in linear system solves. Our theory allows for very coarse linear solves, while still guaranteeing fast convergence of the SQP algorithm. Moreover, the stopping tolerances for linear solves are implemented efficiently, without the need to rely on Lipschitz constants or similar quantities that are difficult to estimate in practice.

Figure 2 showcases the behavior of the developed inexactness-control mechanisms in a critical algorithmic module of our SQP method. We observe that when the SQP iterate is far from the optimum, the algorithm allows rather loose linear solver stopping tolerances. As the algorithm moves toward the optimum, linear solver tolerances are automatically tightened, enabling the satisfaction of the SQP convergence criteria.

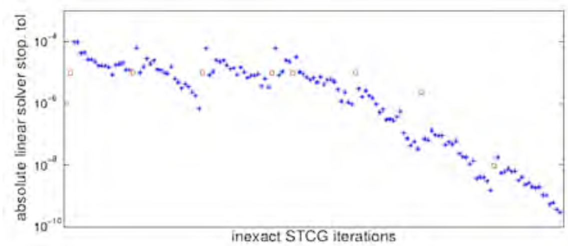

Figure 2. Control of inexactness in linear system solves within a component of a composite-step trust-region SQP algorithm (boundary flow control problem with nonlinear constraints).

A series of numerical experiments, including boundary control of steady flows and optimal design of semiconductor devices, indicates that our approach not eliminates the need for ad-hoc tweaking of stopping tolerances for linear solves, but that it always outperforms the best fixed-tolerance guess in terms of the total number of linear solver iterations. The algorithm is currently being implemented in the “Aristos” large-scale optimization library, developed within the Trilinos project. Aristos will enable the distributed solution of optimal design and control problems involving an unprecedented number (tens to hundreds of millions) of optimization variables.

For further information on this subject contact:

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