Parallel CFD-Based Optimization: Optimal Control and Optimal Design with PDE Toolkits

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ABSTRACT

Our goal is to develop and apply scalable parallel algorithms for the optimization of systems governed by viscous incompressible flows. To facilitate parallel implementation, we would like to build these algorithms from components of such parallel PDE solver toolkits as PETSc and SUNDANCE. Target application classes include optimal control and optimal design. In both settings, a major challenge is the development of numerical optimization algorithms for solving the first-order conditions characterizing optimality. A further major challenge, specific to the shape optimization problem, is the development of algorithms that overcome the difficulties of moving boundaries and shape sensitivities, which are particularly vexing on parallel computers. Below we describe algorithms we have developed that target these problems, and their application to the solution of some viscous flow control and shape optimization problems.

In the first half of our presentation, we review some of our work on fast solvers for optimization problems that are governed by PDEs [1,2,3], and their implementation using components from PETSc, a parallel PDE solver library developed at Argonne National Lab. The method we have developed, which we refer to as *Lagrange-Newton-Krylov-Schur (LNKS)*, solves the full optimality system consisting of state, adjoint, and control equations using an inexact preconditioned Newton-QMR method. The preconditioner is a block factorization that emulates a reduced quasi-Newton SQP method: it approximates the reduced Hessian via suitably-initialized limited memory BFGS updates while discarding other second derivative terms, and replaces the exact state and adjoint solves with application of appropriate preconditioners, e.g. additive Schwarz or multigrid. If sufficient descent cannot be obtained with a line search, then we drop down to the reduced space and take a quasi-Newton step. Experiments with this method on some problems of optimal control of three-dimensional steady Navier-Stokes flows via boundary suction/injection demonstrate high parallel scalability, mesh-independence of Newton iterations, mesh-independence of Krylov iterations (provided an optimal state preconditioner is available), and solution to optimality in four times the cost of a flow solution, for a problem with over 600,000 state and 9000 control variables. This small constant multiple of the state solve cost is due to iterating in the full space, which hides the iterations (linear and nonlinear) needed to converge the flow behind those required for optimization. LNKS is most effective when the state equations are difficult to solve, requiring many iterations.

In the second half of the presentation, we turn our attention to the remaining challenges posed by shape optimization problems. These include difficulties in maintaining a differentiable shape representation, in determining derivatives of response quantities with respect to the shape representation, and in maintaining a mesh that smoothly resolves the changing geometry. All of these are particularly challenging in 3D and on parallel computers. The geometry modeling and meshing complexities of the Lagrangian approach have lead us to pursue an Eulerian formulation, which solves the shape optimization problem with respect to a fixed spatial description. This greatly facilitates parallel implementation.

Our approach integrates several contemporary ideas from scientific computing. From level set methods we borrow the idea of implicit shape representation by the zero isocontour of a level set function. But unlike level set methods, we avoid solving the Hamilton-Jacobi equation that evolves the level set function in "time" (which amounts to a steepest descent optimization method), in favor of direct Newton-Krylov solution of the nonlinear PDEs representing first-order optimality with respect to state, adjoint, and level set variables. Because there exist an infinite number of level set functions for a given shape, the optimization problem is ill-posed, and we must therefore employ a regularization functional to render the solution unique. As in phasefield methods, we use a characteristic function to denote interior and exterior regions. But because the exterior region is represented by boundary conditions, we appeal to distributed Lagrange multiplier variants of fictitious domain methods to incorporate the effect of these conditions.

Several shape optimization model problems, including ones in which the topology of the optimal shape differs from that of the initial, are solved on regular grids to demonstrate the method. Numerical solution is effected through Galerkin finite element approximation of weak statements of the infinite dimensional Newton step. The implementation is done via SUNDANCE, a C++ finite element toolkit for solution of variational problems developed by Kevin Long at Sandia. The blending of ideas from level set/phasefield surface representation, fictitious domain enforcement of boundary conditions, and full-space Newton-Krylov optimization solvers leads to a purely Eulerian method that avoid dynamic mesh (re)generation and shape (re)parameterization. The tradeoff is that the convergence rate of the numerical approximation is suboptimal, but we believe this is a small price to pay for avoiding the significant geometry and parallelism difficulties of Lagrangian methods.

1. G. BIROS, *Parallel Lagrange-Newton-Krylov-Schur methods for PDE-constrained optimization, with application to optimal control of viscous flows*, Ph.D. thesis, Carnegie Mellon University, September 2000.

2. G. BIROS AND O. GHATTAS, *Parallel Lagrange-Newton-Krylov-Schur Methods for PDE-Constrained Optimization. Part I: The Krylov-Schur Solver*, SIAM Journal on Scientific Computing, under revision.

3. G. BIROS AND O. GHATTAS, *Parallel Lagrange-Newton-Krylov-Schur Methods for PDE-Constrained Optimization. Part II: The Lagrange-Newton Solver, and its Application to Optimal Control of Steady Viscous Flows*, SIAM Journal on Scientific Computing, under revision.