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# Final Report - Subcontract B623760

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# Center for Computational Mathematics

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To: Rob Falgout
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Subject: Progress Report – Subcontract B623760
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During my visit to LLNL during July 17–27, 2017, I worked on linear system solvers. The two level hierarchical solver that initiated our study was developed to solve linear systems arising from *hp* adaptive finite element calculations, and is implemented in the $PLTMG$ software package, version 12 [1]. This preconditioner typically requires $3 - 20\%$ of the space used by the stiffness matrix for higher order elements. It has multigrid like convergence rates for a wide variety of PDEs (self-adjoint positive definite elliptic equations, convection dominated convection-diffusion equations, and highly indefinite Helmholtz equations, among others). The convergence rate is not independent of the polynomial degree $p$ as $p \to \infty$, but but remains strong for $p \leq 9$, which is the highest polynomial degree allowed in $PLTMG$, due to limitations of the numerical quadrature rules implemented in the software package. A more complete description of the method and some numerical experiments illustrating its effectiveness appear in [2]. Like traditional geometric multilevel methods, this scheme relies on knowledge of the underlying finite element space in order to construct the smoother and the coarse grid correction.

If an algebraic version for general matrices arising from PDE discretizations could be developed, the small size and simple construction of the preconditioner would be an advantage, and since it is just a two level scheme, only one coarse matrix is required. The development team is Rob Falgout, Randolph Bank, James Brannick, and Shuhao Cao. Because Professors Brannick and Cao were not available during the dates of the visit, progress was slower than anticipated. However, it remains an important avenue to pursue and we expect the make significant progress on it in the future.

In the meantime we made progress on another important problem, related to PDE optimization problems that feature box constraints (simple upper and lower bounds). Box constraints are commonly applied to PDE solutions of obstacle problems, and to the control variables in optimal control problems. There are two main approaches for dealing with such constraints. Interior point methods use a path following algorithm to trace the solution from some interior starting point to the solution that is on the boundary of the feasible region. As a practical matter, the interior point method involves adding penalty-like terms to the some diagonal elements of the Jacobian/Hessian and the corresponding right hand side. The (ironic) disadvantage of interior point methods is that good initial guesses often lead to very short steps in the path following/line search algorithm, resulting in excessive numbers of Newton iterations. This is particularly challenging in the case of adaptive feedback loops, since they automatically provide increasing good initial guesses in each loop.

The main alternative is active set methods, that iterate towards finding the set of constraints that are active at the solution. The current active set is excluded from the Newton calculations, which then locally behaves as it would in an unconstrained optimization problem. Its disadvantage is that the form of the system matrix constantly changes as variables are added to and removed from the current active set. On the positive side, it tends to converge much faster than the interior point method when starting from a good initial guess.

Our approach is a modified interior point method that tries to incorporate the best features of the active set method in order to converge quickly in situations where there is a good initial guess. In the line search loop, variables already near to their upper or lower bounds with update directions that move them in the direction of the boundary, are simply moved to within a small but fixed distance of the boundary. Their updates are then set to zero and they are thus excluded from the remainder of the line search procedure. However, they remain as variables in the overall Newton iteration as in the usual interior point method, so the linear systems are as in the usual interior point method. With some experimentation on the choice a parameters (how close to the boundary is "close"?) we are able to achieve the usual sorts of convergence rates for Newton iteration in the context of adaptive feedback loops.

## References


[1] Randolph E. Bank. PLTMG: A software package for solving elliptic partial differential equations, users' guide 12.0. Technical report, Department of Mathematics, University of California at San Diego, 2016.

[2] Randolph E. Bank. A two level solver for *hp* adaptive finite element equations. *Computing and Visualization in Science*, to appear.