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Final Report: Subcontract B623868 Algebraic Multigrid solvers for coupled PDE systems

J. Brannick

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Algebraic Multigrid solvers for coupled PDE systems
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The Pennsylvania State University ("Subcontractor") continued to work on the design of algebraic multigrid solvers for coupled systems of partial differential equations (PDEs) arising in numerical modeling of various applications, with a main focus on solving the Dirac equation arising in Quantum Chromodynamics (QCD). The goal of the proposed work was to develop combined geometric and algebraic multilevel solvers that are robust and lend themselves to efficient implementation on massively parallel heterogeneous computers for these QCD systems. The research in these areas built on previous works, focusing on the following three topics: (1) the development of parallel full-multigrid (PFMG) and non-Galerkin coarsening techniques in this frame work for solving the Wilson Dirac system; (2) the use of these same Wilson MG solvers for preconditioning the Overlap and Domain Wall formulations of the Dirac equation; and (3) the design and analysis of algebraic coarsening algorithms for coupled PDE systems including Stokes equation, Maxwell equation and linear elasticity.

The proposed research focused mainly on the continued development of an integrated bootstrap--adaptive multigrid method for various discretizations of the Dirac equation in Lattice QCD. In this project we focused on the development of the 4D Wilson solver when using standard full coarsening on the finest level. The project team worked with R. Falgout and J. Schroder in CASC to develop the method in hypre. The main progress made in this component of the project was in terms of code development and, specifically, a first version of the 4D bootstrap solver was was implemented in hypre. The code has been integrated with the QLUA QCD code that generates the Wilson discretization with realistic gauge fields and is now able to work with physically relevant data. Our first tests of the algorithm for the problem are not as promising as the results we obtained for the PFMG-BAMG method that was developed for the 2D Wilson system and current efforts of the team are focusing on debugging the code in order to improve overall performance of the solver.

The project team also continued to develop the classical AMG form of optimal AMG interpolation and the generalized BAMG algorithm for solving general PDE problems, including the linear Elasticity system. In particular, the classical algebraic multigrid form of optimal interpolation that directly minimizes the two-grid convergence rate was derived and compared with the so-called ideal interpolation that minimizes a certain weak approximation property of the coarse space. The team also studied compatible relaxation type estimates for the quality of the coarse grid and derived a new sharp measure using optimal interpolation that provides a guaranteed lower bound on the convergence rate of the resulting two-grid method for a given grid. Also an adaptive coarsening algorithm based on this sharp form of compatible relaxation was developed. The resulting coarsening algorithm aims to find a sparse representation (changing of basis) for the coarse space defined by the optimal interpolation operator.
In addition, a generalized bootstrap algebraic multigrid setup algorithm that computes a sparse approximation to the optimal interpolation matrix was derived and implemented for various PDE problems, showing promising initial results. In particular, it was demonstrated

numerically that the bootstrap algebraic multigrid method with sparse interpolation matrix (and spanning multiple levels) converges faster than the two-grid method with the standard ideal interpolation (a dense matrix) for various scalar diffusion problems with highly varying diffusion coefficient and we show the general usage of our algorithm by applying also to elasticity problem.