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Algebraic Multigrid solvers for coupled PDE systems

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The Pennsylvania State University (“Subcontractor”) worked on the design of multigrid solvers for coupled systems of partial differential equations arising in numerical modeling of various applications, with a main emphasis on the design of new optimal algebraic multigrid interpolation. Generally, the aim of this work was to develop geometric and algebraic multilevel solvers that are robust and lend themselves to efficient implementation on massively parallel heterogeneous computers. The research in these areas built on previous works, focusing on the following topics:

- (1) design and analysis of algebraic coarsening algorithms for coupled PDE systems including Stokes equation, Maxwell equation and linear elasticity;
- (2) development of non-Galerkin coarsening techniques for the Wilson Dirac system; and
- (3) the use of this same Wilson MG solver for preconditioning the Overlap and Domain Wall formulations of the Dirac equation.

Optimal interpolation

One main research focus was on developing a new form of optimal AMG interpolation that directly minimizes the two-grid convergence rate and compare it with the so-called ideal form of interpolation that minimizes a certain weak approximation property of the coarse space.

Various theoretical results on this optimal interpolation were derived and it was shown that for proper choices of the coarse variables a new generalized ideal form of interpolation is equivalent to the optimal form.

Compatible relaxation

Compatible relaxation type estimates for measuring the quality of the coarse grid were studied and a new sharp measure using the new optimal form of interpolation was derived. This new approach provides a guaranteed lower bound on the convergence rate of the resulting two-grid method for a given grid and, hence is useful in studying various coarsening strategies for a variety of PDE systems. A new adaptive coarsening algorithm that uses this optimal form of interpolation in constructing the coarse grid was developed and implemented. The algorithm was tested for scalar and PDE systems, showing promising results in all cases.

Optimal Bootstrap Interpolation

A generalized bootstrap algebraic multigrid G-BAMG setup algorithm that computes a sparse approximation to the optimal interpolation matrix was developed. This optimal form of classical algebraic multigrid interpolation that has as its columns eigenvectors with small eigenvalues of

the generalized eigen-problem involving the system matrix and symmetrized smoother. The new algorithm uses as a main tool a multilevel eigensolver to compute approximations to these generalized eigenvectors. A notable feature of the approach is that it allows for general block smoothers and, as such, is well suited for systems of PDEs. It has also been demonstrated through numerous numerical tests that the G-BAMG method with sparse interpolation matrix (and spanning multiple levels) outperforms the two-grid method with the standard ideal interpolation (a dense matrix) for various scalar diffusion problems with highly varying diffusion coefficient was designed and studied. This work led to one submitted publication:

[arXiv:1703.10240](https://arxiv.org/abs/1703.10240)

Optimal interpolation and Compatible Relaxation in Classical Algebraic Multigrid

James Brannick, Fei Cao, Karsten Kahl, Rob Falgout, Xiaozhe Hu

Comments: 23 pages, submitted to SISC, Subjects: **Numerical Analysis (math.NA)**

Finite Elements for the Dirac equation

Using techniques from the edge averaged finite element technique and the virtual element method we designed a stable and consistent finite element discretization for the simplified 2D Schwinger model of quantum electrodynamics, a model problem that is typically studied when developing numerical algorithms for the full Dirac equation in QCD. Though the stabilization term used in the discretization acts as the glue for continuity, it is still computed locally for each element and then added to the system. Moreover, unlike the Weak Galerkin or Hybridized Discontinuous Galerkin methods, this new approach based on VEM does not require computing on an entirely different data structure (e.g., a skeleton, i.e., edges or faces), and this greatly simplifies the analysis and implementation. The stabilization term guarantees the stability of the method on a discrete level so that the question of stability need only hold for the local VEM approximation space. This allows the VEM to deal with saddle-point systems such as the Dirac equation. Moreover, after the splitting, there is no restriction on element. The intricacy of constructing element basis functions on quadrilateral or hexahedron meshes is gone. This can be extremely useful as well for dimensions higher than 3, due to the difficulty in constructing a triangulation. A paper is currently being written that summarizes these results.

Multigrid for the Dirac equation

Bootstrap algebraic multigrid BAMG setup algorithms were developed for solving the Dirac equation arising in Lattice Quantum Chromodynamics (QCD). Several topics have been studied in this component of project as well. These include: (1) a variety of techniques for constructing a non-Galerkin coarse grid operator for the Wilson-Dirac system of equations; (2) development of a preconditioner for the Wilson system using the VEM discretization of the Dirac equation; (3) the use of the Wilson system to precondition the Overlap discretization. Research on Topics (1) and (3) led to partial results, but this work is still in progress and will continue in the next subcontract. A paper is being written that summarizes the results from Topic (2) and will be submitted to a peer reviewed journal.