Lawrence Livermore National Laboratory

hypre MG for LQFT

Chris Schroeder

LLNL - Physics Division

This work performed under the auspices of the U.S. Department of Energy by
Lawrence Livermore National Laboratory under Contract DE-???

Contributors

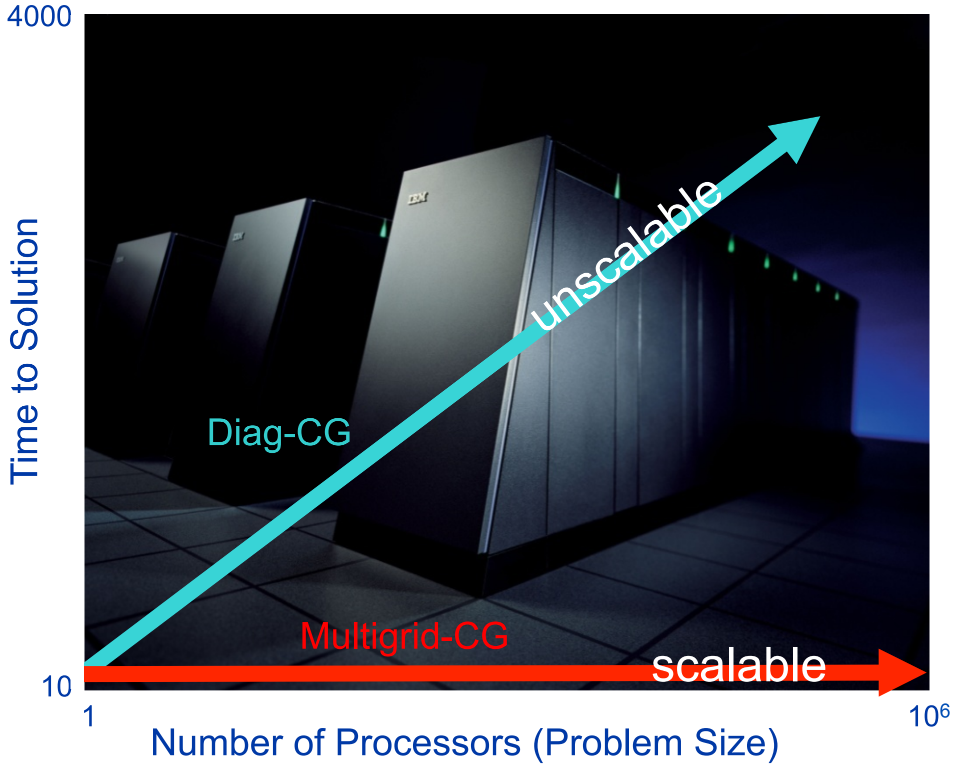
hypre Team

- Rob Falgout (project lead)
- Allison Baker
- Edmond Chow
- Van Emden Henson
- Jim Jones
- Barry Lee
- Jeff Painter
- Charles Tong
- Tom Treadway
- Panayot Vassilevski
- Ulrike Meier Yang

QCD-MG collaboration

- Argonne
  - James Osborn
- Boston University
  - Ron Babich
  - Rich Brower
  - Saul Cohen
  - Claudio Rebbi
- Colorado U., Boulder
  - Marian Brezina
  - Christian Ketelsen
  - Tom Manteuffel
  - Steve McCormick
  - John Ruge
- Harvard
  - Mike Clark
- KAUST
  - David Keyes
- LLNL
  - Rob Falgout
- Penn State
  - James Brannick
  - Ludmil Zikatanov
- Tufts
  - Scott MacLachlan

Multigrid Solvers Scale



- Require *weak scaling* – constant solution time as problem size grows in proportion to the number of processors
- Multigrid solvers succeed because they are O(N)

Multigrid for Lattice QCD

- *Geometric* Multigrid not applicable to Lattice QCD

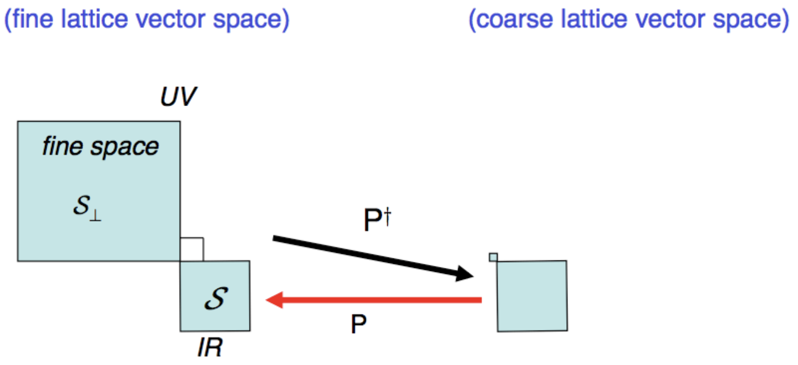
gauge symmetry → covariant derivative
→ nearly random gauge links

  - the system is ***complex*** and ***indefinite***
  - the system can be ***extremely ill-conditioned***
  - the near-null space is ***unknown*** and ***oscillatory***

Multigrid for Lattice QCD

- *Algebraic Multigrid + Adaptive Smooth Aggregation*
  - defines restriction strictly in terms of the matrix

$$P = \begin{pmatrix} v_1 & v_2 & & & \\ v_1 & v_2 & & & \\ \vdots & \vdots & & & \\ v_1 & v_2 & & & \\ & & v_1 & v_2 & \\ & & v_1 & v_2 & \\ & & \vdots & \vdots & \\ & & v_1 & v_2 & \\ & & & & \ddots \end{pmatrix}$$

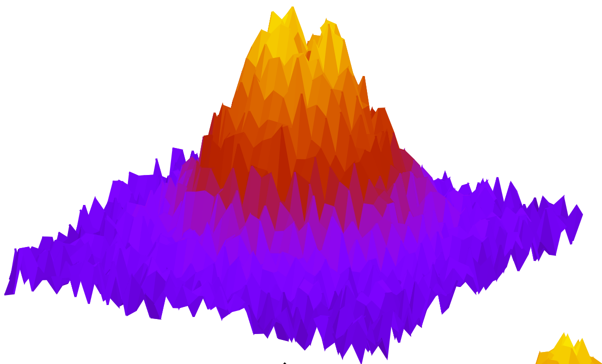


  - discovers the near-null space dynamically & adapts
    - difficult modes ~ near-null modes
    - use error vectors to redefine restriction
    - repeat until all near-null modes are captured

Multigrid Basics

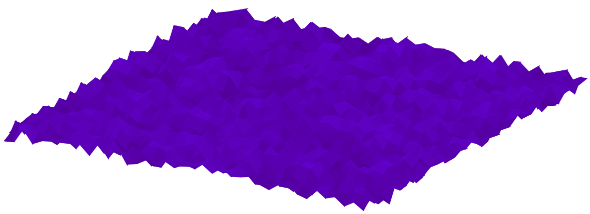
<u>residual</u>: $r_i = b - A\,x_i$

The Multigrid V-cycle



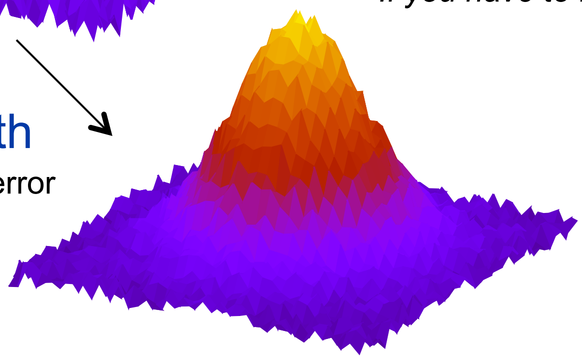
If you have to move a mountain with a shovel,

use a BIG shovel



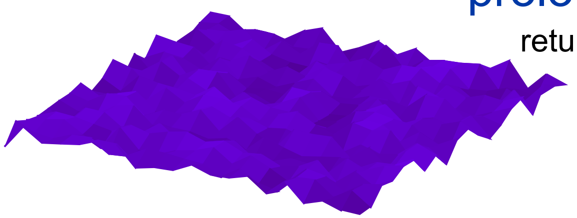
smooth

reduce high freq error



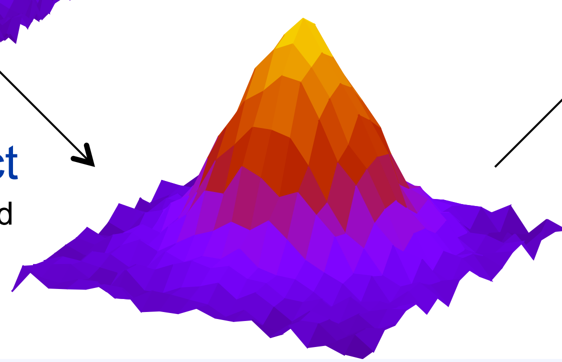
prolong

return to fine grid



restrict

switch to coarse grid



coarse solve

deal with low freq modes on coarse grids

→ fewer nodes, lighter-weight structures

→ fewer iterations

V-cycle is one of several options

Joining Forces: *hypre* Multigrid and Lattice QCD

- ***hypre*** is an advanced and growing suite of parallel linear solvers and preconditioners scalable on massively parallel architectures, including Sequoia
- developed at CASC@LLNL by Rob Falgout et al.
- benefits from extensive work on Algebraic Multigrid
- a vital component of a broad array of application codes both here at LLNL and worldwide (downloaded 10,000 times in 70 countries)

Joining Forces: *hypre* Multigrid and Lattice QCD

- increase impact of ***hypre***
- allow “lattice” direct access to its advanced multigrid algorithms, solve the setup cost problem
- create channel for co-development – new variants for Lattice QCD may well serve the community at large

Project Outline

- Year 1:
  - expand hypre to handle complex numbers. **DONE**
  - expand hypre to handle arbitrary, user-defined dimension. **DONE**
- Year 2:
  - implement the Wilson Dirac operator in hypre **DONE**
  - solve Wilson with hypre's multigrid methods **?**
  - compare to other USQCD codes
- Year 3:
  - implement Domain Wall and Staggered fermion operators in hypre.

Wilson Dslash solves with *hypre*

- *hypre's* pre-existing AMG methods (BoomerAMG, PFMG, …) are ineffective when applied to LQFT
- USQCD method, Adaptive Smoothed Aggregation, is basically incompatible with structure of *hypre*
- Need to develop and implement a new algorithm – compatible with *hypre* **and** effective for LQFT
- Strategy: Extend **PFMG**, which is already in *hypre*, in direction of **Bootstrap AMG**, which is (probably) effective for LQFT

Bootstrap AMG

BOOTSTRAP ALGEBRAIC MULTIGRID FOR THE 2D WILSON DIRAC SYSTEM

J. BRANNICK[‡] AND K. KAHL[§]

Key words. QCD, Wilson discretization, bootstrap AMG, Kaczmarz relaxation, odd-even reduction, multigrid eigensolver.

AMS subject classification. 65F10, 65N55, 65F30

Abstract. We develop an algebraic multigrid method for solving the non-Hermitian Wilson discretization of the 2-dimensional Dirac equation. The proposed approach uses a bootstrap setup algorithm based on a multigrid eigensolver. It computes test vectors which define the least squares interpolation operators by working mainly on coarse grids, leading to an efficient and integrated self learning process for defining algebraic multigrid interpolation. The algorithm is motivated by the γ_5-symmetry of the Dirac equation, which carries over to the Wilson discretization. This discrete γ_5-symmetry is used to reduce a general Petrov Galerkin bootstrap setup algorithm to a Galerkin method for the Hermitian and indefinite formulation of the Wilson matrix. Kaczmarz relaxation is used as the multigrid smoothing scheme in both the setup and solve phases of the resulting Galerkin algorithm. The overall method is applied to the odd-even reduced Wilson matrix, which also fulfills the discrete γ_5-symmetry. Extensive numerical results are presented to motivate the design and demonstrate the effectiveness of the proposed approach.

“Bootstrap PFMG”

- Geometric coarsening:
  - Brannick-Kahl: Red/Black Precon + Full Coarsening
  - Red/Black incompatible
  - Full Coarsening difficult
  - Use Semi coarsening as in PFMG **DONE**
- Kaczmarz smoothing
  - sequential, doesn’t scale; replace with smoother in *hypre*, e.g., Chebyshev polynomial; requires development
- Tune interpolation coefficients to optimize reproduction of [initial] test vectors
- Use [initial] hierarchy to compute eigenvectors (or singular vectors); augment set of test vectors; repeat

Project Outline

- Year 1:
  - expand hypre to handle complex numbers. **DONE**
  - expand hypre to handle arbitrary, user-defined dimension. **DONE**
- Year 2:
  - implement the Wilson Dirac operator in hypre **DONE**
  - solve Wilson with hypre's multigrid methods

    need new algorithm,
    underway,
    potentially on schedule

  - compare to other USQCD codes **To do ASAP**
- Year 3:
  - Domain Wall and Staggered

    input is done, sufficiently general
    B-PFMG *may* be effective
    [with some tuning]