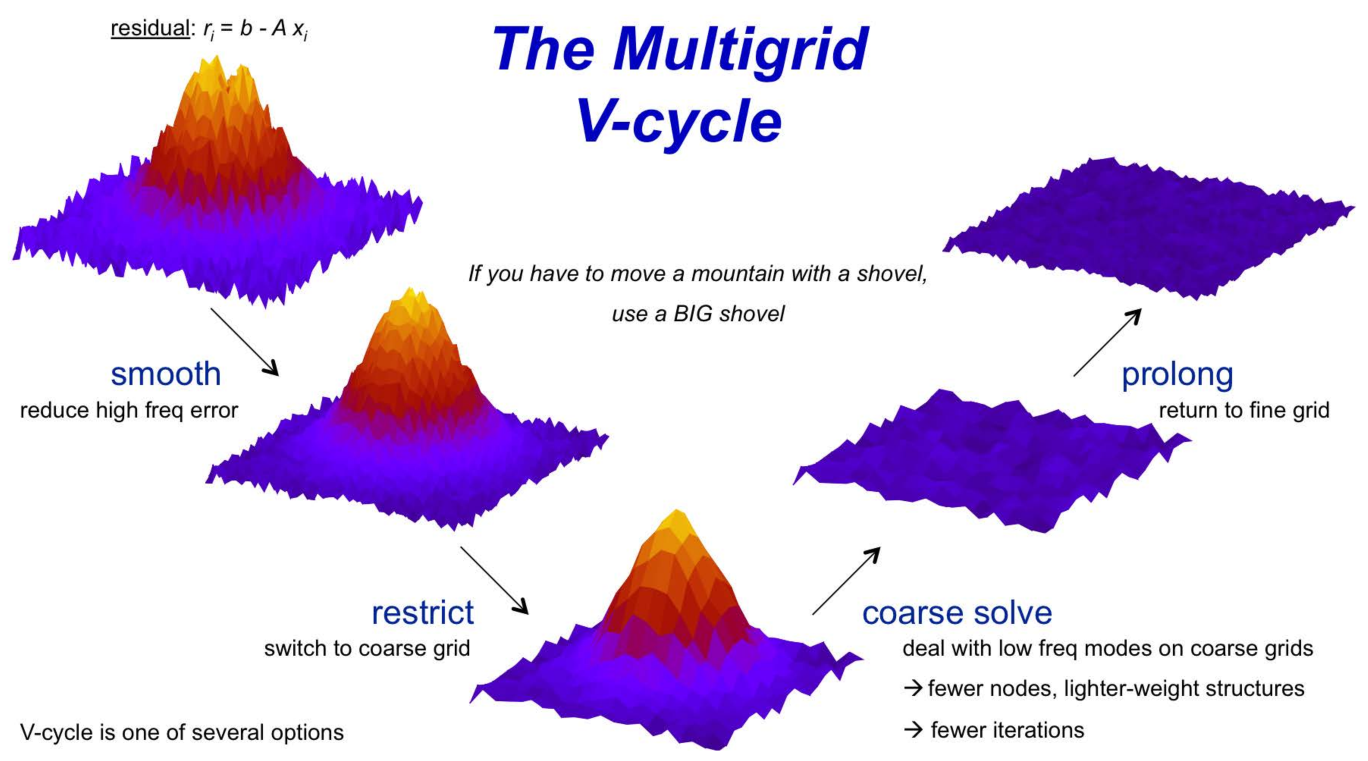
Bootstrap Algebraic Multigrid and Lattice QCD

E. Berkowitz, R. Falgout, C. Schroeder

Lawrence Livermore National Laboratory

Multigrid Methods



- It is hard to shrink errors with nonlocal behavior on a full-sized fine grid of interest.
- Idea:
  - Smooth the noise.
  - Restrict to an easier-to-handle coarse grid.
  - Solve on the coarse grid.
  - Prolong the coarse-grid solution to the fine grid.
- The solve on the coarse grid can, itself, be a multigrid solve.

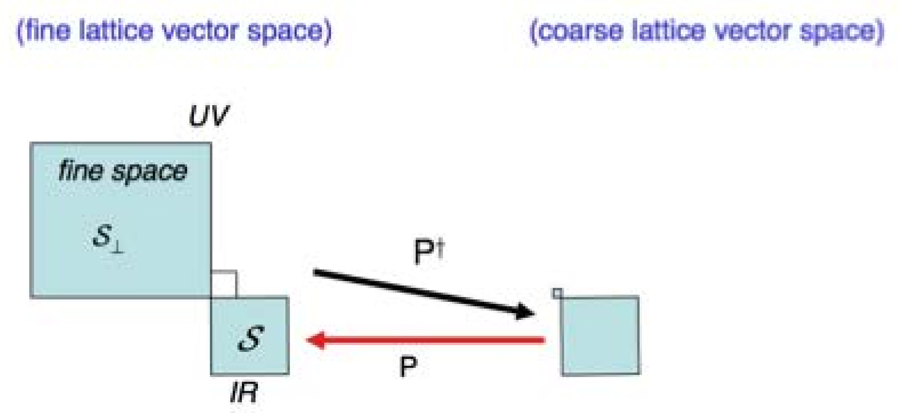
Classical Algebraic Multigrid

- The Ruge-Stüben variant of Classical Algebraic Multigrid (AMG) [Brandt, McCormick, and Ruge, Technical Report, Colorado State University, 1983] exhibits optimal efficiency for many challenging problems
- Often outperforms traditional iterative methods.
- Relies on three properties:
  - The strength of connection used in coarsening and interpolating can be accurately determined from the system matrix.
  - The lowest-eigenvalue modes must be locally smooth in directions of the strong connections.
  - The lowest-eigenvalue modes must provide an accurate local representation of the low modes not explicitly captured.
- Standard AMG approaches break down when applied to a typical lattice QCD system because
  - The algebraically smooth error is locally supported
  - The error is not smooth among neighboring grid points in regions where it is nonzero.
- How can we avoid this issue and recover the advantage of multigrid solvers for lattice QCD?

Adaptive Smoothed Aggregation

- Adaptive Smoothed Aggregation (αSA) is an AMG algorithm developed in 2004 by Brezina, Falgout, MacLachlan, Manteuffel, McCormick, and Ruge [SIAM J. Sci. Comp., 25] and first applied to lattice field theory in 2008 by Brannick, Brower, Clark, Osborn, and Rebbi [PRL, 100].

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

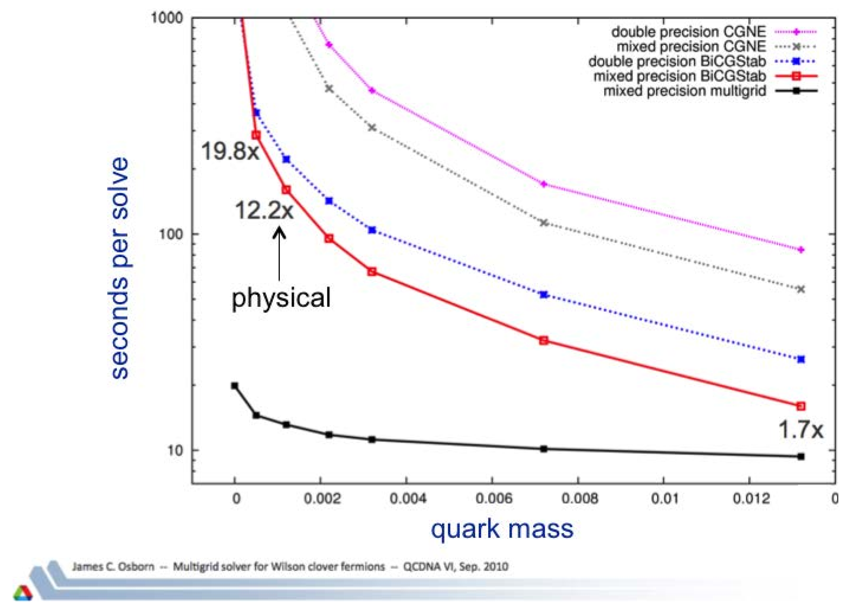


- Discover the near-null space dynamically and adapt.
  - Difficult modes $\sim$ near-null modes.
  - Use residuals to redefine interpolation.
  - Repeat until all near-null modes are captured.

Acknowledgements

- Support for this work was provided through Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Nuclear Physics.
- Prepared by LLNL under Contract DE-AC52-07NA27344.
- LLNL-POST-657546

αSA Performance



- The MG-QCD Collaboration has demonstrated an order-of-magnitude speedup for full QCD in 3+1 dimensions and the implementation, in QOPQDP, is used extensively in current large-scale calculations.
- αSA has a big setup cost, which is particularly expensive for staggered and domain wall fermion discretizations.
- This makes it difficult to use αSA for
  - Monte Carlo evolution
  - calculations where these discretizations are preferred (eg. charge fluctuations)
- Are there algorithms with cheaper setups?

Bootstrap AMG

- Bootstrap AMG (BAMG) is a multigrid variant described by Brandt, Brannick, Kahl, and Livshitz in [SIAM J. Sci. Comp., 33 (2011)] and is expected to perform well for all discretizations and provides an alternative to αSA.
- The essence of the bootstrap approach is the use of the current grid hierarchy iteratively to determine a better hierarchy to reduce sensitivity to system properties.
- The prolongation matrix P is chosen by via a least-squares

$$\min_P \left\| v - P\hat{R}v \right\|$$

over the test vectors v and the naive, geometric restriction operator $\hat{R}$.
- Geometric restriction may make the setup costs cheap enough for use in monte-carlo.

Bootstrap AMG Performance

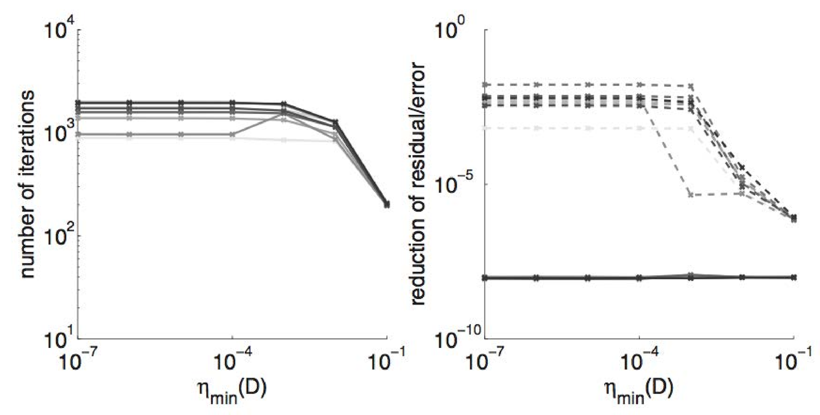


FIG. 9. *Results of CGNR applied to the odd-even reduced system with $N = 128$ and $\beta = 6$. The results for the light to dark lines correspond to different gauge field configurations, going from light to dark with increasing configuration number. On the left, the number of iterations needed to reduce the relative residual by a factor 10^{-8} is plotted against $\eta_{\min}(D)$ defined in (2.4), corresponding to different diagonal shifts m. On the right, the resulting relative residuals (solid lines) and relative errors (dashed lines) are plotted against $\eta_{\min}(D)$.*

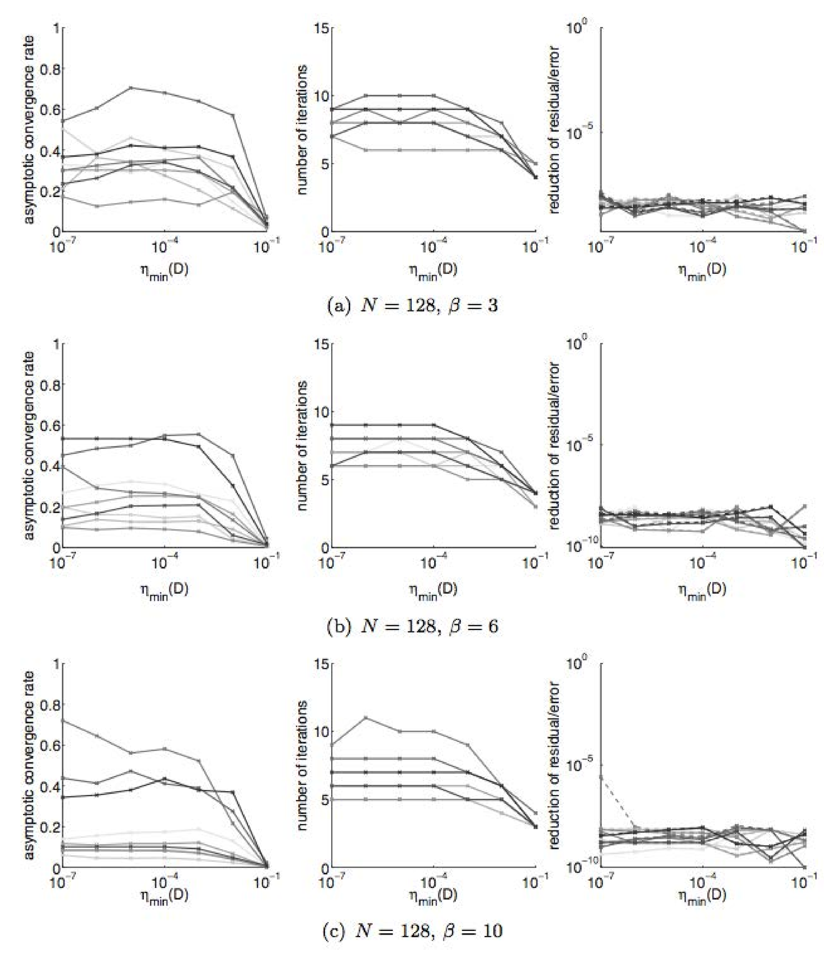


FIG. 11. *Results of BAMG and BAMG preconditioned GMRES(32) applied to the odd-even reduced matrix for $N = 128$ and different values of β. The results for the light to dark lines correspond to different gauge field configurations, going from light to dark with increasing configuration number. On the left, plots of the estimates of the convergence rates ρ for the stand-alone solver versus $\eta_{\min}(D)$ defined in (2.4), corresponding to different diagonal shifts m, are provided. In the middle, the number of BAMG preconditioned GMRES(32) iterations needed to reduce the ℓ_2 norm of the relative residual by a factor of 10^{-8} is plotted against $\eta_{\min}(D)$. The plots on the right contain the ℓ_2 norms of the relative residuals (solid lines) and relative errors (dashed lines) computed using the resulting solution versus $\eta_{\min}(D)$.*

Brannick and Kahl, SIAM J. Sci. Comp., 36.

- Preliminary comparisons with CGNR for 2D Wilson fermions show a 50-200 times speedup and a reduction of residual error by up to six orders of magnitude!

BAMG in *hypre*

- CASC's *hypre* library is a high-performance multigrid library.
- Implementation of BAMG in *hypre* has been underway for roughly 1 year.
  - Should be completed by end of FY2014.