A Multigrid Bases Eigensolver for the Hermitian Wilson Dirac Operator

Gunar Bali[b], Sara Collins[b], Andreas Frommer[a], Karsten Kahl[a], Issaku Kanamori[c], **Matthias Rottmann**[a], and Jakob Simeth[b]

[a]: Bergische Universität Wuppertal
[b]: Universität Regensburg
[c]: Hiroshima University

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Outline

Adaptive Algebraic Multigrid Approach for $D^{\text{(non-Hermitian)}}$

Two-grid error propagator for ν steps of post-smoothing

$$E_{2g}^{(\nu)} = \underbrace{(1 - MD)^{\nu}}_{\text{smoother}} \underbrace{(1 - PD_c^{-1}P^{\dagger}D)}_{\text{coarse grid correction}}, \quad \underbrace{D_c := P^{\dagger}DP}_{\text{coarse operator}}$$

- low accuracy for D_c^{-1} and M is sufficient
- introduce recursive construction for $D_c \rightarrow$ multigrid

To Do: Define interpolation P and smoother M

DD-αAMG[ArXiv:1303.1377,1307.6101]

M: Schwarz Alternating Procedure (SAP)
[Hermann Schwarz 1870; Martin Lüscher 2003]

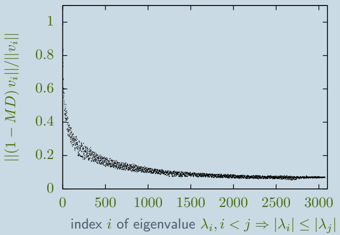
P: Aggregation based Interpolation
[Brannick, Clark et al. 2010]

The Algebraic Multigrid Principle

Smoother: $1 - MD$

- effective on "large eigenvectors"
- "small eigenvectors" remain

SAP



$$Dv_i = \lambda_i v_i \quad \text{with} \quad |\lambda_1| \le \ldots \le |\lambda_{3072}|$$

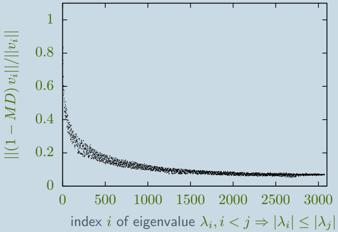
The Algebraic Multigrid Principle

Coarse-grid correction: $1 - P D_c^{-1} P^\dagger D$

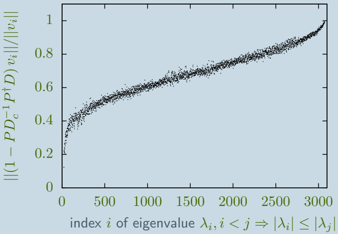
- small eigenvectors built into interpolation P

  $\Rightarrow$ effective on small eigenvectors

SAP



Aggregation + Small EV



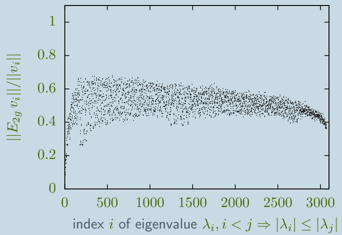
$Dv_i = \lambda_i v_i$ with $|\lambda_1| \le \ldots \le |\lambda_{3072}|$

The Algebraic Multigrid Principle

Two-grid method: $E_{2g} = (1 - MD)(1 - PD_c^{-1}P^\dagger D)$

- complementarity of smoother and coarse-grid correction
- effective on all eigenvectors!

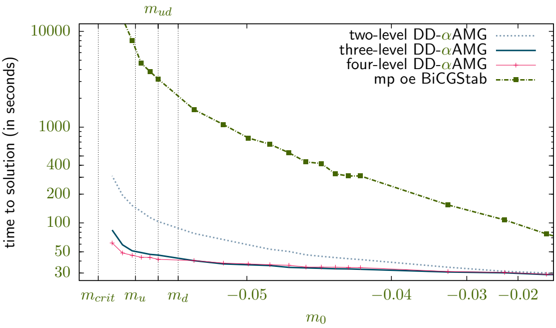
DD-αAMG



$Dv_i = \lambda_i v_i$ with $|\lambda_1| \leq \ldots \leq |\lambda_{3072}|$

AMG for D in Practice: Scaling with the bare quark mass

Configuration: 64×64^3, 128 cores



- lighter quark mass $m_0 \rightarrow$ more ill-conditioned system
- AMG less sensitive to condition number than Krylov subspace methods

Adaptive Algebraic Multigrid Approach for $Q = \gamma_5 D$

Construct P such that $P\gamma_5 = \gamma_5 P$
Replacing $D \to Q = \gamma_5 D$ we obtain the two-grid error propagator

$$\tilde{E}_{2g}^{(\nu)} = \underbrace{(1 - MQ)^\nu}_{\text{requires new smoother}} \underbrace{(1 - PQ_c^{-1}P^\dagger Q)}_{=1-PD_c^{-1}P^\dagger D}, \quad \underbrace{Q_c := P^\dagger QP}_{\text{new coarse operator}}$$

- P is valid for D and Q
- P preserves $Q_c^\dagger = Q_c$ $\to$ recursive application possible
- SAP smoother does not work anymore

Choice: Replace M by GMRES

- AMG for Q in practice a factor of 2 slower than DD-αAMG
- enables to compute $(Q - \sigma)^{-1}$ with AMG and thus to compute small eigenvectors of Q *(application $\to$ J. Simeth)*

Calculating Eigenvectors of Q

Algorithm 1: Rayleigh Quotient Iteration + AMG

input: number of eigenvectors N, desired accuracy ε
output: eigenvectors $v_1, \dots, v_N$

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let v_1, ..., v_N orthonormalized set of random vectors and
λ_i = 0, ε_i = 1 ∀i = 1, ..., N
build P from v_1, ..., v_N
while ∃ε_i : ε_i > ε do
    for all i = 1, ..., N with ε_i > ε do
        σ ← λ_i · max(1 − ε_i, 0)
        v_i ← (Q − σ)^{-1} v_i
        v_i ← v_i − Σ_{j=1}^{i−1} (v_j^† v_i) v_j
        v_i ← v_i / ||v_i||
        update v_i in interpolation P
        λ_i = v_i^† Q v_i
        ε_i = ||Q v_i − λ_i v_i||
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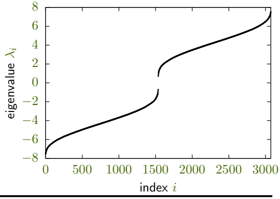
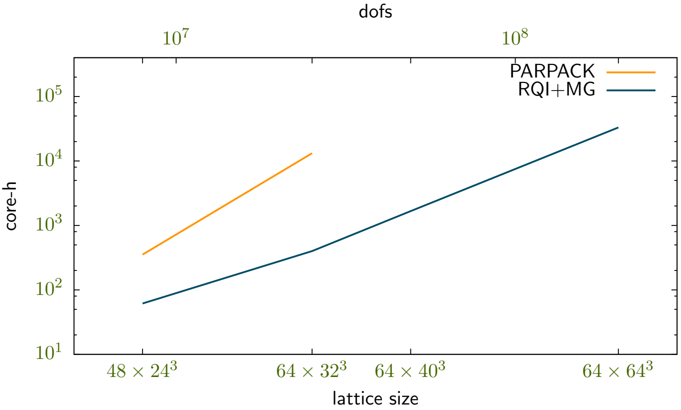
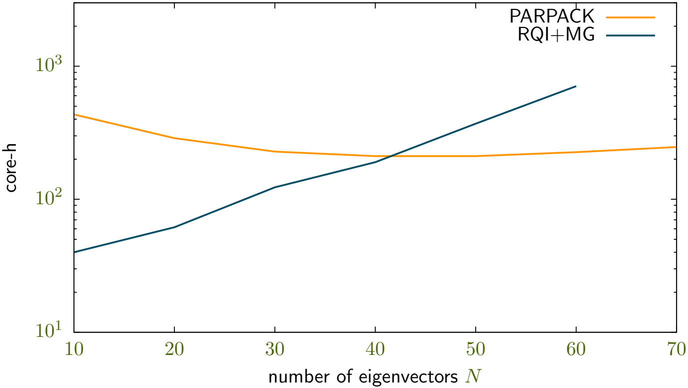


Comparison with PARPACK: Scaling with Lattice Size



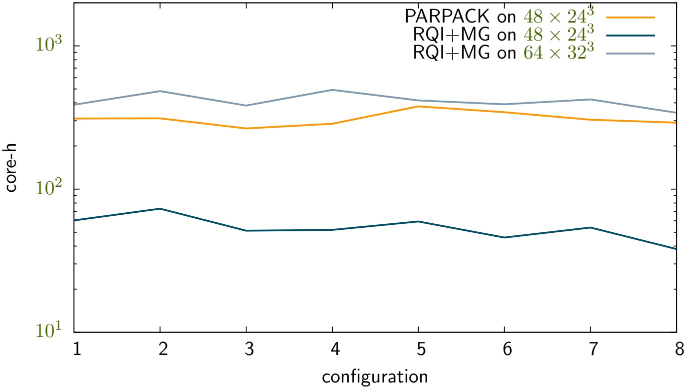
- 20 smallest eigenpairs (λ_i, v_i) with $\varepsilon < 10^{-8}$
- different lattice sizes at constant physics
- Krylov subspace dimension for PARPACK: 100
- only two level multigrid solver, yet
- PARPACK for 64×40^3 did not converge within $2.4 \cdot 10^4$ core-h

Comparison with PARPACK: Scaling with the Number of Eigenvectors N



- 48×24^3 lattice
- Krylov subspace dimension for PARPACK: 200
- operator complexities: P is $\mathcal{O}(N)$, Q_c is $\mathcal{O}(N^2)$
  $\rightarrow$ coarse grid correction/Q_c^{-1} is at least $\mathcal{O}(N^2)$
- multigrid eigensolver more beneficial for small N

Comparison with PARPACK: Gauge Configuration Fluctuations



- 2 ensembles of configurations generated by a hybrid Monte-Carlo simulation
- 8 stochastically independent configurations from each ensemble
- only minor fluctuations in run-time

AMG for Lattice QCD

Rayleigh Quotient Iteration + AMG

Numerical Results

Summary & Outlook

Summary

Summary

- multigrid based eigensolver performs well for
  - large lattice sizes
  - moderate number of eigenpairs
- speed up can be orders of magnitudes

Application

- calculating $\mathrm{tr}(Q^{-1})$ via low mode averaging $\rightarrow$ talk of J. Simeth (coming up next)
  - deflated stochastic algorithm
  - small number of deflated modes
  - low accuracy modes

Outlook

Improve Eigensolver

- explore possible benefits of employing more than two levels in AMG solver
- try other shifted inversion based eigensolver approaches as
    - Jacobi-Davidson
    - shift-and-invert Arnoldi
    - FEAST

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