

The DD- α AMG Solver Library

A Multigrid Solver Library for Wilson-Clover Fermions

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contributions by: A. Frommer, K. Kahl, B. Leder, S. Krieg, A. Strebel, S. Heybrock,
S. Bacchio, K. Szabo, W. Söldner and many others

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Outline

Introduction

Library Features

Progress Report

Summary & Outlook



Adaptive Algebraic Multigrid Approach

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

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

- low accuracy for D_c^{-1} and M is sufficient
- allows for introducing recursive construction for D_c

To Do: Define interpolation P and smoother M

DD- α AMG

M : Schwarz Alternating Procedure (SAP)

[Lüscher 2003]

P : Aggregation Based Interpolation

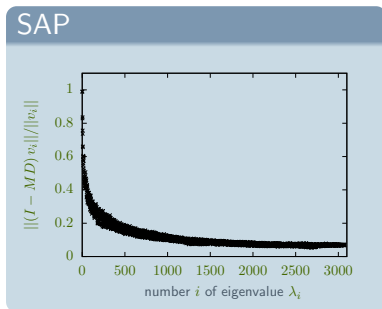
[Brannick, Clark et al. 2010]



The Algebraic Multigrid Principle

Smoother: $1 - MD$

- ▶ effective on “large” eigenvectors
- ▶ “small” eigenvectors remain



$$Dv_i = \lambda_i v_i \quad \text{with} \quad |\lambda_1| \leq \dots \leq |\lambda_{3072}|$$

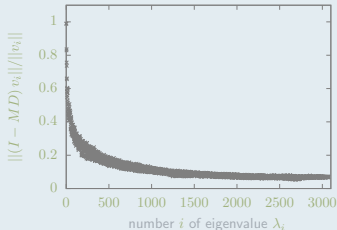


The Algebraic Multigrid Principle

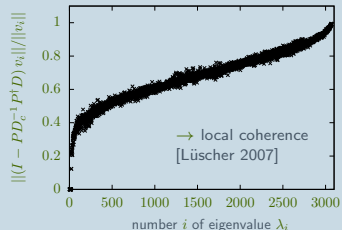
Coarse-grid correction: $1 - PD_c^{-1}P^\dagger D$

- **small eigenvectors** w_1, \dots, w_N built into interpolation P
 \Rightarrow effective on **small eigenvectors**

SAP



Aggregation + Low Modes



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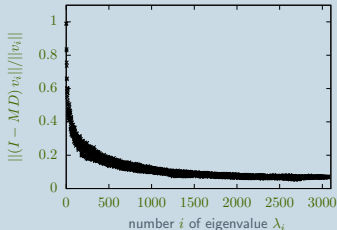


The Algebraic Multigrid Principle

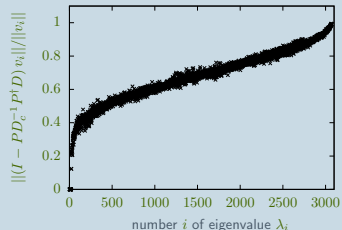
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Aggregation + Low Modes



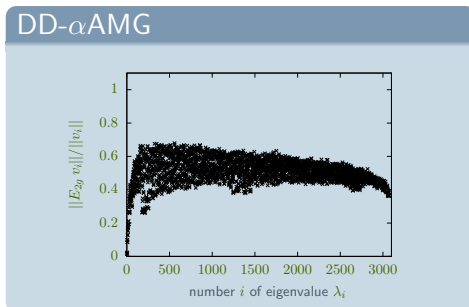
$$Dv_i = \lambda_i v_i \quad \text{with} \quad |\lambda_1| \leq \dots \leq |\lambda_{3072}|$$



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!**

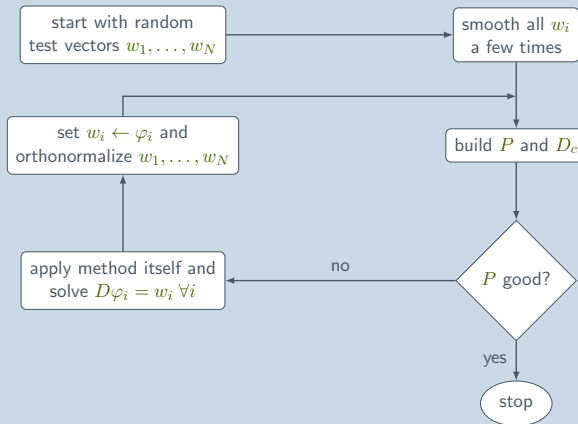


$$Dv_i = \lambda_i v_i \quad \text{with} \quad |\lambda_1| \leq \dots \leq |\lambda_{3072}|$$



Adaptive Setup: How to Obtain Information about Small Eigenvectors

Inverse iteration with the method itself



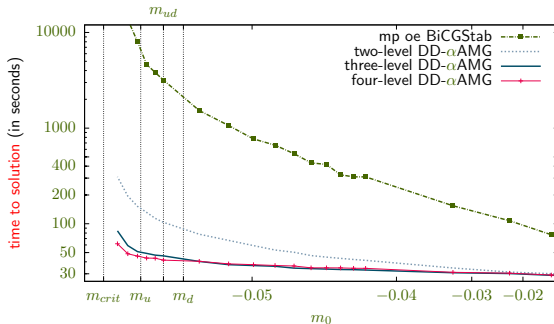
add recurrence scheme \rightarrow multilevel setup

two level setup: [DD-HMC/OpenQCD]



Performance and Setup Costs

BMW-c cnfg, 3HEX-smearcd 64×64^3 , 128 cores



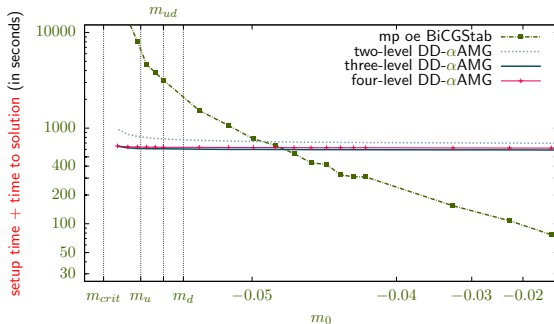
A. Frommer, K. Kahl, S. Krieg, B. Leder, R.

→ arXiv:1303.1377,1307.6101



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The DD- α AMG Solver Library

available on github.com/DDalphaAMG

Technical Features

- ▶ C-code
- ▶ MPI + OpenMP
- ▶ SSE intrinsics
- ▶ library interface
- ▶ integrated profiling
- ▶ small parameter set for users
- ▶ large parameter set for developers
- ▶ debug information
- ▶ GNU GPL

Code Features

- ▶ Wilson+Clover
- ▶ AMG with arbitrary number of levels
- ▶ idling processes
- ▶ different smoothers: SAP, additive Schwarz, GMRES
- ▶ reference methods: BiCGStab, CGN, GMRES
- ▶ mixed precision, odd-even preconditioned



The DD- α AMG Library Interface

available on github.com/DDalphaAMG

Interface Features

- ▶ conversion routines for configurations and vectors
- ▶ setup routine (initial setup)
- ▶ configuration update routine (\rightarrow HMC)
- ▶ setup update routine (\rightarrow HMC)
- ▶ mass update routines (\rightarrow Hasenbusch trick)
- ▶ solver routine (inversion for 1 RHS)
- ▶ GNU GPL \rightarrow feel free to adjust it to your needs



Progress Report: Existing Branches

DD- α AMG for KNC/KNL

- ▶ SAP smoother implemented from scratch
- ▶ coarse grid correction from DD- α AMG
- ▶ DD- α AMG inherited SIMD vectorization from KNC-code

S. Heybrock, D. Richtmann, P. Georg, T. Wettig, R.

→ arXiv:1512.04506,1601.03184, talk by T. Wettig, poster

DD- α AMG for twisted mass fermions

- ▶ the interpolation P in DD- α AMG respects $\gamma_5 P = P \gamma_5^c$
 $\implies D + i\mu\gamma_5 \rightsquigarrow D_c + i\mu\gamma_5^c$

S. Bacchio, J. Finkenrath, C. Alexandrou, A. Frommer, K. Kahl, R.

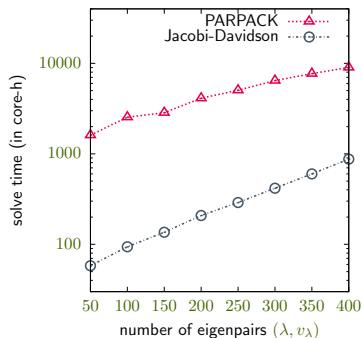
→ talk by S. Bacchio



Progress Report: Future Branch – Eigensolver for $\gamma_5 D$

48×24^3 CLS cnfg, $m_\pi \approx 290$ MeV

- ▶ Jacobi-Davidson with a multigrid solver
- ▶ outperforms PARPACK for 400 eigenpairs
- ▶ improved scaling with lattice volume



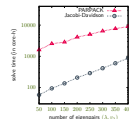
A. Strebel, J. Simeth, G. Bali, S. Collins, A. Frommer, K. Kahl, I. Kanamori, B. Müller, R.

→ arXiv:1509.06865, talk by A. Strebel

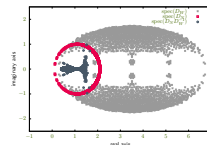


Outlook

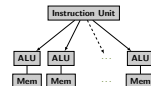
- ▶ eigensolver: improve algorithm (clever restart strategies, etc.)
 ⇒ publication



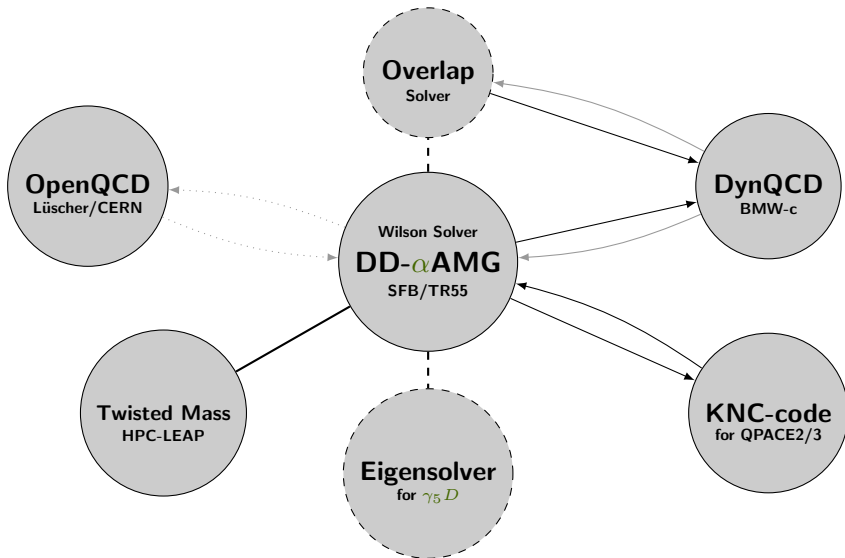
- ▶ overlap solver: prepare code for publication
 J. Brannick, A. Frommer, K. Kahl, B. Leder, A. Strebel, R.
 → arXiv:1410.7170



- ▶ vectorization: generalization, integrate AVX



Summary & Outlook

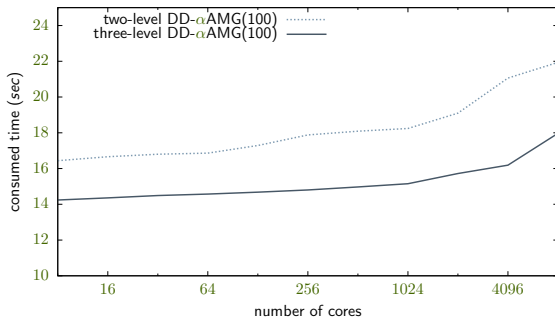


github.com/DDalphaAMG

Appendix



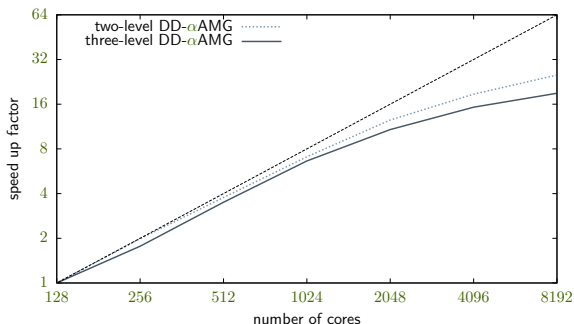
Weak Scaling: 2 and 3 Levels



- ▶ 100 V-Cycles for 2 and 3 levels
- ▶ 16×8^3 local lattice per process
- ▶ Scaling behavior almost independent of number of levels
- ▶ Coarse solver: GMRES(32); profiling shows: slow down mainly caused by allreduce operations $\rightarrow \log(p)$ scaling



Configuration: BMW-c, 64×64^3 , 3Hex-Smeared, m_π physical



- Scaling behavior only slightly corrupted by adding an additional level, although there are
 - Idle times on third level
 - Worse data/comm ratio on third level

