The DD-αAMG Solver Library

A Multigrid Solver Library for Wilson-Clover Fermions

Matthias Rottmann

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

Bergische Universität Wuppertal

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Outline

Adaptive Algebraic Multigrid Approach

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

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

- 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-αAMG

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

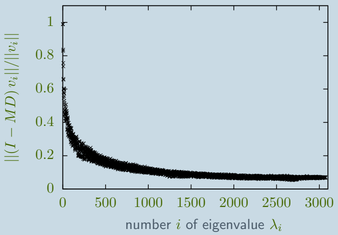
P: Aggregation Based Interpolation
[Brannick, Clark et al. 2010]

The Algebraic Multigrid Principle

Smoother: $1 - MD$

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

SAP

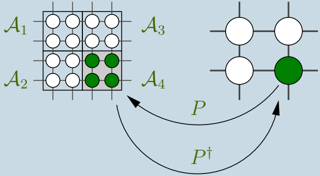


$$Dv_i = \lambda_i v_i \quad \text{with} \quad |\lambda_1| \leq \ldots \leq |\lambda_{3072}|$$

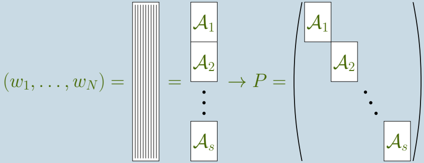
Aggregation Based Interpolation

Construction

- define aggregates: domain decomposition $\mathcal{A}_1, ..., \mathcal{A}_s$



- calculate test vectors $w_1, ..., w_N$
- decompose test vectors over aggregates $\mathcal{A}_1, ..., \mathcal{A}_s$



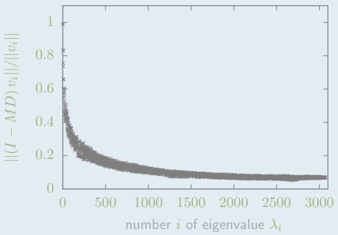
The Algebraic Multigrid Principle

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

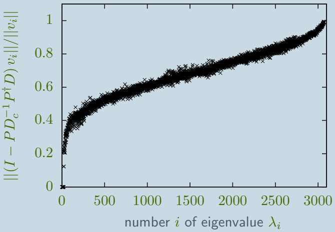
- small eigenvectors $w_1, \dots, w_N$ built into interpolation P

  $\Rightarrow$ effective on small eigenvectors

SAP



Aggregation + Low Modes



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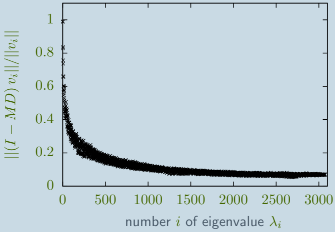

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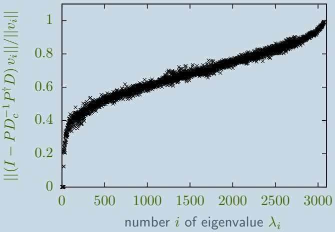


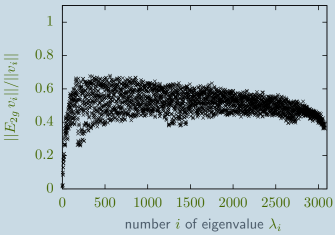
$Dv_i = \lambda_i v_i$ with $|\lambda_1| \leq \ldots \leq |\lambda_{3072}|$

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!

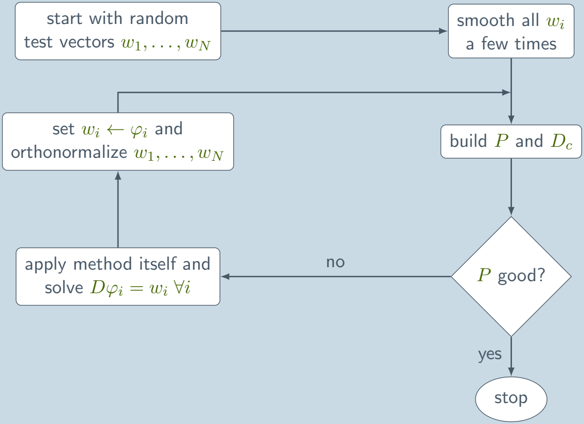
DD-αAMG



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

Adaptive Setup: How to Obtain Information about Small Eigenvectors

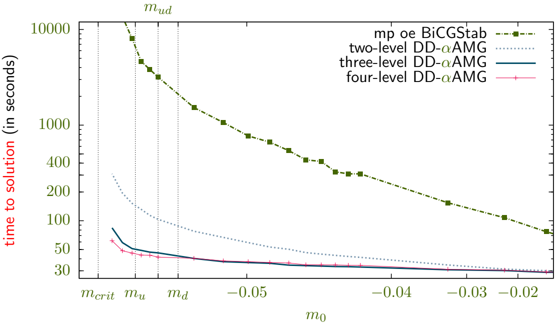
Inverse iteration with the method itself



add recurrence scheme $\rightarrow$ multilevel setup

Performance and Setup Costs

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



A. Frommer, K. Kahl, S. Krieg, B. Leder, R.
→ arXiv:1303.1377,1307.6101

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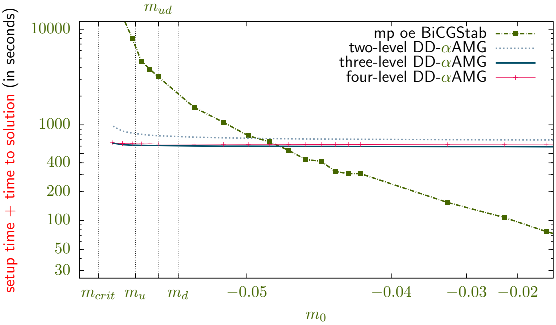

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The DD-αAMG Solver Library

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-αAMG 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-αAMG for KNC/KNL

- SAP smoother implemented from scratch
- coarse grid correction from DD-αAMG
- DD-αAMG inherited SIMD vectorization from KNC-code

S. Heybrock, D. Richtmann, P. Georg, T. Wettig, R.
$\rightarrow$ arXiv:1512.04506,1601.03184

DD-αAMG for twisted mass fermions

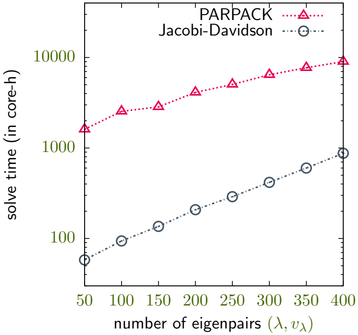
- the interpolation P in DD-αAMG respects $\gamma_5 P = P\gamma_5^c$
  $\implies D + i\mu\gamma_5 \rightsquigarrow D_c + i\mu\gamma_5^c$

S. Bacchio, J. Finkenrath, C. Alexandrou, A. Frommer, K. Kahl, R.
$\rightarrow$ Talk by S. Bacchio

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

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

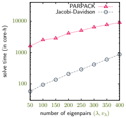
- Jacobi-Davidson with a multigrid solver
- outperforms PARPACK for 400 eigenpairs
- improved scaling with lattice volume



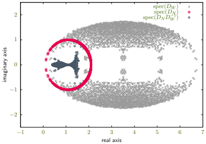
A. Strebel, J. Simeth, G. Bali, S. Collins, A. Frommer, K. Kahl, I. Kanamori, B. Müller, R.
$\rightarrow$ arXiv:1509.06865

Outlook

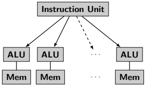
- eigensolver: improve algorithm (clever restart strategies, etc.)
  $\Longrightarrow$ publication



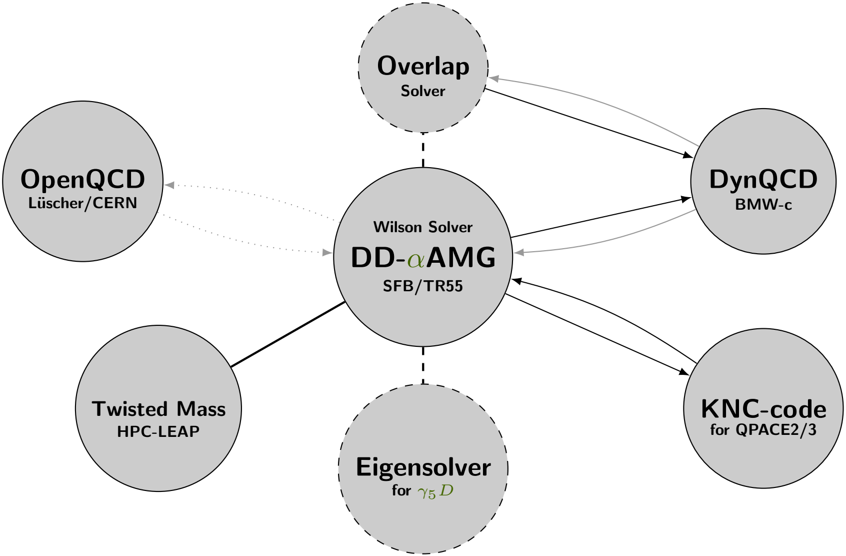
- overlap solver: prepare code for publication
  J. Brannick, A. Frommer, K. Kahl, B. Leder, A. Strebel, R.
  $\rightarrow$ arXiv:1410.7170



- vectorization: generalization, integrate AVX



Summary & Outlook



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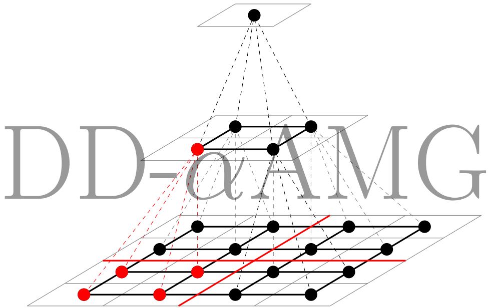

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