# Adaptive Aggregation-based Domain Decomposition Multigrid

for Twisted Mass Fermions with $N_f = 2$

C. Alexandrou [a, b], S. Bacchio [a, c], J. Finkenrath [b]
A. Frommer [c], K. Kahl [c], M. Rottmann [c]

[a] University of Cyprus
[b] The Cyprus Institute
[c] University of Wuppertal

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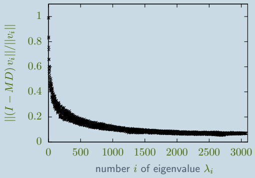
# Overview

# DD-$\alpha$AMG[1]: main ingredients

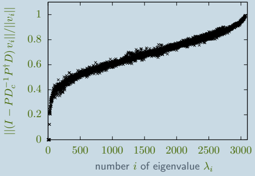
- **The smoother:** *red-black Schwarz Alternating Procedure,* designed to treat the UV-modes of the Wilson Dirac operator $D$.

- **The coarse-grid correction:** $\epsilon \leftarrow \left(\mathbb{1} - PD_c^{-1}P^\dagger D\right)\epsilon$, where $P$ is designed to project the IR-modes of $D$ in $D_c = P^\dagger DP$.

**Smoother**




**Coarse-grid correction**




[1] Andreas Frommer et al. "Adaptive Aggregation Based Domain Decomposition Multigrid for the Lattice Wilson Dirac Operator". In: *SIAM J. Sci. Comput.* 36 (2014), A1581–A1608. DOI: 10.1137/130919507.

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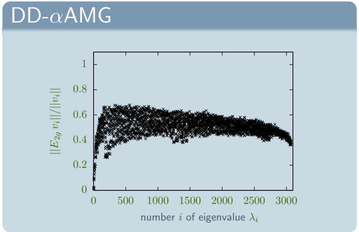


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- **Standard aggregation:** *$P$ is $\Gamma_5$-compatible, i.e.* $\Gamma_5 P = P \Gamma_{5,c}$, and then $D_c$ is $\Gamma_{5,c}$-hermitian as $D$ is with $\Gamma_5$,

$$\Gamma_{5,c}\, D_c = \Gamma_{5,c}\, P^\dagger D P = P^\dagger D^\dagger P\, \Gamma_{5,c} = D_c^\dagger\, \Gamma_{5,c}.$$

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# Standard aggregation: $\Gamma_5$-compatibility

Using a spin-wise aggregation as

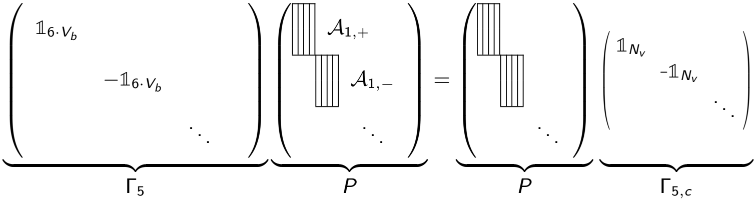
$$\mathcal{A}_{j,+} = \mathcal{V}_j \times \mathcal{S}_{0,1} \times \mathcal{C} \quad \text{and} \quad \mathcal{A}_{j,-} = \mathcal{V}_j \times \mathcal{S}_{2,3} \times \mathcal{C},$$

the movement from fine grid to coarse grid is given by

$$D:\ \mathcal{V} \times \mathcal{S} \times \mathcal{C} \quad \underset{P}{\overset{P^\dagger}{\rightleftharpoons}} \quad D_c:\ \mathcal{V}_c \times 2 \times N_v$$

$$\Gamma_5 = \mathbb{1}_\mathcal{V} \otimes \gamma_5 \otimes \mathbb{1}_\mathcal{C} \quad \underset{P}{\overset{P^\dagger}{\rightleftharpoons}} \quad \Gamma_{5,c} = \mathbb{1}_{\mathcal{V}_c} \otimes \tau_3 \otimes \mathbb{1}_{N_v}.$$

The $\Gamma_5$-compatibility can be represented as



# DD-$\alpha$AMG for twisted mass fermions

For TM fermions with $N_f = 2$, we are interested in the solution of

$$\begin{bmatrix} D + i\mu\Gamma_5 & 0 \\ 0 & D - i\mu\Gamma_5 \end{bmatrix} \begin{bmatrix} \psi_u \\ \psi_d \end{bmatrix} = \begin{bmatrix} \eta_u \\ \eta_d \end{bmatrix}$$

where the u- and d-propagators are uncoupled.

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where the u- and d-propagators are uncoupled.

Thus, we consider two different operators for the u- and d-quarks, $D(\pm\mu)$, obtaining a DD-$\alpha$AMG approach similar to the Wilson clover fermions:

$$D(\pm\mu) = D \pm i\mu\Gamma_5 \quad \underset{P}{\overset{P^\dagger}{\rightleftharpoons}} \quad D_c(\pm\mu) = P^\dagger DP \pm i\mu\Gamma_{5,c}$$

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$$D_c^\dagger(\pm\mu) = P^\dagger(D \pm i\mu\Gamma_5)^\dagger P = P^\dagger(\Gamma_5 D\Gamma_5 \mp i\mu\Gamma_5)P = \Gamma_{5,c}\, D_c(\mp\mu)\Gamma_{5,c}$$

**Note:** the last property is valid only if the same $P$ is used for both $D(\pm\mu)$ and it can be done without affecting the iterations/time to solution.

# DD-$\alpha$AMG parameters

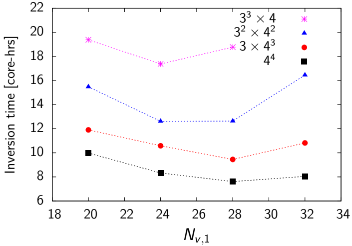
| | parameter | | optimal |
|---|---|---|---|
| Multigrid | number of levels | $n_\ell$ | 3 |
| | number of setup iterations | $n_{setup}$ | 5 |
| | number of test vectors on level 1 | $N_{v,1}$ | 28 |
| | number of test vectors on level 2 | $N_{v,2}$ | 28 |
| | size of lattice-blocks for aggregates on level 1 | $V_{b,1}$ | $4^4$ |
| | size of lattice-blocks for aggregates on level $\ell$, $\ell > 1$ | $V_{b,2}$ | $2^4$ |
| Solver | mixed precision FGMRES | | |
| | relative residual tolerance (restarting criterion) | | $10^{-6}$ |
| Smoother | red-black multiplicative SAP | | |
| | size of lattice-blocks | | $2^4$ |
| | number of post-smoothing steps | | 5 |
| | MINRES iterations to invert the blocks | | 3 |
| K-cycle | with single precision FGMRES | | |
| | restart length | | 5 |
| | maximal restarts | | 2 |
| | relative residual tolerance (stopping criterion) | | $10^{-1}$ |
| Coarsest grid | solved by FGMRES even-odd preconditioned | | |
| | twisted mass parameter | $\mu_c$ | $5.2 \cdot \mu$ |
| | restart length | | 100 |
| | maximal restarts | | 5 |
| | relative residual tolerance (stopping criterion) | | $10^{-1}$ |

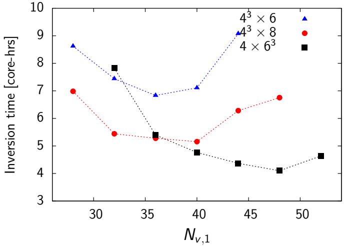
# Analysis of the aggregation parameters

We study[1]

- the number of test vectors used on the fine level, $N_{v,1}$
- the aggregation-block size on the fine level, $V_{b,1}$

$$\dim\left(D_{c,1}\right) = \left(2 \times N_{v,1} \times \frac{V}{V_{b,1}}\right)$$




[1] on a $96 \times 48^3$ lattice, $a = 0.0931(10)$ fm and $m_\pi = 131(1)$ MeV from $cA2.09.48$ [Abdel-Rehim et al, 2015].

# Analysis of the aggregation parameters

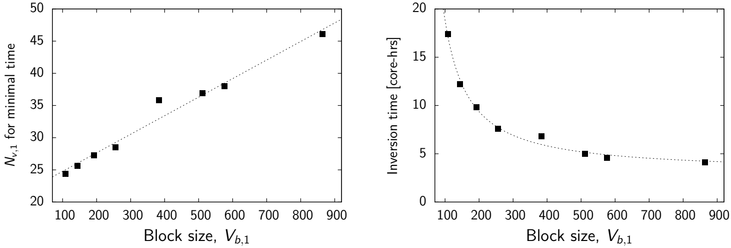
Extracting the minima, we obtain

- a linear behavior which relates the optimal $N_{v,1}$ and $V_{b,1}$,

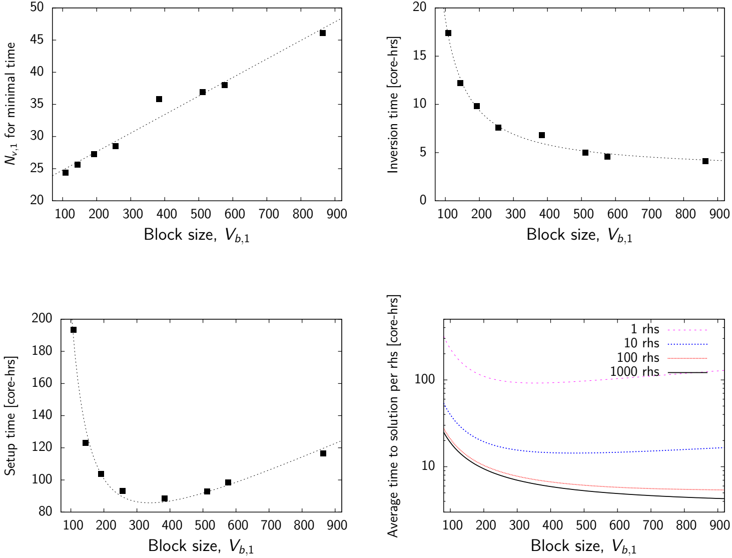
$$N_{v,1} = \alpha + \beta \, V_{b,1}$$

- a predictable behavior for the time to solution, which remarks the stability of the method

$$t_{solve} = \gamma + \delta \dim(D_{c,1}) + \epsilon \dim(D_{c,1})^2.$$



# Analysis of the aggregation parameters



# Comparison with Wilson Clover fermions

**Results for Wilson Clover fermions** on a $48^3 \times 64$ configuration:

| Solver | Setup time [core-hrs] | Inversion time [core-hrs] | Total applications of Dirac operator | Total applications of coarse grid operator |
|---|---|---|---|---|
| CG | – | 174.8 | 26 937 | – |
| DD-$\alpha$AMG | 13.3 | 0.9 | 16 | 2 988 |

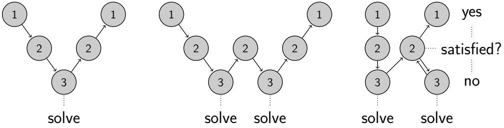
Speed-up versus CG, inversion time: $\sim$ 194x

**Results for Twisted Mass fermions** on a $48^3 \times 96$ configuration:

| Solver | Setup time [core-hrs] | Inversion time [core-hrs] | Total applications of Dirac operator | Total applications of coarse grid operator |
|---|---|---|---|---|
| CG | – | 338.6 | 34 790 | – |
| DD-$\alpha$AMG | 28.5 | 7.6 | 16 | 124 999 |

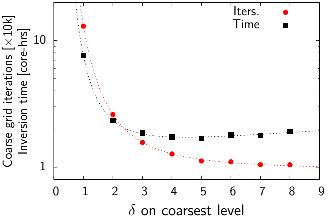
Speed-up versus CG, inversion time: $\sim$ 45x

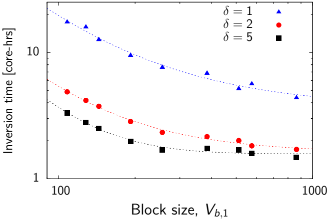
# An interesting trick



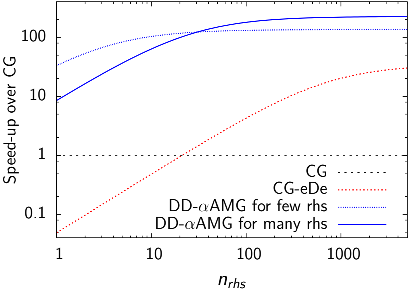

We increase the twisted mass parameter on the coarsest level (3) as

$$\mu_c = \delta\mu$$



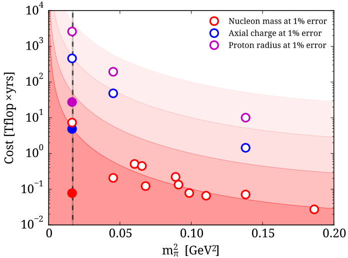



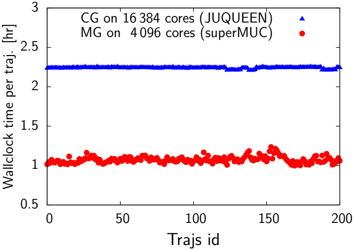
# Final performance




| Solver | Setup time [core-hrs] | Inversion time [core-hrs] | Total applications of Dirac operator | Total applications of coarse grid operator |
|---|---|---|---|---|
| CG | – | 338.6 | 34 790 | – |
| CG-eDe | 6 941.1 | 9.8 | 695 | – |
| DD-$\alpha$AMG for few rhs | 7.7 | 2.5 | 28 | 16 619 |
| DD-$\alpha$AMG for many rhs | 38.3 | 1.5 | 15 | 11 574 |

# Outcomes of this work




- *A novel insight of the aggregation parameters*
- *Employment of DD-αAMG solver for computing observables*
- *Speed-up of the HMC simulations for* $N_f = 2$
- *Public available code and interface to tmLQCD*

# The DDalphaAMG library for TM fermions

- Original package [M. Rottmann, prev. talk]:
  https://github.com/DDalphaAMG
- TM version:
  https://github.com/sbacchio/DDalphaAMG
- Interface to tmLQCD:
  https://github.com/Finkenrath/tmLQCD
  @ branch DDalphaAMG

Addition features in the TM version:

- $N_f = 2$ TM operator
- Twisted boundary conditions
- TM parameter on even and odd sites
- Improved linkage to the library

**tmLQCD interface:**

```
BeginDDalphaAMG
  MGBlockX = 4
  MGBlockY = 4
  MGBlockZ = 4
  MGBlockT = 4
  MGSetupIter = 5
  MGCoarseSetupIter = 3
  MGNumberOfVectors = 24
  MGNumberOfLevels = 3
  MGCoarseMuFactor = 5
EndDDalphaAMG

Begin ...
  ...
  Solver = DDalphaAMG
  SolverPrecision = 1e-14
End ...
```

Information available in the software doc.

# Future developments and acknowledgments

## *We look forward to*

- Extending to $N_f = 2+1+1$ operator

$$\begin{bmatrix} D + i\bar{\mu}\Gamma_5 & -\bar{\epsilon}\,\mathbb{1} \\ -\bar{\epsilon}\,\mathbb{1} & D - i\bar{\mu}\Gamma_5 \end{bmatrix} \begin{bmatrix} \psi_c \\ \psi_s \end{bmatrix} = \begin{bmatrix} \eta_c \\ \eta_s \end{bmatrix}.$$

- Studying new strategies for simulating with $N_f = 2+1+1$.

## *We kindly thank*


**Horizon 2020** for founding S.B. under the Marie Sklodowska-Curie grant agreement No 642069.

**G. Koutsou** for discussions and for helping with the access to various machines where the tests were run.

**B.Leder** for suggesting to shift the coarse grid $\mu_c$ to speed up the coarse grid solver.

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