A Jacobi Davidson Method with a Multigrid Solver for the Hermitian Wilson-Dirac Operator

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Joint Work

This project is joint work with:

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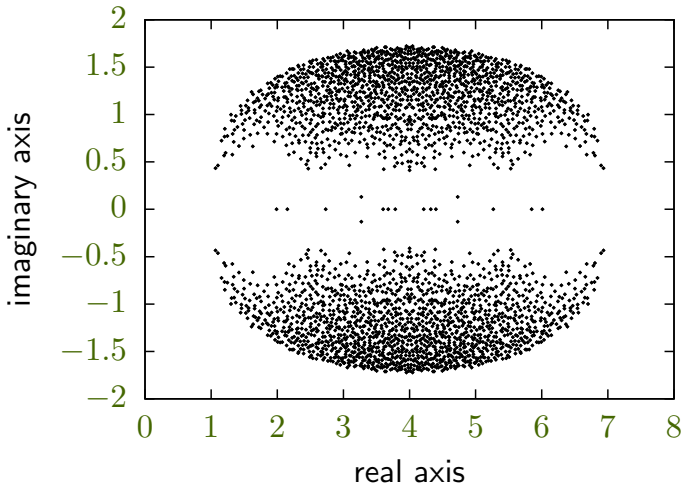
Outline

Lattice QCD: The Wilson Discretization

FD Discretization:

- $N_s^3 \times N_t$ regular lattice $\mathcal{L}$
  (parallelized by distributing sub-blocks)
- nearest neighbor coupling
- 12 variables per site and four 12×12 coupling matrices
- periodic boundary conditions
- γ_5-symmetry: $\gamma_5 D = (\gamma_5 D)^\dagger$
  ($\gamma_5 := \gamma_1\gamma_2\gamma_3\gamma_4,\ \gamma_5^2 = I$)



$\mathrm{spec}(D)$

$\mathrm{spec}(D)$ is in the right half plane and symmetric to the real axis

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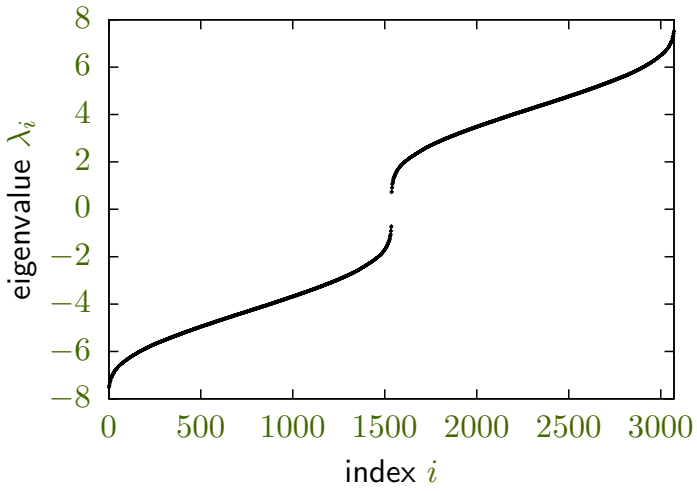


$\mathrm{spec}(\gamma_5 D)$

$\mathrm{spec}(\gamma_5 D)$ is real and maximally indefinite, we denote

$$Q := \gamma_5 D$$

Lattice QCD: Tasks

Application:

- calculating physical observables
  - oftentimes requires $\mathrm{tr}(Q^{-1})$
  - $\mathrm{tr}(Q^{-1}) = \sum \lambda_i^{-1}$
  - compute small eigenvectors exactly
  - treat remainder of spectrum with stochastic algorithm

Challenges:

- todays matrix sizes: $10^7 \times 10^7$ and larger
- (shifted) linear systems with either D or Q to be solved
- small EVs of Q ($=$ singular vectors of D) highly desired

Approaches:

- multigrid approaches for inverting D and Q
- Jacobi-Davidson method $+$ multigrid approach for Q
  $\rightarrow$ cheap eigensolver

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

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

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

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

To Do: Define interpolation P and smoother M

DD-αAMG[ArXiv:1303.1377,1307.6101]

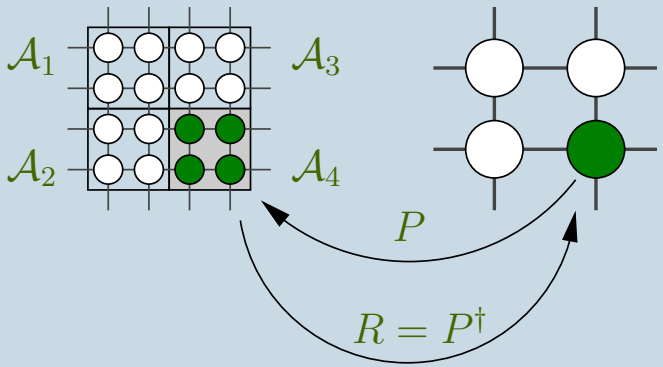
M: Schwarz Alternating Procedure (SAP)
[Lüscher 2003]

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

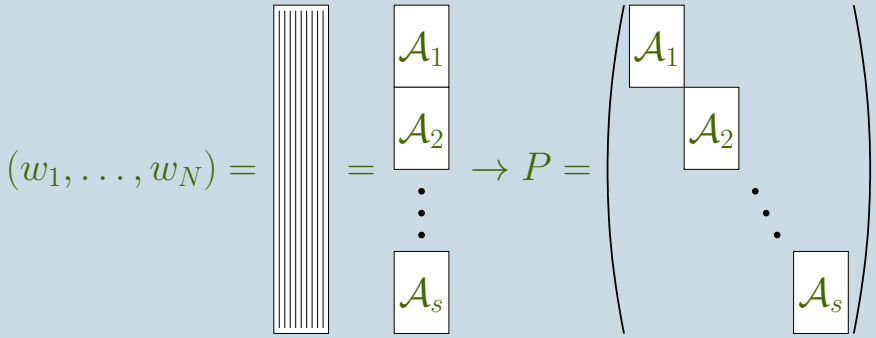
Aggregation Based Interpolation

Construction

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



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



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

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

- 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

γ_5-Preconditioning

- AMG for Q in practice a factor of 2 slower than DD-αAMG
  $\rightarrow$ can be remedied by "γ_5-preconditioning":

$$\begin{aligned} & (Q - \sigma I)\varphi &= \psi \\ \Leftrightarrow \quad & \gamma_5 (Q - \sigma I)\varphi &= \gamma_5 \psi \\ \Leftrightarrow \quad & (D - \sigma\gamma_5)\varphi &= \gamma_5 \psi \end{aligned}$$

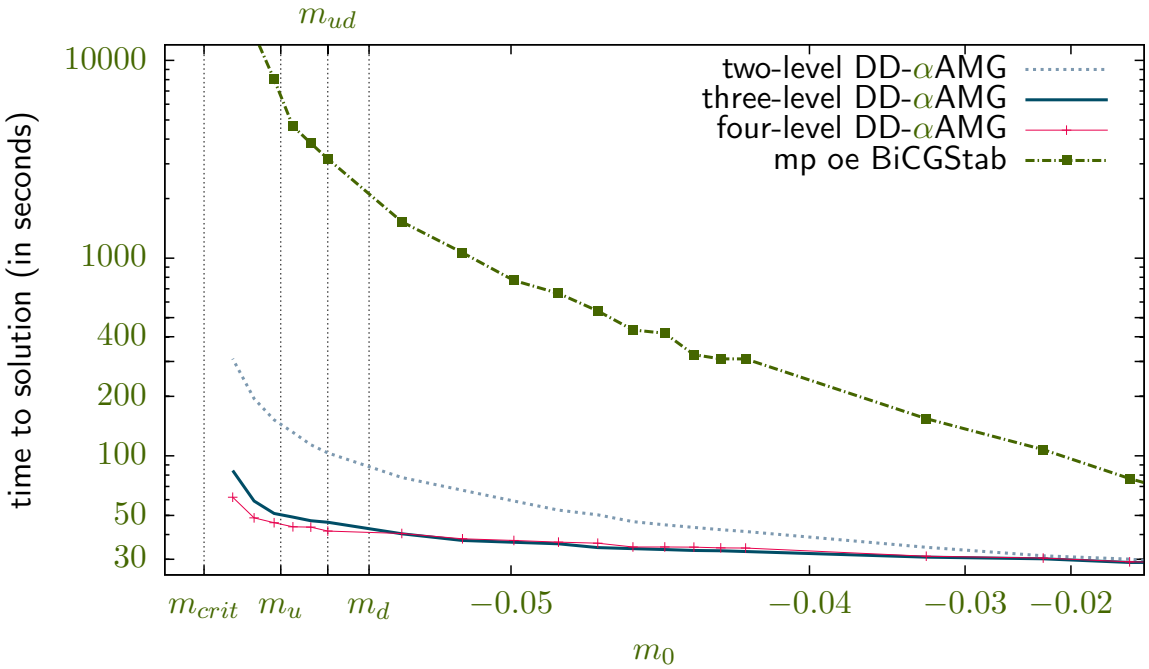
- error propagator of smoother now reads:

$$\tilde{E}_S^{(\nu)} = (I - M(D - \sigma\gamma_5))^\nu$$

- enables to compute $(Q - \sigma)^{-1}$ with AMG efficiently and thus to compute small eigenvectors of Q

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

An Introduction to Eigensolver Methods

- Applying a matrix A to an arbitrary vector v multiple times converges to *largest* eigenvector
  $\rightarrow$ Power method
- If λ is an eigenvalue of A, then $(\lambda - \sigma)^{-1}$ is an eigenvalue of $(A - \sigma I)^{-1}$
  $\rightarrow$ Inverse iteration
  $\rightarrow$ Now we can compute any eigenpair we want
- Given a normalized vector v the *Rayleigh Quotient* is defined as

$$r(x) = v^{\dagger} A v$$

  $\rightarrow$ $r(x)$ is the best-approximation to an eigenvalue of v
  $\rightarrow$ Rayleigh quotient iteration (cubic convergence for hermitian matrices)

An Introduction to the Jacobi-Davidson Method

The Jacobi-Davidson method combines two ideas

- *Davidson*: Impose Galerkin Condition $AVs - \theta s \perp V$ on eigenvalue problem to some subspace $V = \{v_1, v_2, \ldots, v_n\}$, which leads to

  $$V^\dagger AVs - \theta s = 0$$

  If (θ_i, s_i) is a solution of this equation then $(\theta_i, u_i = Vs_i)$ is called a *Ritz pair* w.r.t. the subspace V
- (θ_i, u_i) approximates eigenpairs $\rightarrow$ How to construct V?
- *Jacobi*: Given an eigenvector approximation u_i, choose an orthogonal correction $t \perp u_i$ such that

  $$A(u_i + t) = \lambda(u_i + t)$$

  We find that t fulfills the equation

  $$(I - u_i u_i^\dagger)(A - \lambda I)(I - u_i u_i^\dagger)t = -(A - \theta_i I)u_i := -r$$

  λ unknown $\rightarrow$ replace by θ_i

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$$(I - u_i u_i^\dagger)(A - \theta_i I)(I - u_i u_i^\dagger)t = -(A - \theta_i I)u_i =: -r$$

  Solve inexactly for t and add result to V

The Jacobi-Davidson Method

Algorithm 1: Jacobi-Davidson (basic)

input: initial guess t, desired accuracy ε
output: eigenpair (λ, x)

```
for all m = 1, 2, ... do
    t = t − V V^† t,  v_m = t / ||t||_2
    M = V^† A V
    compute smallest eigenpair (θ, s) of M
    u = V s
    r = A u − θ u
    if ||r||_2 ≤ ε then
        λ = θ,  x = u
    solve (approximately) for t ⊥ u in
        (I − u u^†)(A − θ I)(I − u u^†) t = −r
```

The Jacobi-Davidson Method with AMG

Algorithm 2: Jacobi-Davidson + AMG

input: no. of eigenvalues n, subspace size ℓ, initial guess $[v_0, v_1, \ldots, v_k, t]$, desired accuracy ε

output: set of n eigenpairs (Λ, X)

```
for all m = k+1, k+2, ... do
    t = t - VV^†t, v_m = t/||t||_2
    compute all (θ_i, s_i) with (AV)^†(AV)s_i = θ_i(AV)^†Vs_i
    find smallest θ_i ∉ Λ
    u = Vs_i, r = Au - θ_i u
    if ||r||_2 ≤ ε then
        Λ = [Λ, θ_i], X = [X, u]
        if m ≥ ℓ + n_conv then
            jd_restart
        find smallest θ_i ∉ Λ
        rebuild interpolation
    solve (approximately) (A - θ_i I)t = r
```

Restarting

Goal: Limit the amount of work (and memory) per iteration
$\rightarrow$ control dimension of search space V

Algorithm 3: jd_restart

input: look ahead m, number of converged eigenpairs n_{conv}, search space V
output: new search space V and Ritz pairs (θ_i, s_i)

1 $[\sim, \pi] = \texttt{sort}(|\Theta|, \text{ascending})$
2 **for all** $i = 1, \ldots m + n_{conv}$ **do**
3 $\quad V_i = V s_{\pi(i)}$
4 $V = V(1 : m + n_{conv})$
5 orthogonalize V
6 compute all (θ_i, s_i) with $(AV)^\dagger (AV) s_i = (AV)^\dagger V s_i$

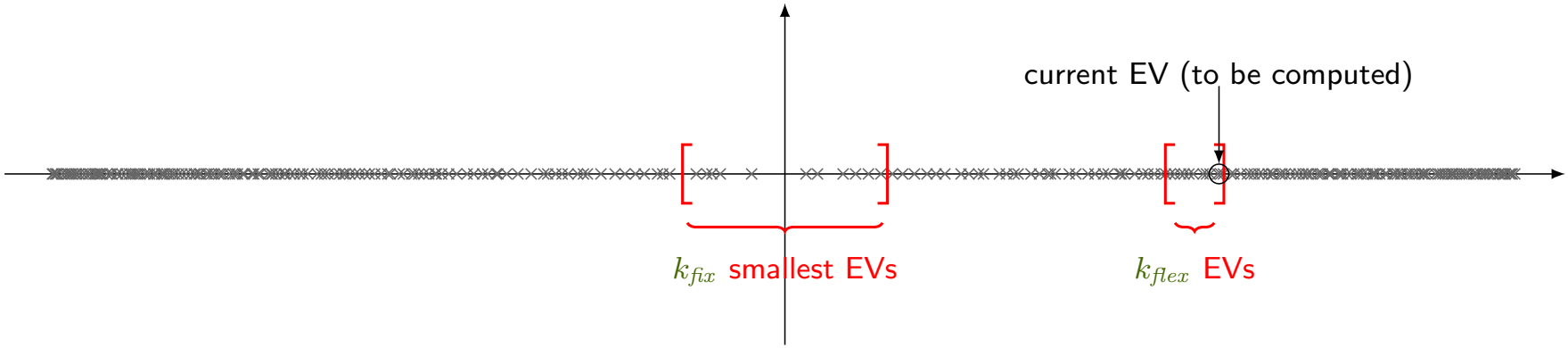
- look ahead m preserves search space information in spirit of thick restarting
- subspace size is bound by $n + \ell$

Interaction between Jacobi-Davidson and AMG

Rebuilding the interpolation

- JD computed all eigenvectors up to some point σ
- AMG needs small eigenvectors of $(A - \sigma I)$ for interpolation P

Idea: Use converged vectors to improve P dynamically:



Build interpolation P with:

- k_{fix} smallest eigenvectors
- current eigenvector approximation u
- k_{flex} converged eigenvectors closest to u

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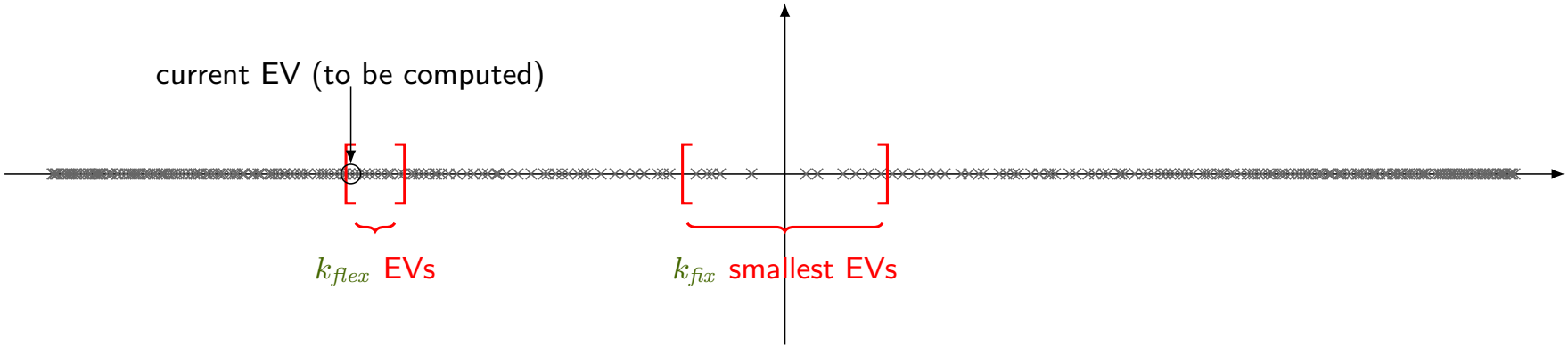

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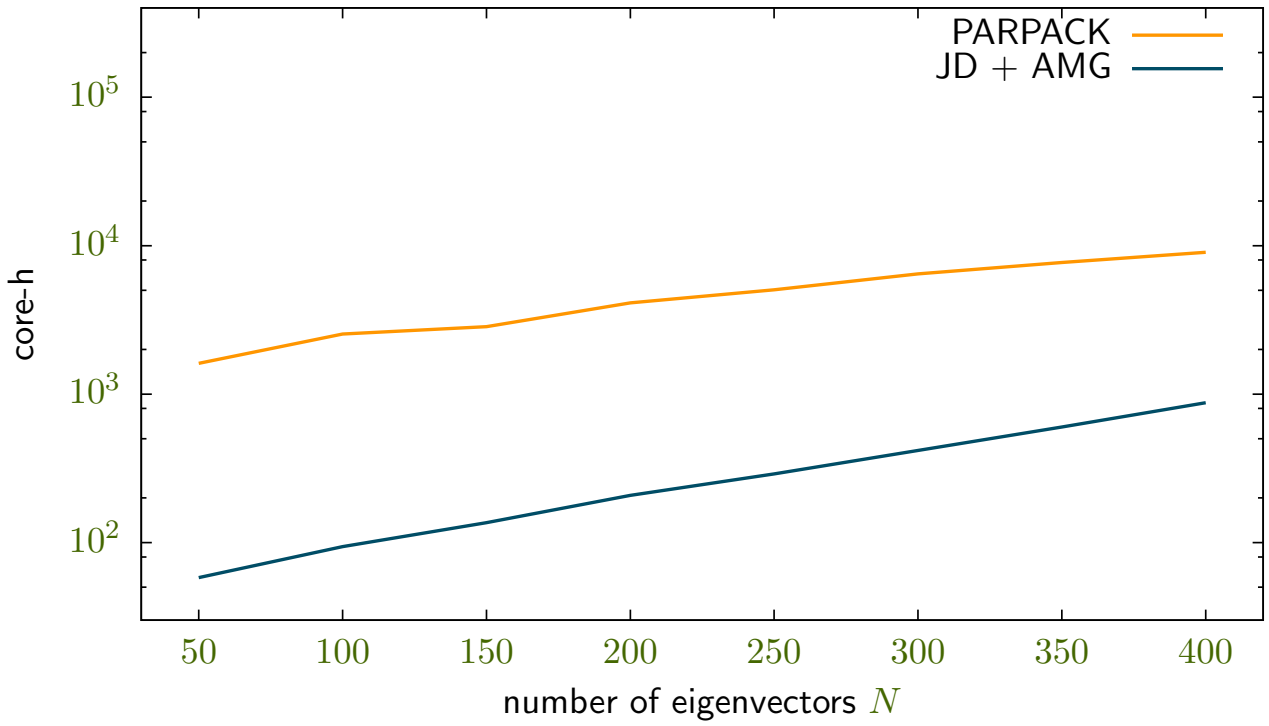
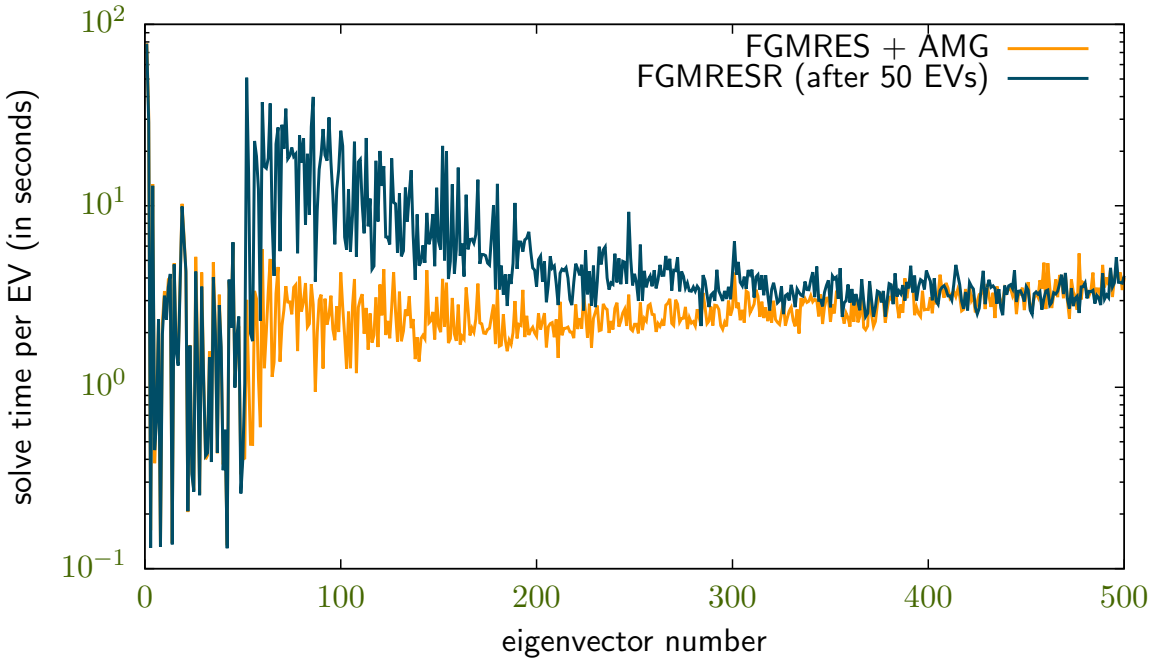
Comparison with PARPACK: Scaling with the Number of Eigenvectors N



- 48×24^3 lattice ($\approx 8 \times 10^6$ unknowns)
- 648 cores on JURECA
- PARPACK: Krylov subspace dimension $4N$
- JD: $k_{fix} = 8$, $k_{flex} = 16$, search space dimension 150 orthogonalization cost $n_{conv} + 150$

Effectiveness of AMG Solves



- coarse grid correction switched off after 50 converged eigenvectors
- clear loss in solve time for first 400 eigenvectors
- afterwards coarse grid effectiveness deteriorates
  - better interpolation strategy?
  - hybrid approach?
  - different preconditioner at some point?

Summary & Outlook

Summary

- Jacobi-Davidson type algorithm with multigrid support
- good scaling with number of eigenvalues
- scalability mostly depends on solver performance
- speed up can be orders of magnitudes

Improve Eigensolver

- explore possible benefits of AMG with more levels
- study orthogonal projections for solves
- find optimal restarting strategy
- improve interaction between JD and interpolation
- explore scaling behavior with lattice size
  (former approach scaled better than PARPACK)
- compare with other eigensolver approaches (e.g. FEAST)

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