Multigrid Preconditioning for the Overlap Operator

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Motivation

Task: Find solution of $D_N \varphi = \eta$ where

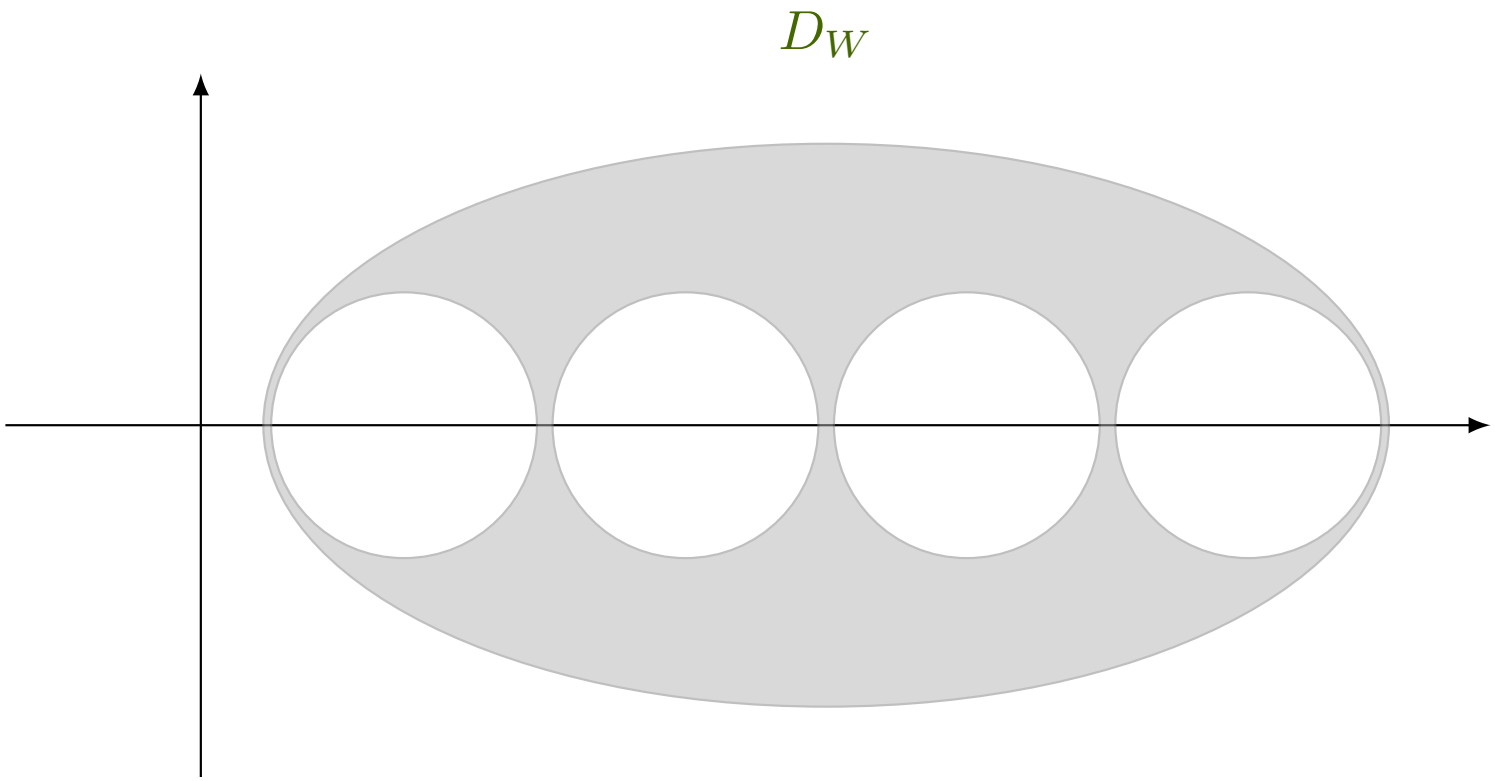
$$\begin{aligned} D_N =& (m_0^N - \frac{m}{2})(1 + \gamma_5 \operatorname{sign}(\overbrace{\gamma_5 (D_W - m_0^N)}^{H_W})) + m \\ =& (m_0^N - \frac{m}{2})(1 + \gamma_5 (H_W^\dagger H_W)^{-\frac{1}{2}} H_W) + m \end{aligned}$$

Challenges:

i) Evaluating $(H_W^\dagger H_W)^{-\frac{1}{2}} x$ is quite costly

ii) Iteration counts of $\mathcal{O}(1{,}000)$ for $D_N \varphi = \eta$

Overlap construction – assuming normality of D_W



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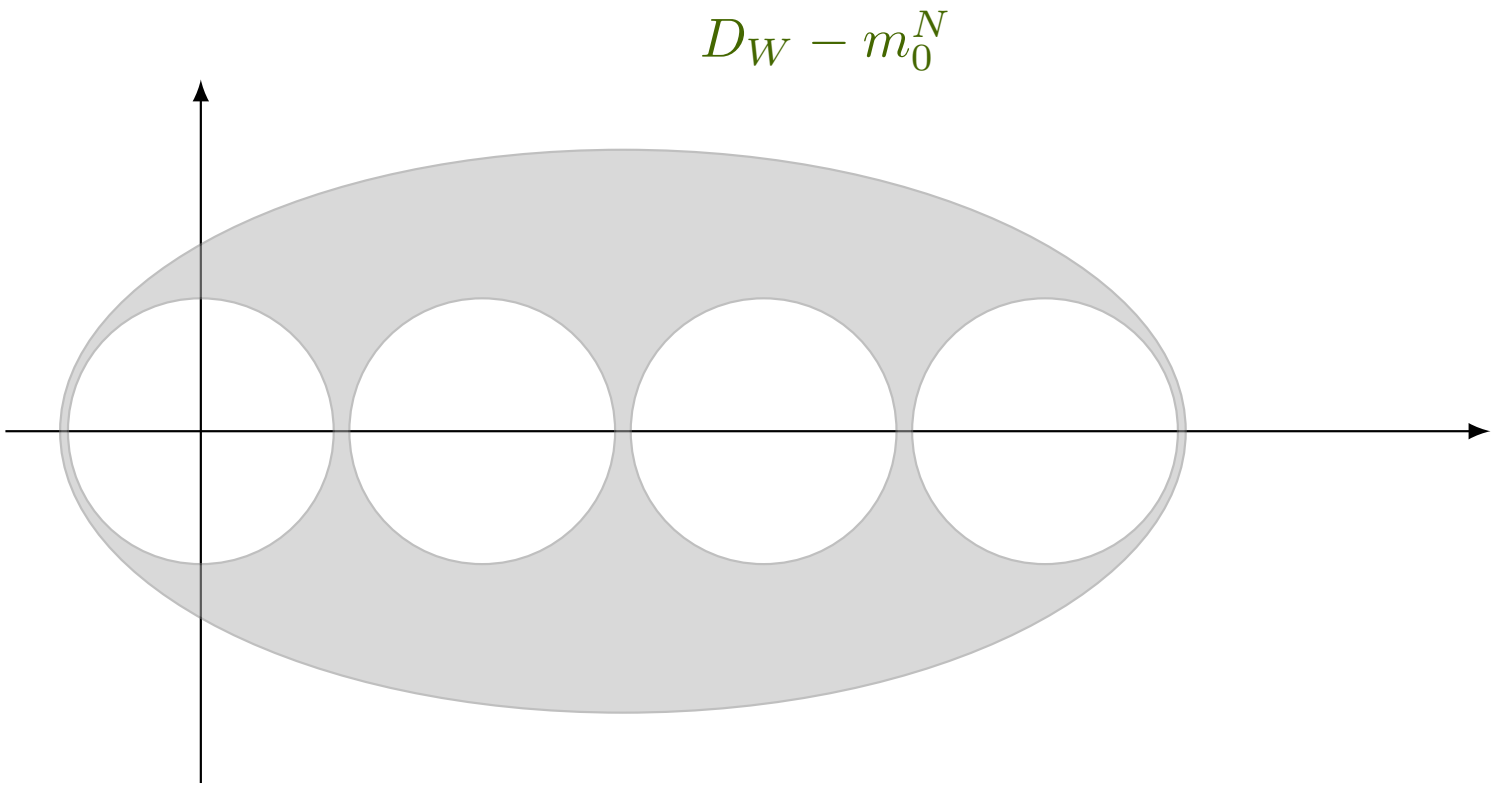
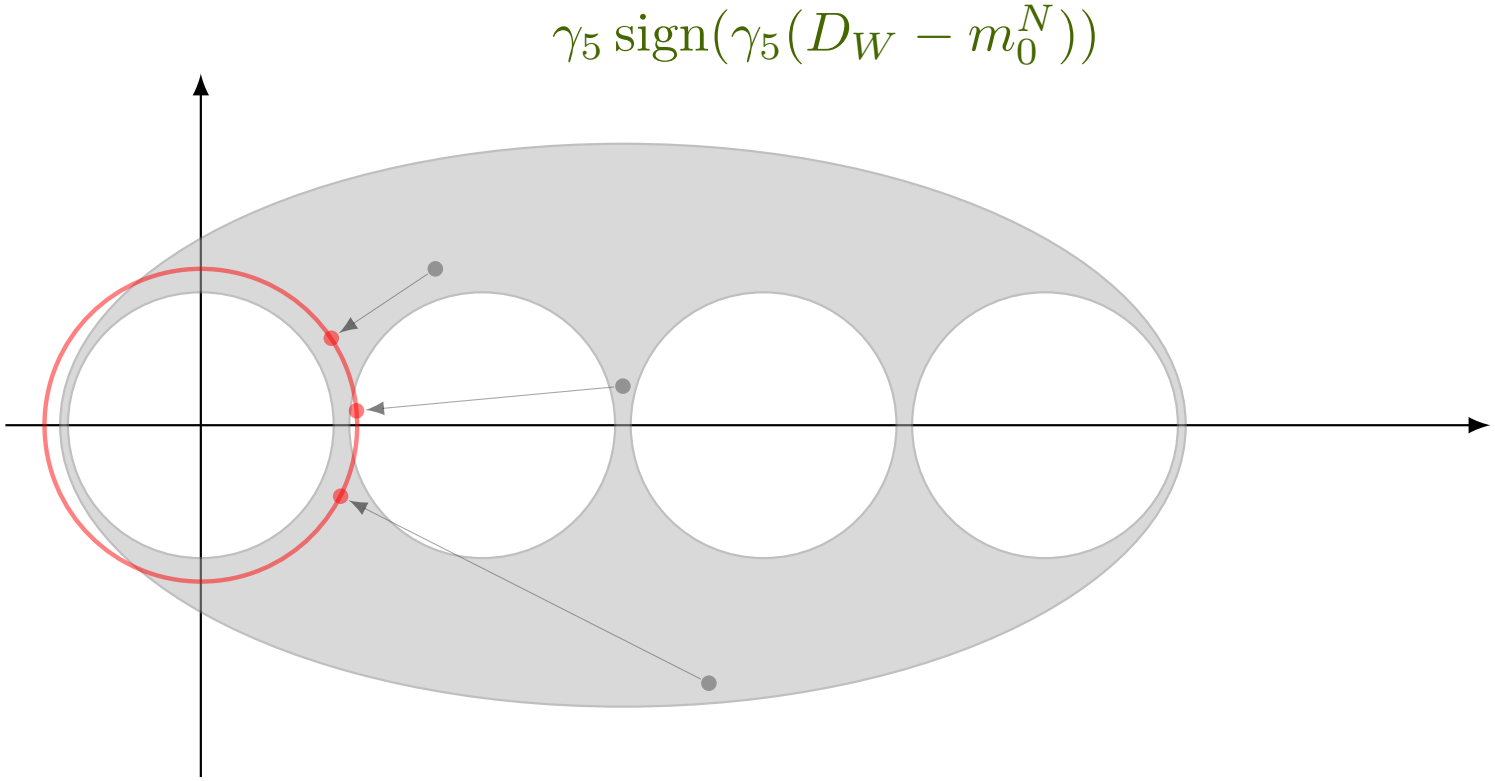
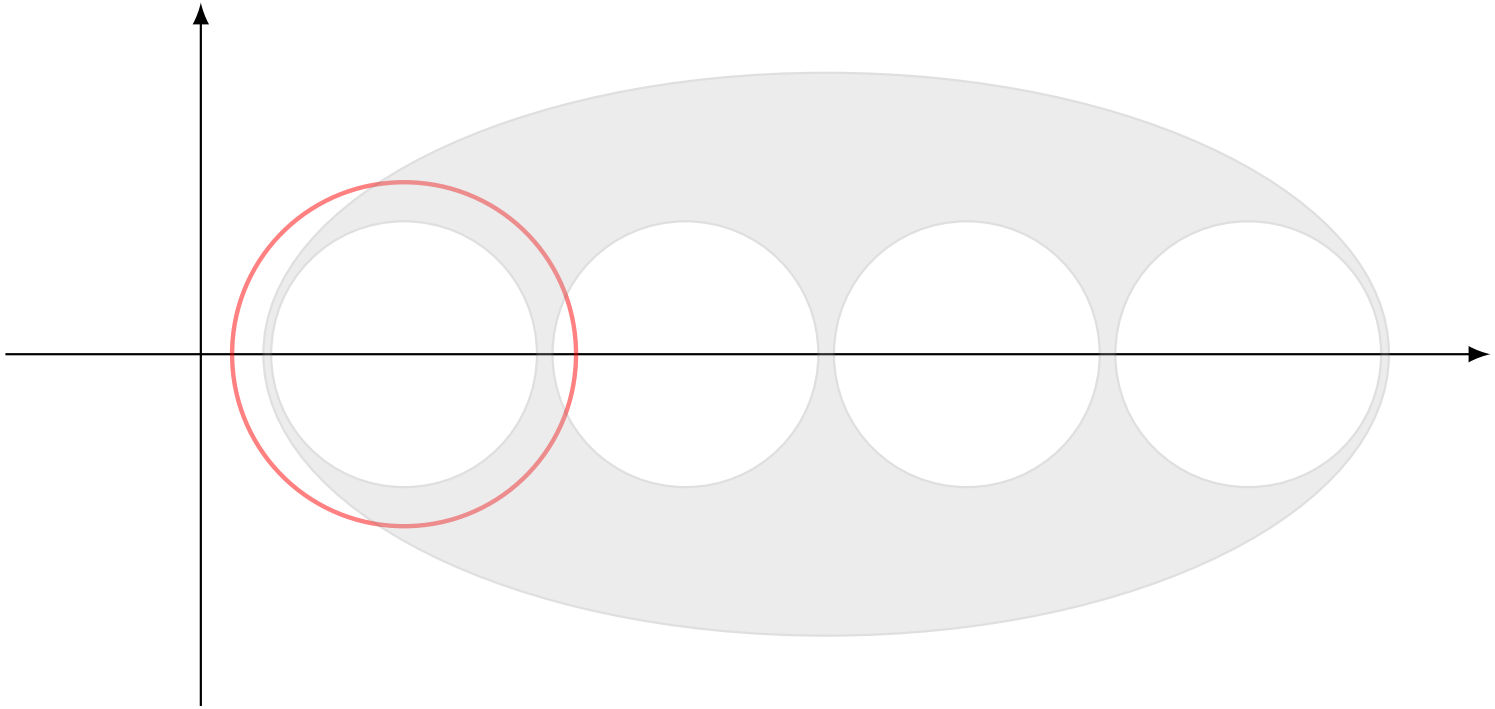


Overlap construction – assuming normality of D_W



Overlap construction – assuming normality of D_W

$$D_N = (m_0^N - \tfrac{m}{2})(1 + \gamma_5 \operatorname{sign}(\gamma_5(D_W - m_0^N)) + m$$



Preconditioning with the Wilson-Dirac operator

Challenge ii): Reduce number of iterations for $D_N \varphi = \eta$

Idea: Preconditioning (what else?)

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What is a suitable preconditioner for D_N?

The kernel operator of D_N, i.e., the Wilson-Dirac operator D_W

$$D_N D_W^{-1} \psi = \eta \text{ with } \varphi = D_W^{-1} \psi$$

- Computing D_W^{-1} is done by DD-αAMG [arXiv:1303.1377]
- D_W^{-1} is cheap

Why is D_W a good preconditioner for D_N?

Assuming normality of D_W (i.e., $D_W^\dagger D_W = D_W D_W^\dagger$) we find

Relation between low modes of D_W and D_N

Let λ be a small eigenvalue of D_W, i.e., $D_W x = \lambda x$ with $|\lambda|$ small. W.l.o.g. assume $m = 0$. Then

$$\begin{aligned} D_N x &= m_0^N \big(1 + \gamma_5 \operatorname{sign}(\gamma_5 (D_W - m_0^N))\big) x \\ &= m_0^N \big(1 + \gamma_5 ((D_W - m_0^N)^\dagger (D_W - m_0^N))^{-\frac{1}{2}} \\ &\quad \cdot (\gamma_5 (D_W - m_0^N))\big) x \\ &= m_0^N x + m_0^N (\lambda - m_0^N) \big((\lambda - m_0^N)(\overline{\lambda - m_0^N})\big)^{-\frac{1}{2}} x \\ &= m_0^N \big(1 + \operatorname{sign}(\lambda - m_0^N)\big) x \end{aligned}$$

Deviation from normality of non-chiral discretizations

Quality of preconditioner depends on normality?!

Measure for the deviation of normality

$$\delta_N := ||D_W^\dagger D_W - D_W D_W^\dagger||_F,$$

where $||X||_F^2 = \sum_{i,j=1}^n x_{ij}^2,\ X \in \mathbb{C}^{n\times n}$.

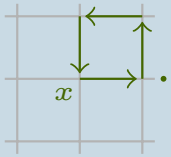
Theorem

The deviation of normality of D_W is given by

$$\delta_N = 16 \sum_x \sum_{\mu>\nu} \mathrm{Re}(\mathrm{tr}(I - Q_x^{\mu,\nu})),$$

where $Q_x^{\mu,\nu}$ is the plaquette defined by

$$Q_x^{\mu,\nu} = U_\nu(x) U_\mu(x+\hat{\nu}) U_\nu^H(x+\hat{\mu}) U_\mu^H(x) =$$



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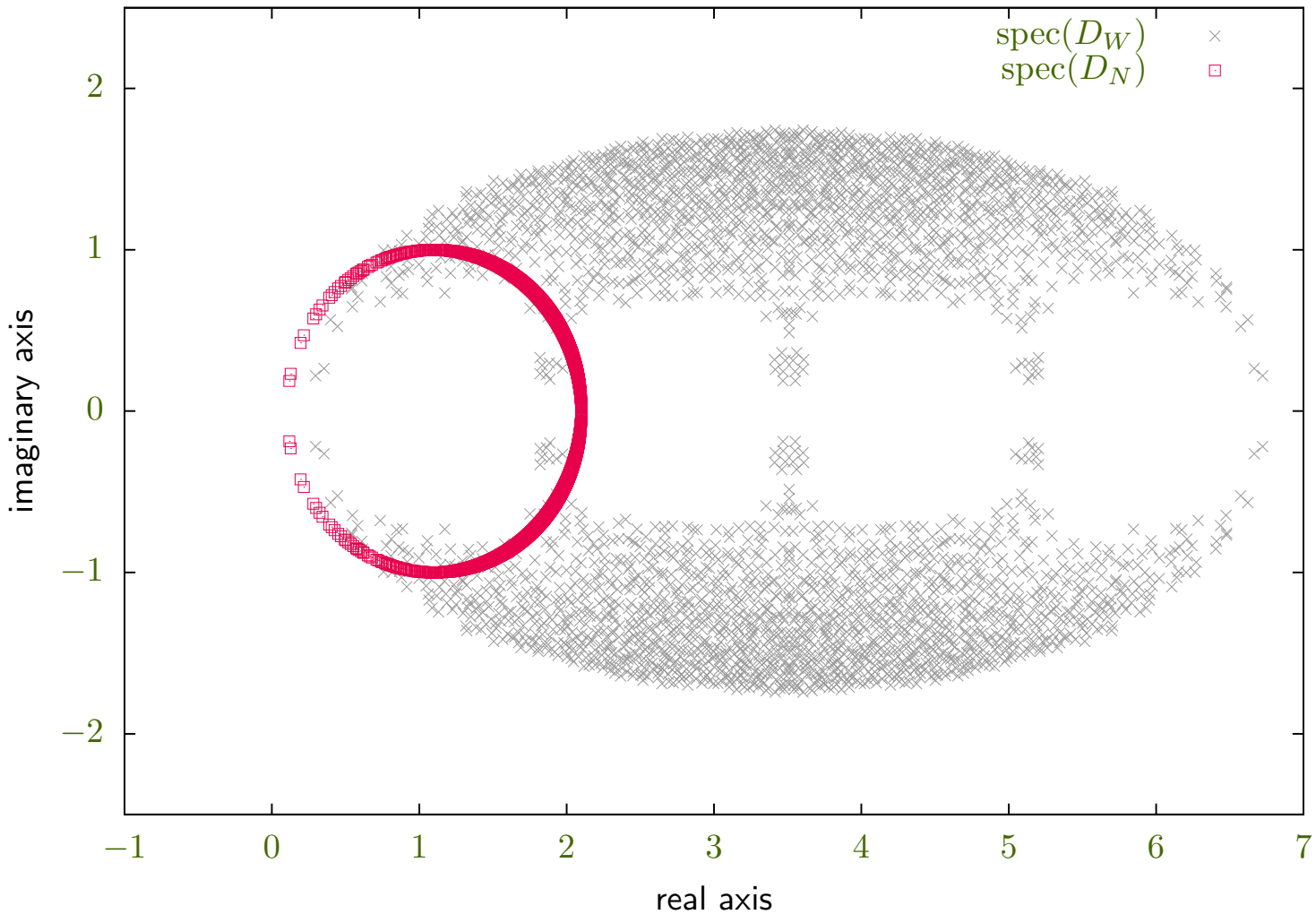

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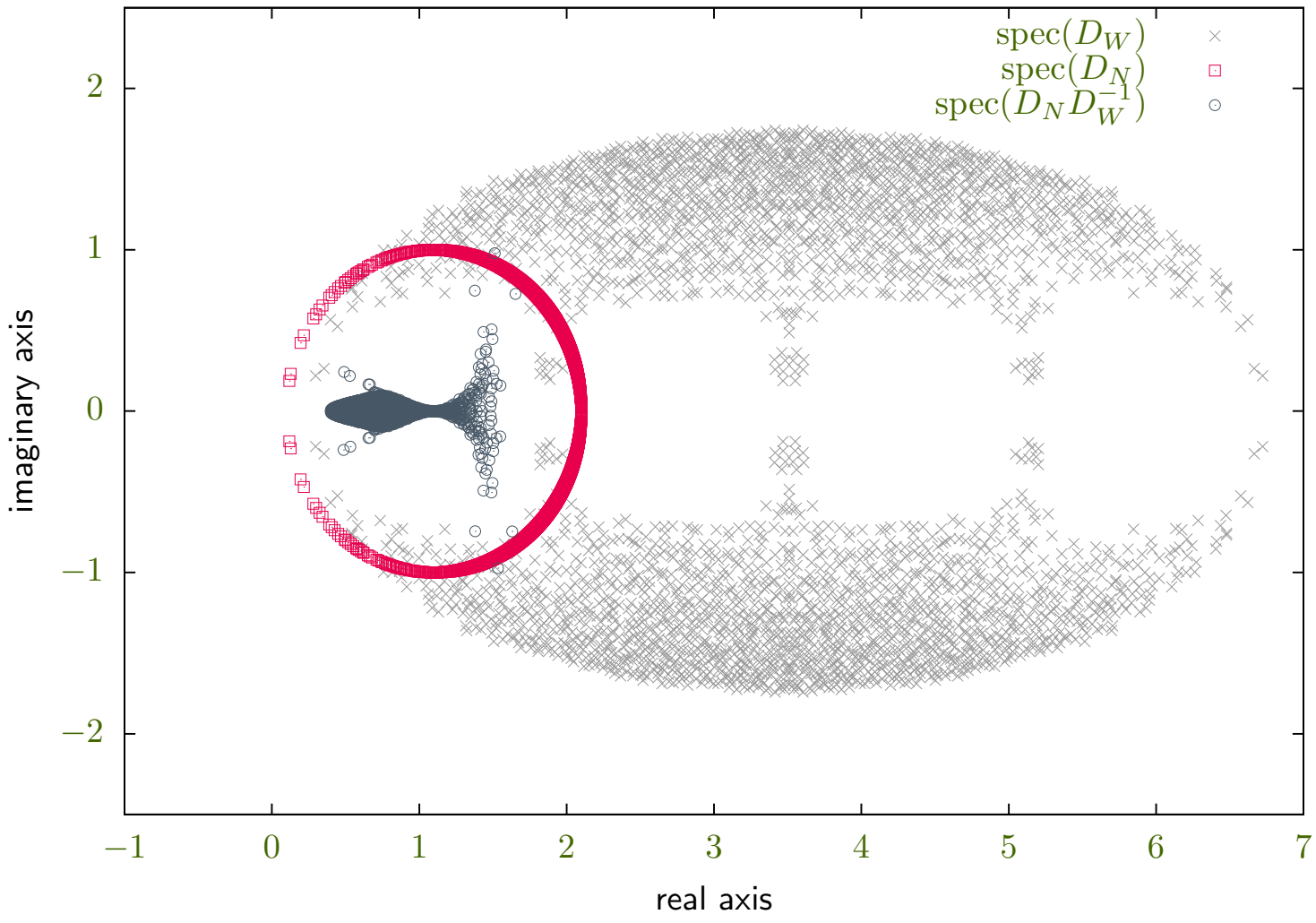
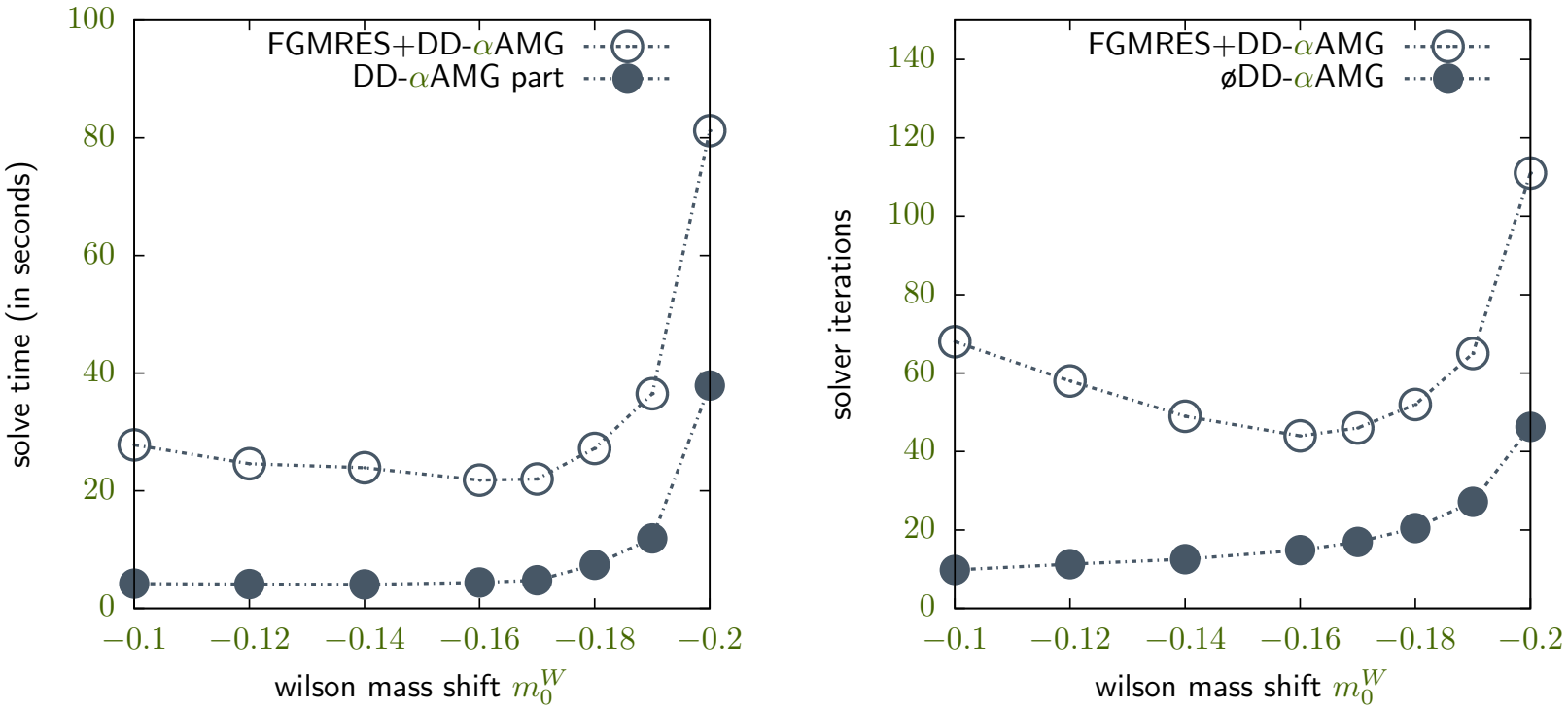
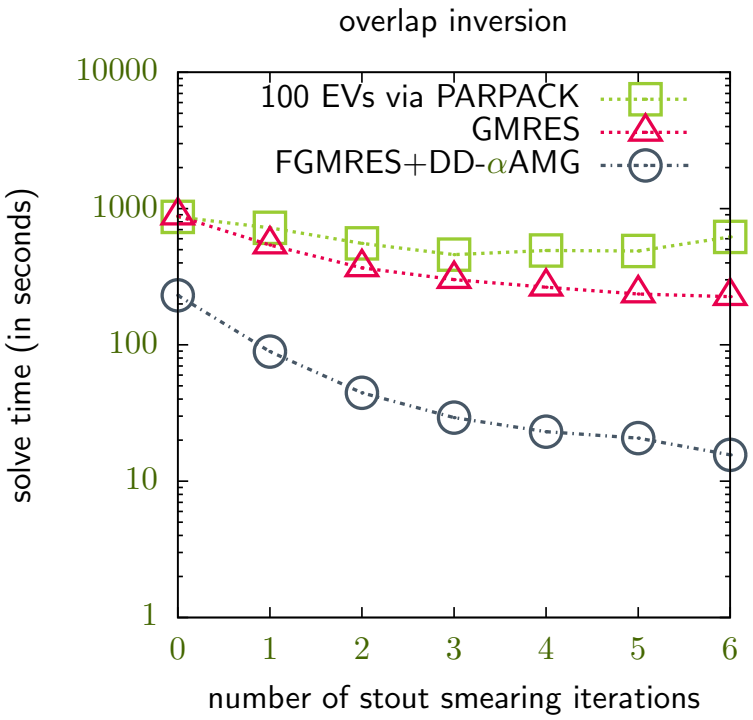


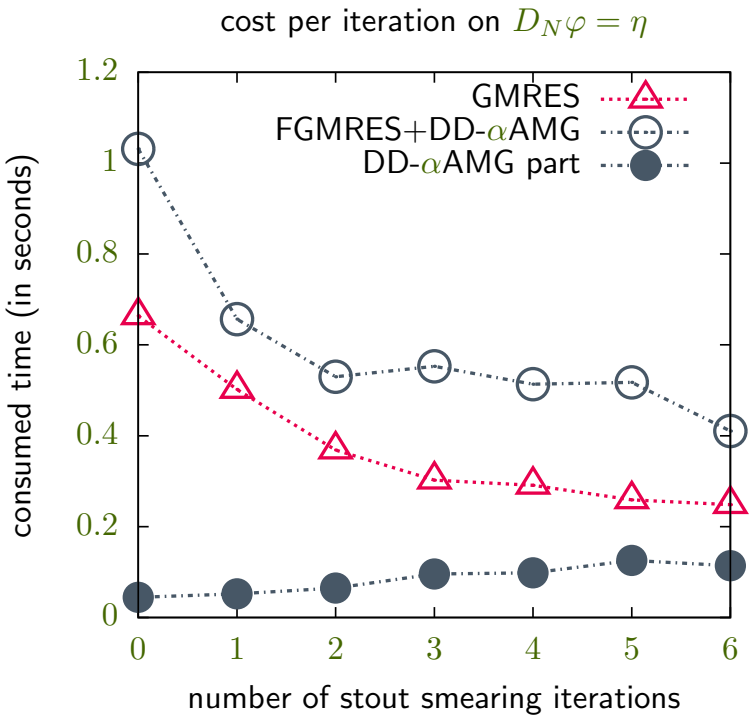
Scanning the Optimal Wilson Preconditioner Mass Shift m_0^W



- 32^4 lat, 3HEX smeared BMW-c cnfg (unpublished), $m_\pi \approx 350$ MeV, $1{,}024$ processes
- overlap tol 10^{-8}, Wilson tol 10^{-2}, sign fct with explicit deflation and relaxed tol
- optimal $m_0^W \approx 0.16$

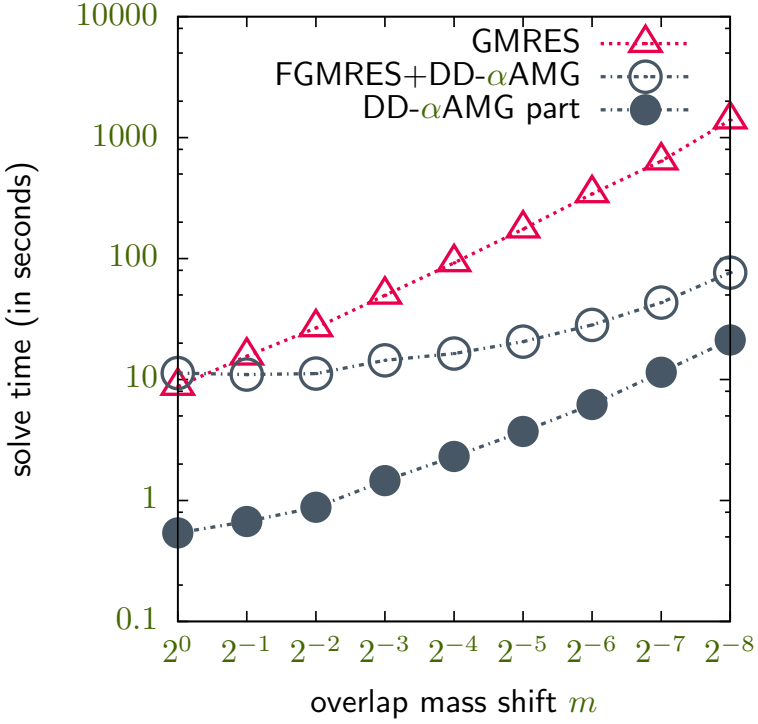
Smearing Study

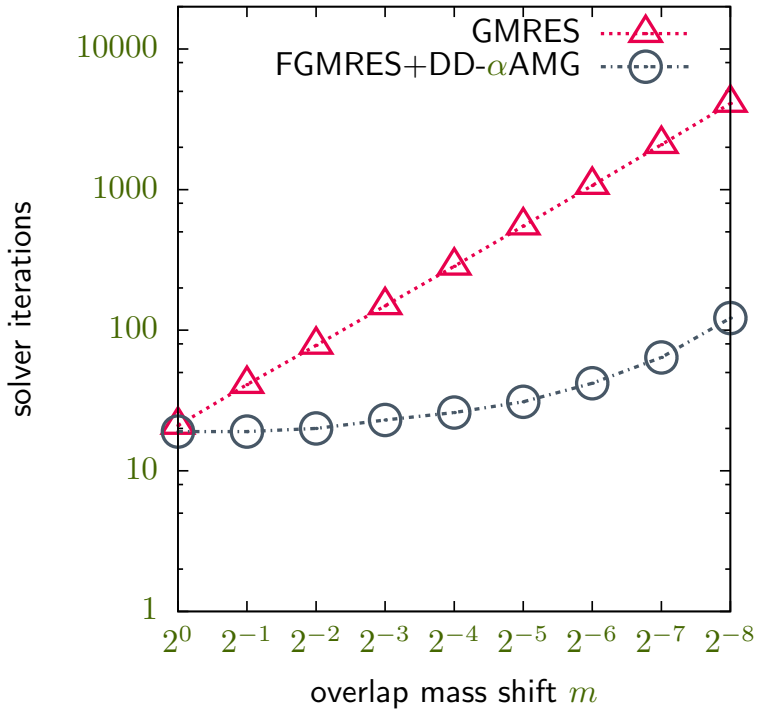




- 32^4 lattice, $1{,}024$ processes
- no smearing $\rightarrow$ $\times 5$ speedup
- 3–6 steps of stout smearing $\rightarrow$ $\times 20$–$\times 30$ speedup
- cost per iteration for preconditioned method only slightly higher
- preconditioner cost almost negligible

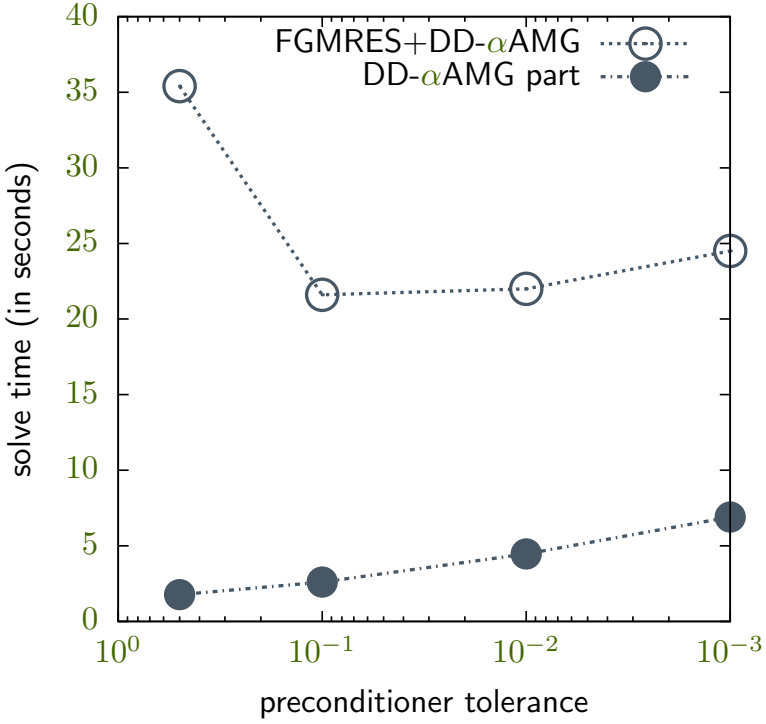
Scaling with the Overlap Mass Shift

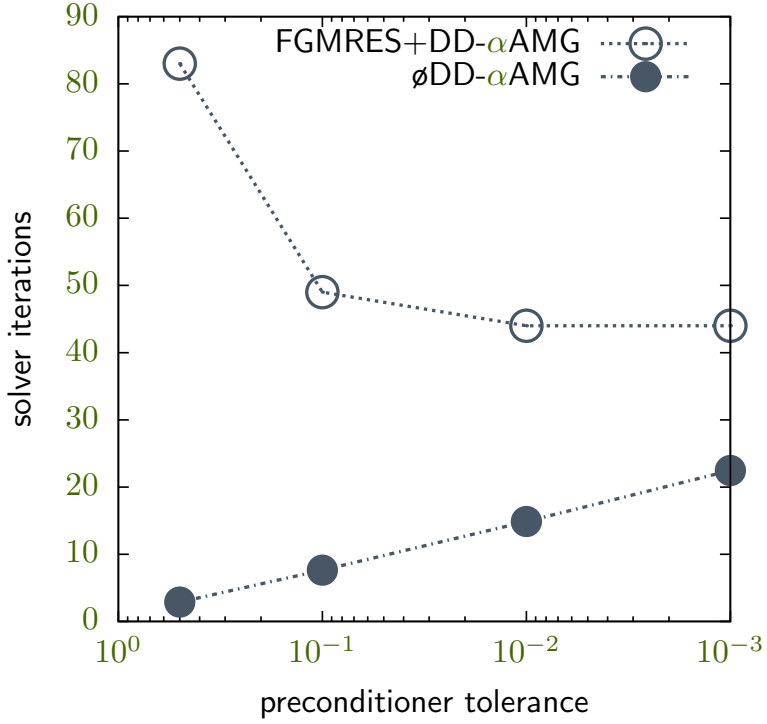




- 32^4 lat, 3HEX smeared BMW-c cnfg
- cnfg generated at approx. $m = 2^{-6}$ ($m_\pi \approx 350$ MeV)
- smaller masses $\longrightarrow$ bigger gain

Influence of the Preconditioner Accuracy





- 32^4 lat, 3HEX smeared BMW-c cnfg
- $tol = 10^{-2}$ optimal in terms of iteration count
- $tol = 10^{-1}$ optimal in terms of solve time

Solving the inverse square root

Challenge i): Evaluating $(H_W^\dagger H_W)^{-\frac{1}{2}} x$

Good convergence without explicit calculation of low modes of H_W?

Idea: Use implicit low mode information via *thick restarts* (cf. [Eiermann, Ernst, Güttel 2011]).

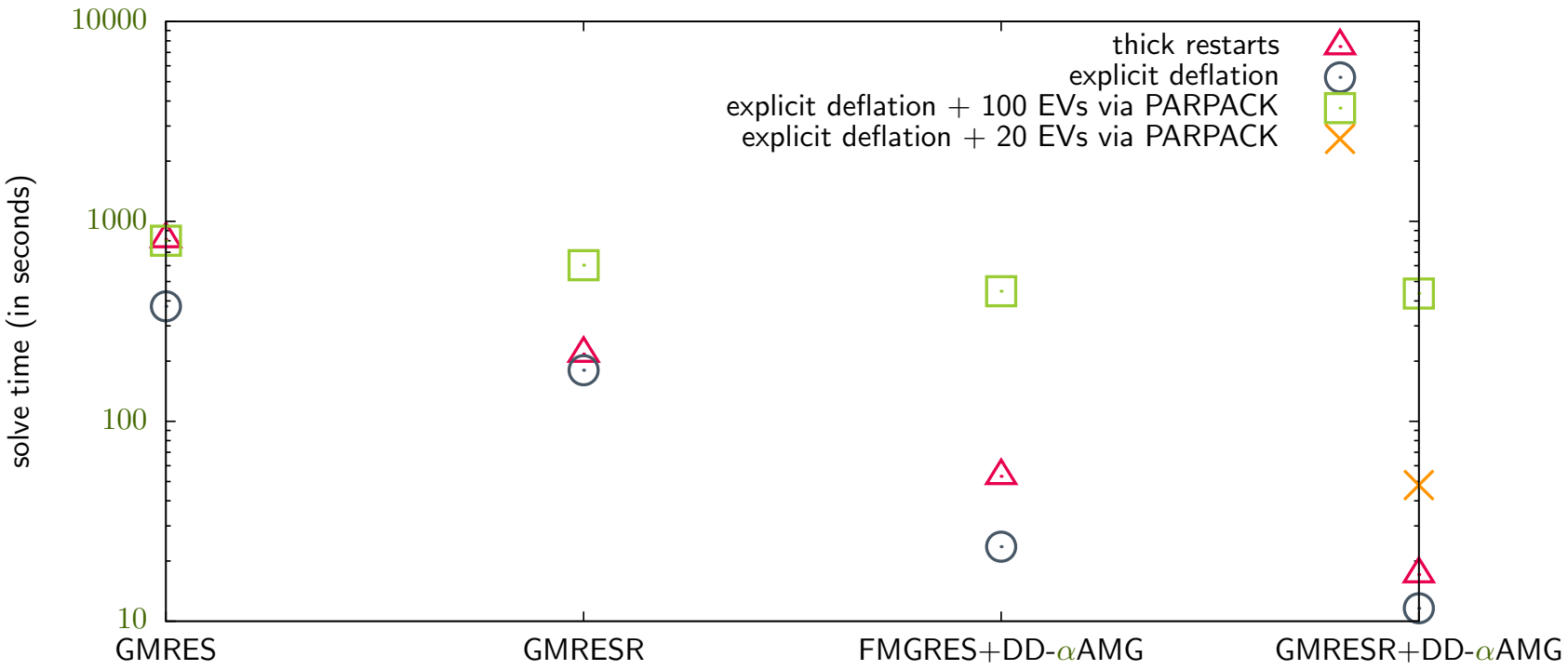
With the Cauchy integral representation

$$f(A) = A^{-\frac{1}{2}} = \int_\Gamma g(t)(tI - A)^{-1}\,\mathrm{d}t$$

and a Lanczos decomposition of $H_W^\dagger H_W$ we can compute the k-th error propagator by numerical quadrature (cf. [Frommer, Güttel, Schweitzer 2014]):

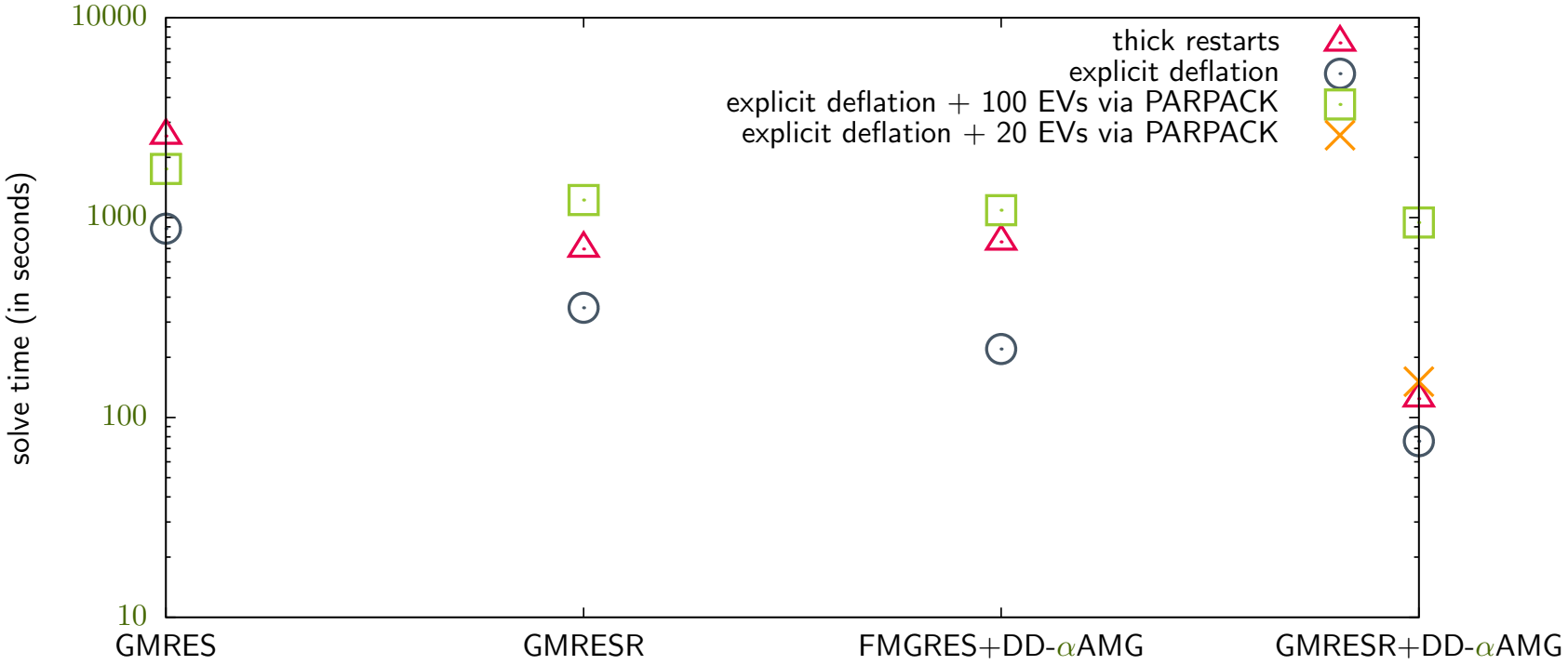
$$e^{(k)}(T) = c \sum_{i=1}^{l} \rho(T, x_i) \frac{\omega_i}{-\beta(1 - x_i) - T(1 + x_i)}$$

Thick Restarts and Explicit Deflation



- 32^4 lat, 3HEX smeared BMW-c cnfg, $1{,}024$ cores
- GMRESR := FGMRES-64bit + GMRES-32bit
- GMRESR+DD-αAMG := FGMRES-64bit + FGMRES-32bit + DD-αAMG

Thick Restarts and Explicit Deflation



- 32^4 lat, no smearing, $1{,}024$ cores
- one RHS: preconditioning + thick restarts
- many RHS: preconditioning + explicit deflation

Summary & Outlook

Summary:

- Preconditioning overlap equation leads to fewer iterations for the solution of $D_N \varphi = \eta$
- Preconditioner is cheap
- Efficiency of preconditioner improves
  - when approaching normality
  - for smaller masses
- For few RHS: thick restarts instead of EV computation

Outlook:

- Incoorporate solver into production codes of collaborators
- Further optimization of preconditioner
- Overall performance improvement of the method

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