Chiral Rank-k Truncation of the Multigrid Subspace for Wilson Fermions

Travis Whyte [1]

[1]Hamilton Mathematics Institute and School of Mathematics, Trinity College Dublin

[2]William & Mary, Department of Computer Science

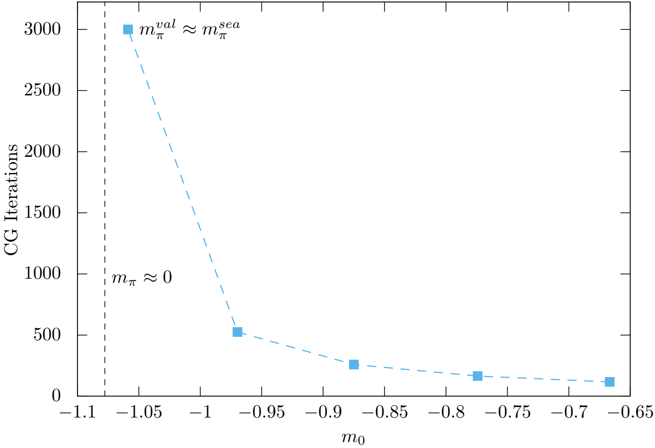
[3]Thomas Jefferson National Accelerator Facility

In collaboration with Andreas Stathopoulos [2] and Eloy Romero [3]

Lattice 2024, University of Liverpool

Motivation

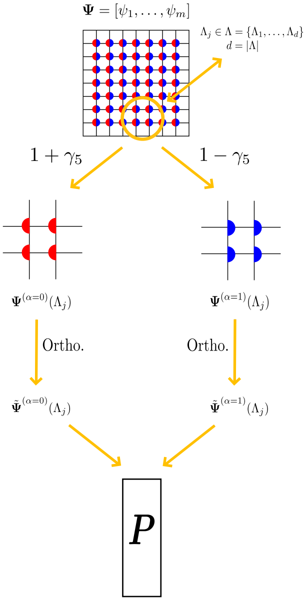
- The generation of propagators is **expensive**: modern spectroscopy studies approaching $O(10^4)$ right hand sides per configuration
- Near physical pion mass, iterative solvers experience "critical slowing down"



Multigrid for the lattice Wilson-Dirac Operator

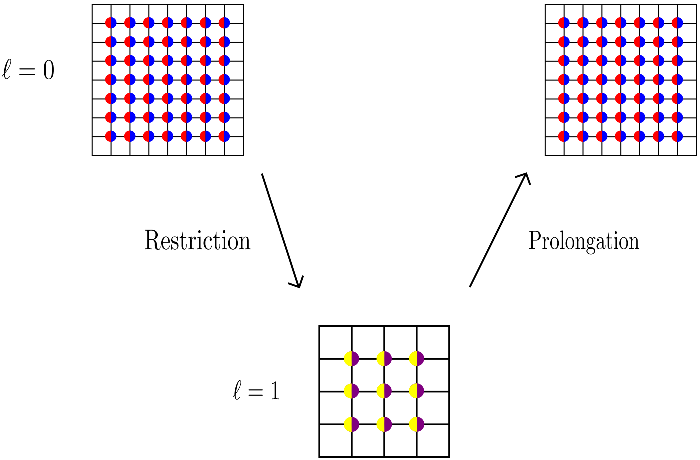
Babich et al Phys. Rev. Lett. 2010

1. For $\ell = 0, \ldots, \ell_{max}$
2. For $i = 1, \ldots, m$
   Smooth on $D_\ell \psi_i \approx 0$ with random initial guess
3. end for
4. Apply the projectors $(1 \pm \gamma_5^\ell)$ to $\Psi = [\psi_1, \ldots, \psi_m]$
5. For $\alpha = 0, 1$
6. For $j = 1, \ldots, d$
7. Orthonormalize $\Psi^\alpha(\Lambda_j)$
8. end for
9. end for
10. Form P take $R = P^\dagger$
11. Form $D_{\ell+1} = R D_\ell P$
12. end for



Multigrid for the lattice Wilson-Dirac Operator

$$x_{i+1} = x_i + \boldsymbol{M}^{-1}(b - \boldsymbol{D}(x_i + \boldsymbol{P}x_c))$$



$$x_c = (\boldsymbol{RDP})^{-1}\boldsymbol{R}(b - \boldsymbol{D}x_i)$$

Multigrid for the lattice Wilson-Dirac Operator

- The choice of m is important!
  - m too small $\rightarrow$ bad preconditioner
  - m too large $\rightarrow$ expensive preconditioner to apply

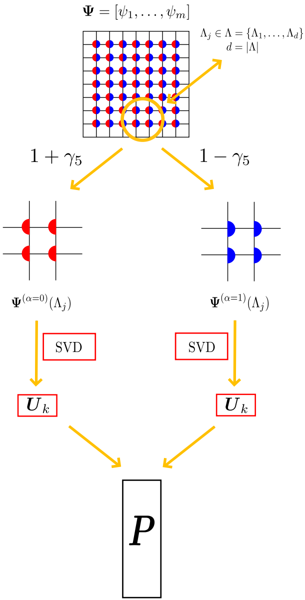
- Typical choice of m for modern lattices is $\approx 24 - 32 \rightarrow$ potential loss of information

- SVD is a natural remedy to this Chow SIAM J. Sci Comp 2006, D'Ambra and Vassilevski 1907.04417

  1. Consider $\hat{\boldsymbol{P}}$ from the m null vectors
  2. Compute $\boldsymbol{U}_k \boldsymbol{\Sigma}_k \boldsymbol{V}_k^\dagger \approx \hat{\boldsymbol{P}}(\Lambda_j)$ (locally on each domain)
  3. Set $\boldsymbol{P}(\Lambda_j) = \boldsymbol{U}_k$

Multigrid for the lattice Wilson-Dirac Operator

1. For $\ell = 0, \ldots, \ell_{max}$
2. For $i = 1, \ldots, m$
   Smooth on $\boldsymbol{D}_\ell \psi_i \approx 0$ with random initial guess
3. end for
4. Apply the projectors $(1 \pm \gamma_5^\ell)$ to $\boldsymbol{\Psi}$
5. For $\alpha = 0, 1$
6. For $j = 1, \ldots, d$
7. $[\boldsymbol{U}, \boldsymbol{\Sigma}, \boldsymbol{V}] = \boldsymbol{\Psi}^\alpha(\Lambda_j)$
8. end for
9. end for
10. Form $\boldsymbol{P}$ take $\boldsymbol{R} = \boldsymbol{P}^\dagger$
11. Form $\boldsymbol{D}_{\ell+1} = \boldsymbol{R}\boldsymbol{D}_\ell \boldsymbol{P}$
12. end for

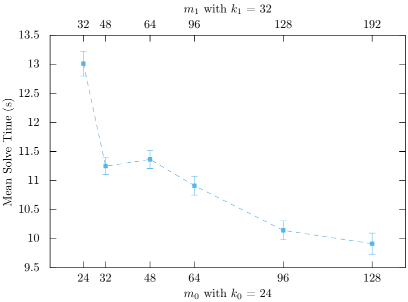


Experimental Setup

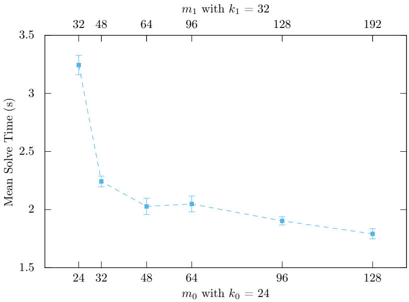
- Simulations performed with two separate gauge configurations on 8 nodes with with Intel Xeon Gold 6130 processors (2×16 cores)
  1. GFA: $32^3 \times 256$ anisotropic lattice with $m_\pi \approx 280$ MeV from the HadSpec Collaboration with the Wilson Clover action Edwards et al 0803.3960, H W Lin et al 0810.3588
  2. GFI: $32^3 \times 64$ isotropic lattice with $m_\pi \approx 220$ MeV from the MILC Collaboration with the Clover-on-HISQ action MILC Collab 1004.0342, 1212.4768 PNDME Collab 1806.09006
- A multigrid hierarchy of three levels is used with domain sizes of 4^4 and 2^4 for the levels $\ell = 0$ and $\ell = 1$, respectively
- The multigrid preconditioner is applied in a K-cycle
- FGMRES is used as both smoother and outer solver for each level
- Results are averaged over 10 random right hand sides

The Number of Near Null Vectors: (m_0, m_1)

GFA



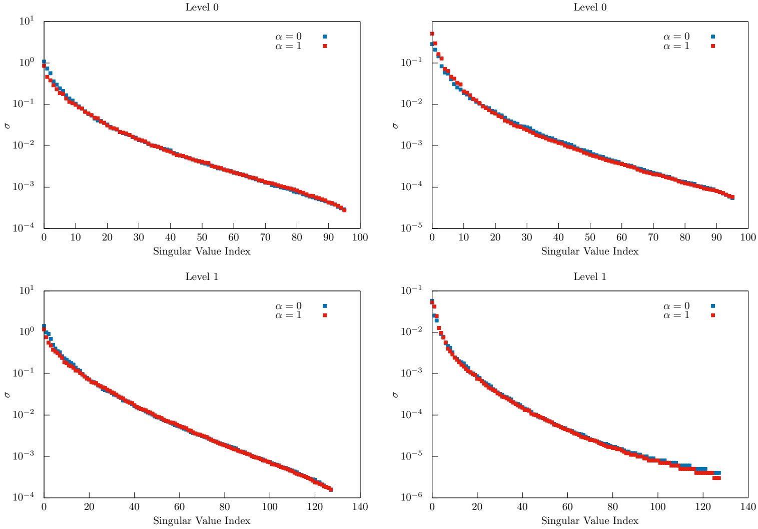
GFI



- We consider only $(k_0, k_1) = (24, 32)$, and we explore a set of predefined pairs of (m_0, m_1).
- Very little improvement observed beyond $(m_0, m_1) = (96, 128)$ for both gauge configurations

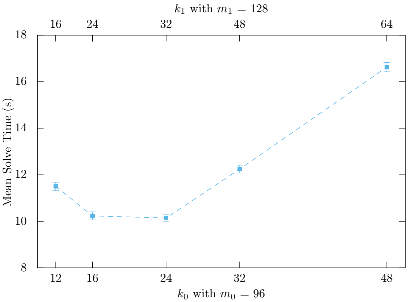
Optimal Truncation: (k_0, k_1)

GFA GFI

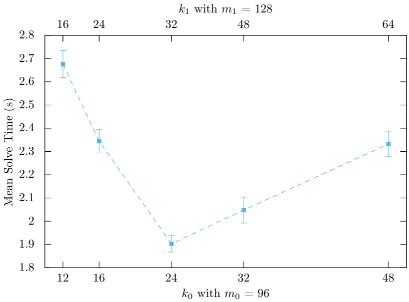


Optimal Truncation: (k_0, k_1)

GFA

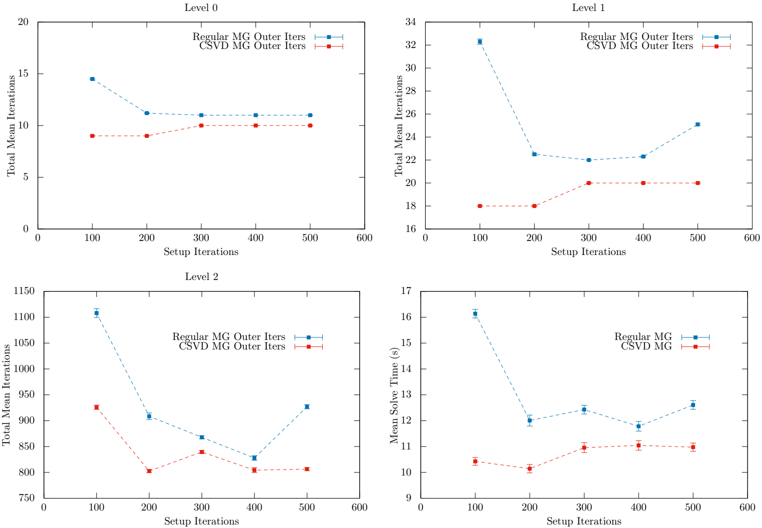


GFI



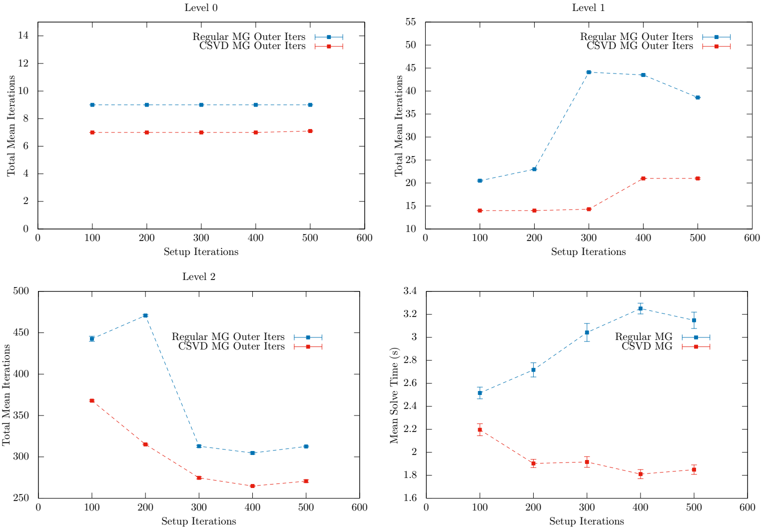
- We consider only $(m_0, m_1) = (96, 128)$, and we explore a set of predefined pairs of (k_0, k_1).
- Clear minima show a preference for $(k_0, k_1) \approx (24, 32)$

Setup Iterations: GFA



- SVD less sensitive to setup iterations used; overall solve time decreased

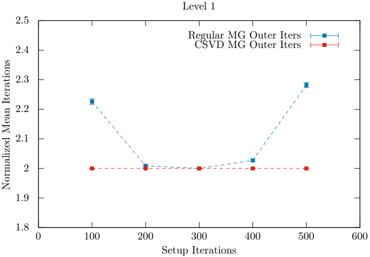
Setup Iterations: GFI

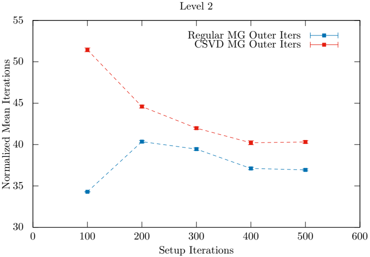


- SVD less sensitive to setup iterations used; overall solve time decreased

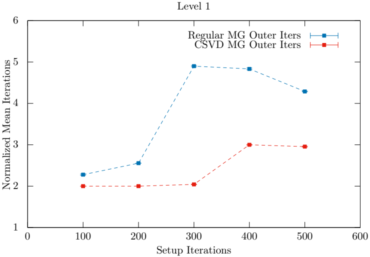
Coarse Grid Performance

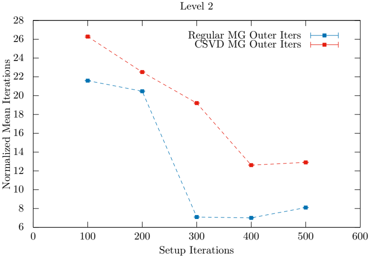
GFA



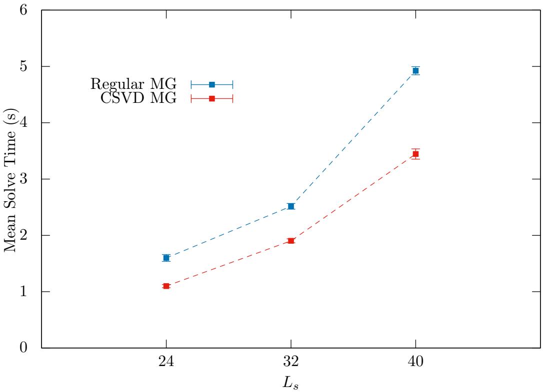


GFI





Scaling with Volume



- MILC lattices with $a \approx 0.12$ fm and $m_\pi \approx 220$ MeV MILC Collab 1004.0342, 1212.4768 PNDME Collab 1806.09006
- Near optimal set up parameters obtained for the $L_s = 32$ lattice used for all three volumes

Summary and Future Work

- The chiral rank-k truncation is able to capture components of the near null space not captured by the conventional set up method
- Less sensitive to setup parameters than conventional multigrid; may be promising for HMC
- Integration with QUDA
- Combine the chiral rank-k truncation with Least Squares Interpolation to incorporate information lost as a result of the truncation

Acknowledgments

- Thank you to my collaborators for all of their work in this project and thank you to Steve Gottlieb, Walter Wilcox and colleagues in the HadSpec Collaboration for access to the gauge configurations
- Calculations performed on DiRAC, Jefferson Lab and W&M compute facilities and funded through the ECP, Royal Society, UKRI SFTC and SFI

- Thanks for your attention!