Multigrid Methods for Lattice QCD

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on Numerical Analysis and Lattice QCD

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Presentation Plan

* Model problems - solver challenges
  * Dirac Wilson system of QCD
  * Schwinger model of QED
* Smoothed Aggregation (A)MG
* Adaptive (A)MG Approaches
* Numerical Results
* Future Work

4D Dirac Wilson system

$$(M\phi)(x) = \phi(x) - \kappa\Bigg(\sum_{\mu=1}^{4}(I-\gamma^{\mu})\otimes U_{\mu}(x)\phi_{x+e_{\mu}} + (I+\gamma^{\mu})\otimes U_{\mu}^{*}(x-e_{\mu})\phi_{x-e_{\mu}}\Bigg)$$

* For fixed x, $U_{\mu}(x) \in SU(3)$: $\beta \to \infty \Rightarrow U_{\mu} \to I$
* $\gamma^{\mu} \in \mathbb{C}^{4\times 4}$: sparse matrices with 4 nonzero entries, $\pm 1, \pm i$
* $M \in \mathbb{C}^{n\times n}$, $n = 12 \cdot n_1 \cdot n_2 \cdot n_3 \cdot n_4$
* M is positive for $0 \leq \kappa < \kappa_c$ and M becomes very ill-conditioned for $\kappa \approx \kappa_c$
* $\gamma^5 M = M^* \gamma^5$

Simplification: 2D Dirac Wilson system

$$M = \frac{1}{2}\left(\sum_{\mu=1}^{2} \sigma_\mu (\nabla_\mu^+ + \nabla_\mu^-) + \nabla_\mu^- - \nabla_\mu^+ \right) + m$$

* Cov. finite difference operators ($U_\mu \in U(1)$):

$$(\nabla_\mu^+ f)(x,s) = U_\mu(x) f(x + e_\mu, s) - f(x,s)$$

$$(\nabla_\mu^- f)(x,s) = f(x,s) - U_\mu^*(x - e_\mu) f(x - e_\mu, s)$$

* $H = \sigma_3 M = M^* \sigma_3 = H^*$, with $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

2D Hermitian Dirac Wilson System $Hf = \psi$

$$\begin{pmatrix} A & B \\ B^* & -A \end{pmatrix} \begin{pmatrix} f(x,1) \\ f(x,2) \end{pmatrix} = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

Taking $a = \frac{1}{N}$ on a fixed domain and setting $U_\mu \equiv 1$ gives

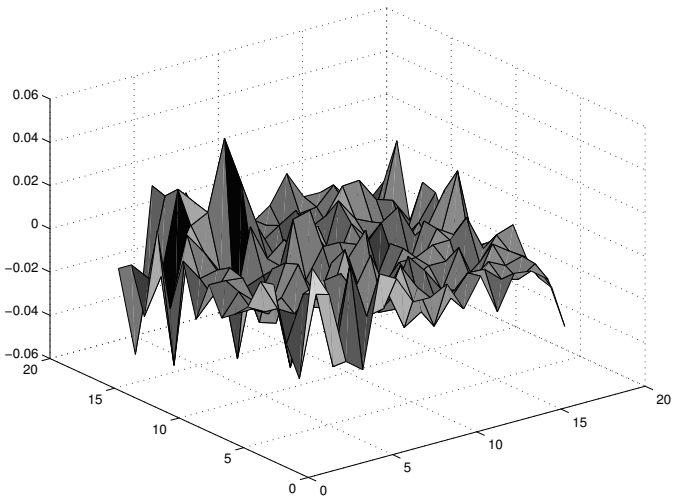
$$\begin{pmatrix} A & B \\ B^* & -A \end{pmatrix}^2 = \begin{pmatrix} (mI - \frac{a}{2}\Delta_a)^2 - \Delta_a & 0 \\ 0 & (mI - \frac{a}{2}\Delta_a)^2 - \Delta_a \end{pmatrix}$$

For $m = 0$, $\mathbf{1} \in \mathrm{Null}(H)$ and $(mI - \frac{a}{2}\Delta_a)^2 - \Delta_a = -\Delta_a(I - \frac{a^2}{4}\Delta_a)$, with

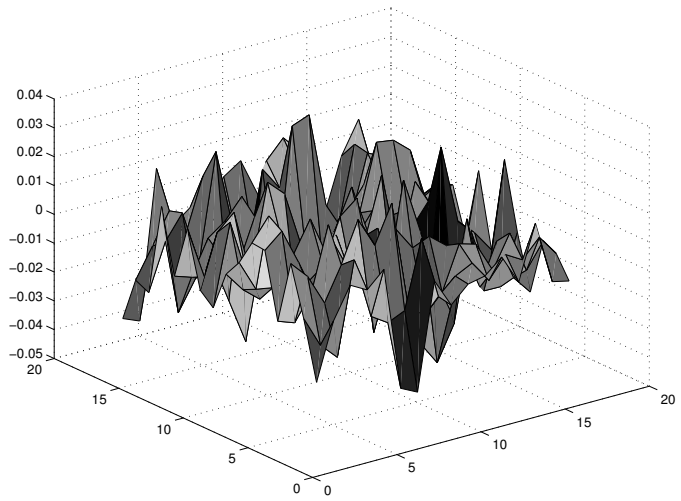
$$\sigma(-\Delta_a) \subseteq [0, \frac{8}{a^2}] \quad \text{and} \quad \sigma(I - \frac{a^2}{4}\Delta_a) \subseteq [1, 3]$$

General case: Lowest eigenmode of H^2

Real



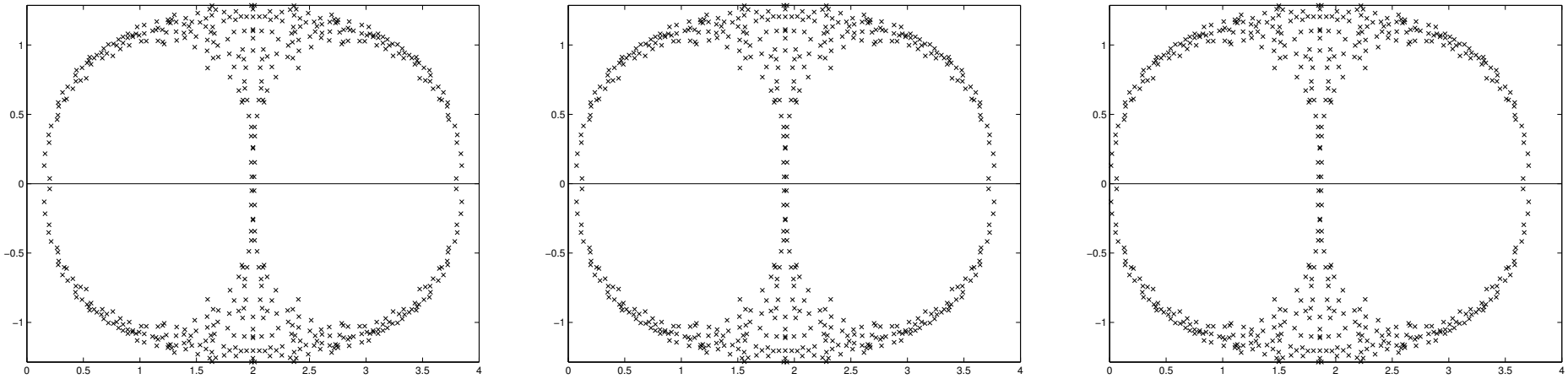
Imag



$m \approx m_{cr}, \beta = 3$, $n = 2 \cdot 16 \cdot 16$ lattice

Spectrum of M

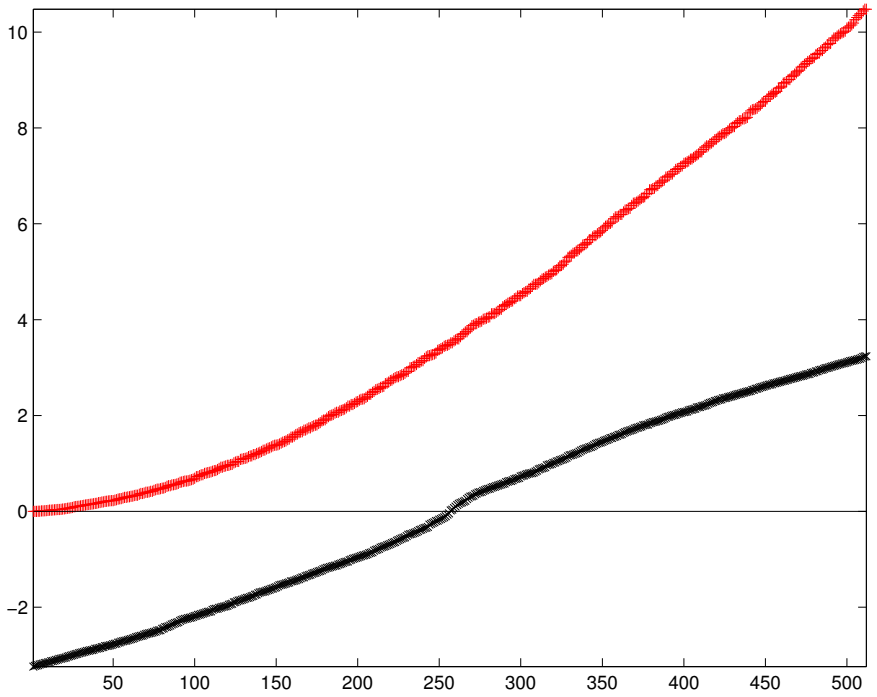
$m = 0$ $m = -.1$ $m = -.2$



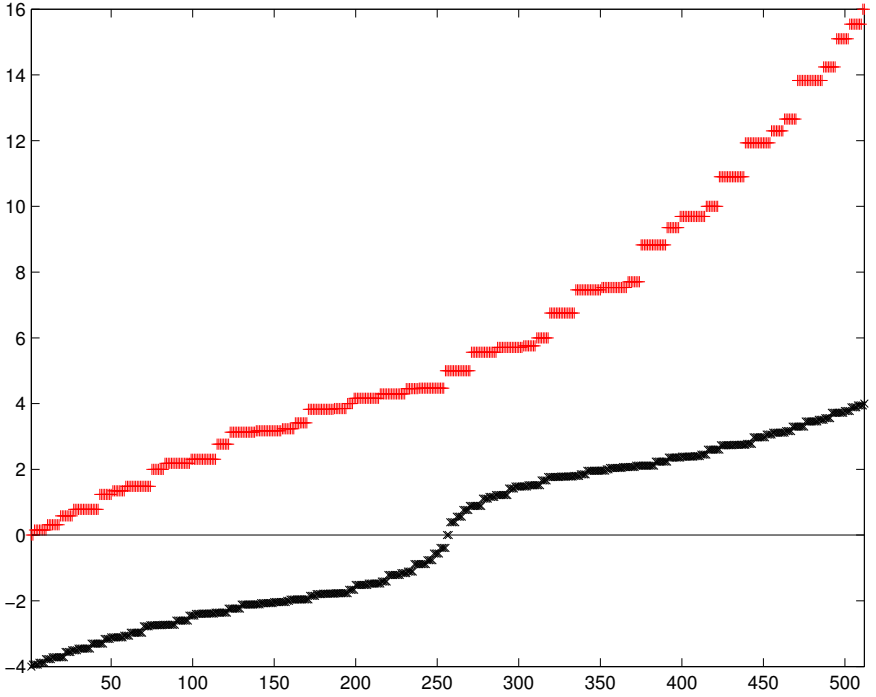
$\beta = 3, m_{cr} \approx -.21, n = 2 \cdot 16 \cdot 16$

Spectrum of H and H^2

Free Field



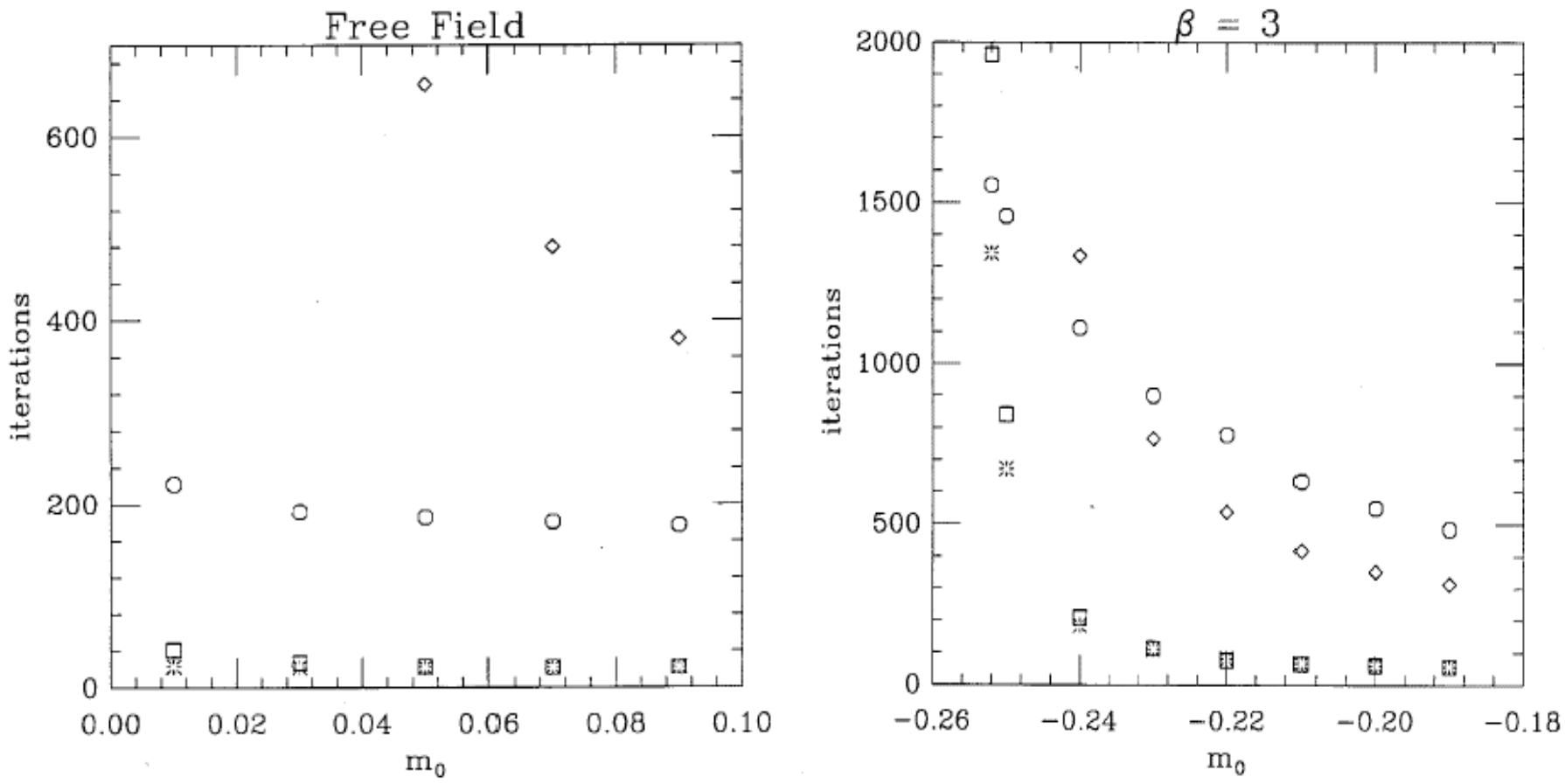
$\beta = 3$



$m \approx m_{cr}$, $n = 2 \cdot 16 \cdot 16$

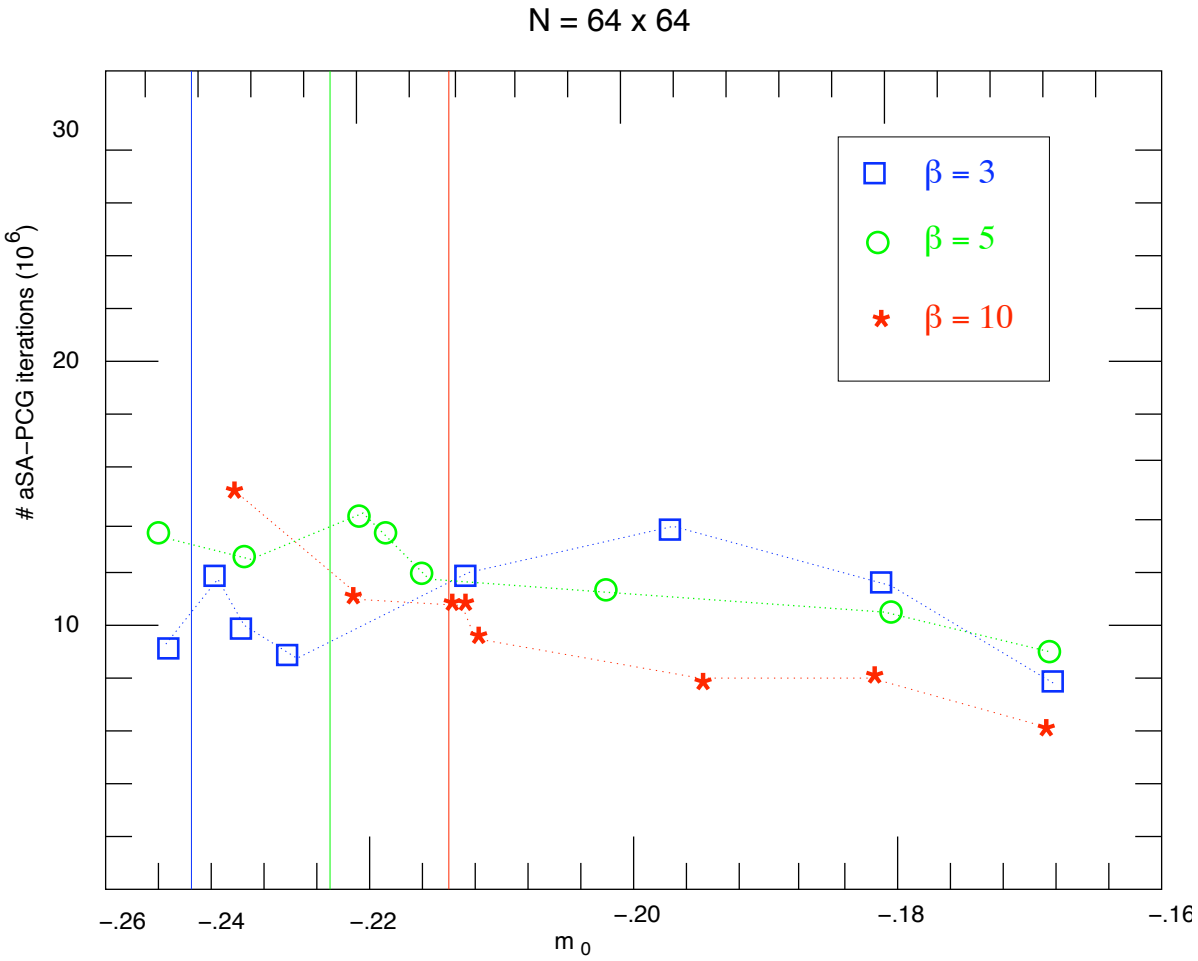
MG for lattice fermions circa 2000

* R. Ben-Av, et al, *Fermion simulations using parallel transported multigrid*, Phys. Lett. **B**253 (1991), pp. 185–192
* R. Ben-Av, M. Harmatz, S. Solomon, and P. G. Lauwers, *Parallel* transported multigrid for inverting the dirac operator: Variants of the method and their efficiency, Nucl. Phys. **B**405 (1993), pp. 623–666
* A. Brandt, *Multigrid methods in lattice field computations*, Nucl Phys. Proc. Suppl. **2**6 (1992), pp. 137–180
* R. C. Brower, R. G. Edwards, C. Rebbi, and E. Vicari, *Projective multigrid for Wilson fermions*, Nucl. Phys. **B**366 (1991), pp. 689–705
* P. Hasenfratz, *Prospects for perfect actions*, Nucl. Phys. Proc. Suppl. **6**3 (1998), pp. 53–58
* Many others ...



$N = 64$, Jacobi (Diamond), CG (circle), MG V-cycle (square), W-cycle (star)

Brower, et. al., *Projective multigrid for Wilson fermions* (1991)

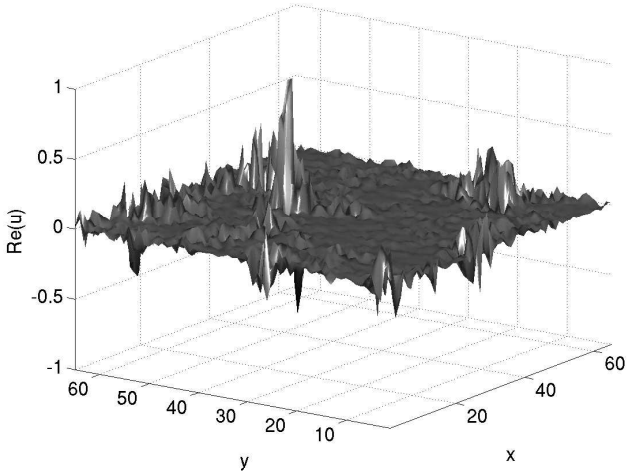


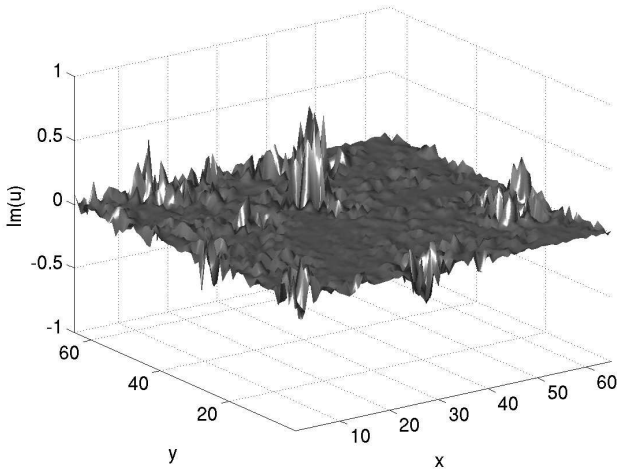
Brannick, et. al., *Adaptive smoothed aggregation in lattice QCD*, Lecture Notes Comp. Sci. Eng., Springer-Verlag, 2006

Extreme simplification: Gauge Laplacian

$$L = \sum_{\mu} \nabla_{\mu}^{-} - \nabla_{\mu}^{+} + m$$

* Scaling by $\frac{1}{2(2+m)}$ gives $L = I - \kappa D$, $D = \begin{pmatrix} 0 & D_{eo} \\ D_{oe} & 0 \end{pmatrix}$ with $L > 0$ for $0 \leq \kappa < \kappa_{cr} := \frac{1}{\lambda_{\max}(D)}$





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Method of subspace corrections

* Abstract problem: Find $u \in V$ such that $Au = f$, $f \in V^*$, $A > 0$
* Space decomposition: $V = \sum_i V_i$

  Idea: Correct the error in each subspace by solving $A_i e_i = r_i$ for $i = 1 : J$

  * exactly, if each of the subspaces is small (e.g., multiplicative Schwarz)
  * approximately, if the subspaces are of large dimension (e.g., multigrid)

  Algorithm MSC With $u \leftarrow u^0$, for $i = 1 : J$ repeat the subspace correction $u \leftarrow u + e_i$ where $e_i \in V_i$ is given by

$$e_i = M_i^{-1} \Pi_i (f - Au)$$

* **Examples**: (1) $V = \mathbb{R}^n$ with $V_i := \text{span}\{\delta_i\}$ and $M_i = A_i = a_{ii}$ gives Gauss-Seidel; (2) $V_J \supset V_{J-1} \supset \ldots \supset V_1$ and $M_i \approx A_i$ results is MG

Let $T_i = M_i^{-1} A_i \pi_i$, then $u - u^\ell = E_J(u - u^{\ell-1})$,

$$E_J = (I - T_J)(I - T_{J-1}) \dots (I - T_1)$$

Theorem.[XU AND ZIKATANOV, J. of AMS (2003)] The convergence factor is obtained via $\|E_J\|_A^2 = 1 - \frac{1}{c_0+1}$,

$$c_0 = \sup_{\|v\|=1} \inf_{\sum_i v_i = v} \sum_{i=1}^{J} (\bar{T}_i^{-1} T_i^* w_i, T_i^* w_i)_A \text{ with } w_i = \sum_{j=i}^{J} v_j - T_i^{-1} v_i$$

where $\bar{T}_i \equiv T_i^* + T_i - T_i^* T_i$ SPD $\Rightarrow c_0 < \infty$

Application to MG

* For finite element spaces and regular refinement $V_J \supset V_{J-1} \supset ... \supset V_1$. In such settings, under appropriate assumptions, it is straightforward to show that the convergence depends logarithmically on the number of levels
* If nested finite element meshes are not available, then the standard arguments do not apply!
* Motivated by success of MG methods algebraic versions were proposed to handle general problems. Originally for second-order elliptic equations with discontinuous coefficients on unstructured grids
* "Algebraic" stands for the fact that all the tools of the method are constructed solely on the basis of the original matrix A, in a setup phase
* In AMG, the subspaces are built "on the fly", making multilevel theory for the convergence of such algorithms very difficult

AMG estimates ($J = 2$)

Two-grid error propagator:

$$E_{tg} = (I - M^{-t}A)(I - \pi_A)(I - M^{-1}A)$$

with $\pi_A := P(P^tAP)^{-1}P^tA$. Two-level convergence factor is obtained via

$$\|E_{tg}\|_A^2 = 1 - \frac{1}{K}; \quad K(P) = \sup_v \frac{\|(I - \pi_{\bar{M}})v\|_{\bar{M}}}{\|v\|_A}$$

where $\bar{M} := M^t(M^t + M - A)^{-1}M$. Analysis of recursive multi–level method depends in addition on stability:

$$\|PR\|_A < \eta; \quad RP = I_c$$

What does it mean to choose $V_c = \mathrm{Range}(P) \subset V$?

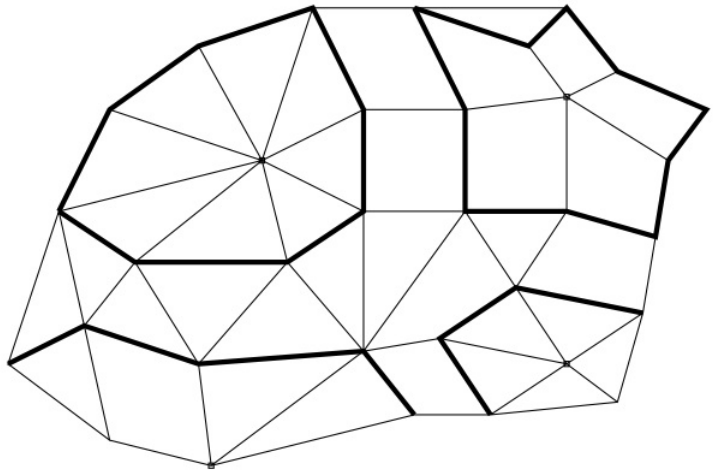
Coarse space is constructed automatically within the algorithm, level by level, in a (hopefully) computationally optimal setup procedure which involves

1. Picking a set of coarse variables, i.e., set of indices
   $\mathcal{N}_c = \{i_1, \ldots, i_{n_c}\} \rightarrow$ graph theoretic approaches

2. Definiing $V_c = \mathrm{span}\{\psi_k\}_{k=1}^{n_c}$ such that each ψ_k is supported in Ω_k, for a vector:
   $\Omega_k \subset \{1, \ldots, n\} \rightarrow$ null space of the system matrix

$*$ Each of the V_c (or V_i obtained recursively) must satisfy certain properties, related to the convergence of the overall algorithm.

Smoothed Aggregation



* Define *strong* nbhd. of dof $i \in \Omega = \{1, .., n\}$ as

$$N_i(\epsilon) := \{j \neq i : \epsilon a_{ij}^2 > a_{ii} a_{jj}\}$$

* Using N_i and ind. set algorithm, Ω partitioned into set of disjoint aggregates $\{\mathcal{A}_i\}_{i=1}^{n_c}$ such that $\cup_{i=1}^{n_c} \mathcal{A}_i = \Omega$

$\text{agg}(\Omega, A)$

do $i \in \bar{\Omega}$

if $N_i(\epsilon) \geq 1$

$\mathcal{A}_j = N_i(\epsilon) \cup \{i\}$

$\bar{\Omega} \leftarrow \bar{\Omega} \setminus \mathcal{A}_j$

$j \leftarrow j + 1$

end if

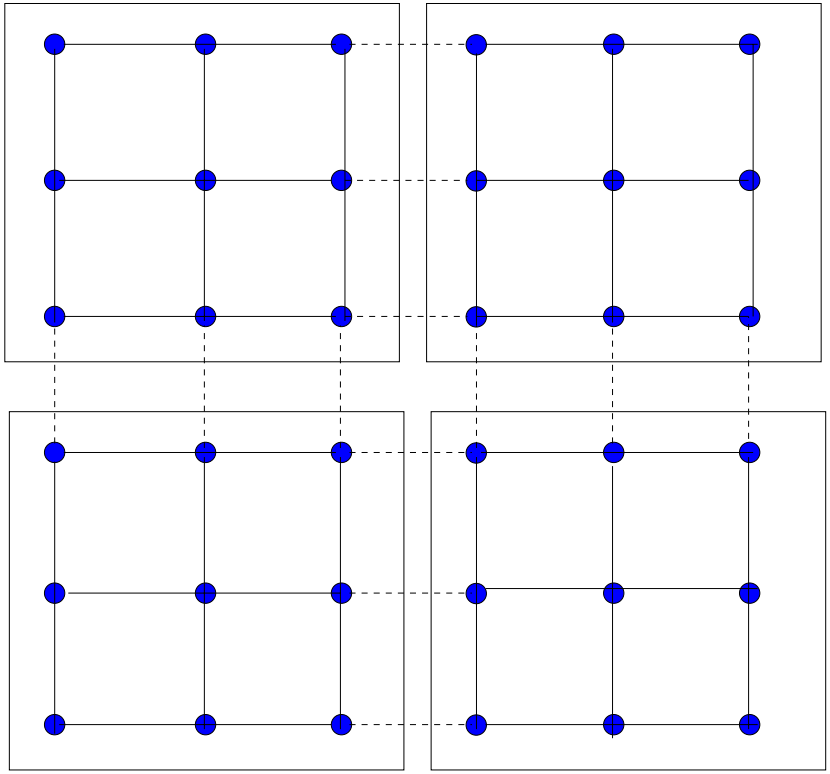
end do

Smoothed Aggregation MG on a lattice

* On structured lattices we define $\{\mathcal{A}_i\}_{i=1}^{n_c}$ using simple geometric blocking, again such that

$$\cup_{i=1}^{n_c} \mathcal{A}_i = \Omega$$

* This *fixes* the sparsity pattern of P and hence also of $A_c = P^t A P$



Smoothed Aggregation (A)MG

Given $B = [x],\ x \in \mathbb{R}^n$, and the set of aggregates, $\{\mathcal{A}_i\}_{i=1}^{n_c}$

$$\tilde{P} = \left(\begin{array}{c|c|c} x_1 & & \\ \vdots & & \\ x_{l_1} & & \\ \hline & \vdots & \\ \hline & & x_{n_{l_c}} \\ & & \vdots \\ & & x_n \end{array}\right) \begin{array}{l} \}\mathcal{A}_1 \\ \\ \vdots \\ \\ \}\mathcal{A}_{n_c} \end{array}$$

* $n_{l_c} = n - l_{n_c} + 1,\ l_i = |\mathcal{A}_i|$
* $\tilde{P}$ scaled: $\tilde{P}^t\tilde{P} = I,\ \tilde{P}x_c = x$
* $P = (I - \tau A)\tilde{P}$

Multiple vector preserving interpolation

For $B := [x^{(1)}, ..., x^{(r)}]$, $x^{(i)} \in \mathbb{R}^n$,

$$\tilde{P} = \left(\begin{array}{c|c|c} X_1 & & \\ \hline & \vdots & \\ \hline & & X_{n_c} \end{array}\right) \begin{array}{l} \} \mathcal{A}_1 \rightarrow Q_1 R_1 \\ \\ \vdots \\ \\ \} \mathcal{A}_{n_c} \rightarrow Q_{n_c} R_{n_c} \end{array}$$

* $X_i \in \mathbb{R}^{l_i \times r}$
* $\tilde{P}^t \tilde{P} = Q^t Q = I$
* $\tilde{P} B_c = \tilde{P} R = B$

Smoothed Aggregation (A)MG convergence theory

Theorem: (P. Vanek, M. Brezina, J. Mandel, 2001) Assume that there exists a constant, $C_a > 0$, such that for every $u \in \mathbb{R}^n$ and every $l \in \{1, , , L\}$, the following approximation property holds:

$$\sum_i \min_{w \in \mathbb{R}^r} \|u - B^1 w\|^2_{\mathcal{A}_i^l} \leq C_a \|u\|^2_A$$

Then

$$\|\tilde{x} - \mathbf{MG}_1(x, b_1)\|_A \leq \left(1 - \frac{1}{c(L)}\right) \|\tilde{x} - x\|_A$$

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The need for adaptive (A)MG method(s)

For $G_c \approx A_c^{-1}$ we have the standard error transfer iteration

$$x \leftarrow (I - M^{-t}A)(I - PG_cP^tA)(I - M^{-1}A)x$$

The smoother is typically fixed, e.g. (block) Gauss Seidel. Thus, the sources of potential failure of the above V–cycle are:

* either the interpolation error $x - Px_c$ is large, or
* the coarse solver G_c cannot handle the coarse component x_c of the current level error x

Hence, the need for adapting the MG cycle and thus the coarse-level hierarchy.

To guide the adaptation on the basis of a current algebraically smooth error vector x, represents the main feature of the "adaptive (algebraic) multigrid methods"

The idea of incorporating "smooth vector(s)" in the construction of a method was first introduced by Brandt, McCormick, and Ruge (1983)

Some recent references:

A. Brandt, "Bootstrap AMG", 2001

M. Brezina, R. Falgout, S. MacLachlan, T. Manteuffel, S. McCormick, and J. Ruge, "Adaptive smoothed aggregation (αSA)," SIAM J. Sci. Comp., **25** (2004), pp 1896–1920

M. Brezina, R. Falgout, S. MacLachlan, T. Manteuffel, S. McCormick, and J. Ruge, "Adaptive algebraic multigrid methods," SIAM J. Sci. Comp., **27** (2006), pp 1261–1286

J. Brannick and L. Zikatanov, "A compatible relaxation and trace minimimization based AMG setup algorithm," DD16 Proceedings (2006)

A basic adaptive (A)MG algorithm

[(T)] For a target $\rho \in (0,1)$ test the method G by applying it to $Ax = 0$:

$$x \leftarrow (I - M^{-t}A)(I - PG_cP^tA)(I - M^{-1}A)x \qquad (1)$$

If $x^tAx \leq \varrho^{2\nu}\, x_0^tAx_0$ **break**,

else set $P = [P,\ P_{\text{new}}]$, $A_c = P^tAP$

for $k = 2 : L-1$

(i) set $x = x_c$, $A = A_k$, $A_c = A_{k+1}$, $M = M_k$, $P = P_k$, $G_c = G_{k+1}$, and update x_c using γ applications of (1)

(ii) $P = [P,\ P_{\text{new}}]$, $A_c = P^tAP$

end for

goto step [(T)] to test the new solver

end if

A basic adaptive (A)MG algorithm ...

In summary, based on a existing (A)MG code, using adaptation, one improves the solver quality by changing its components one level at a time

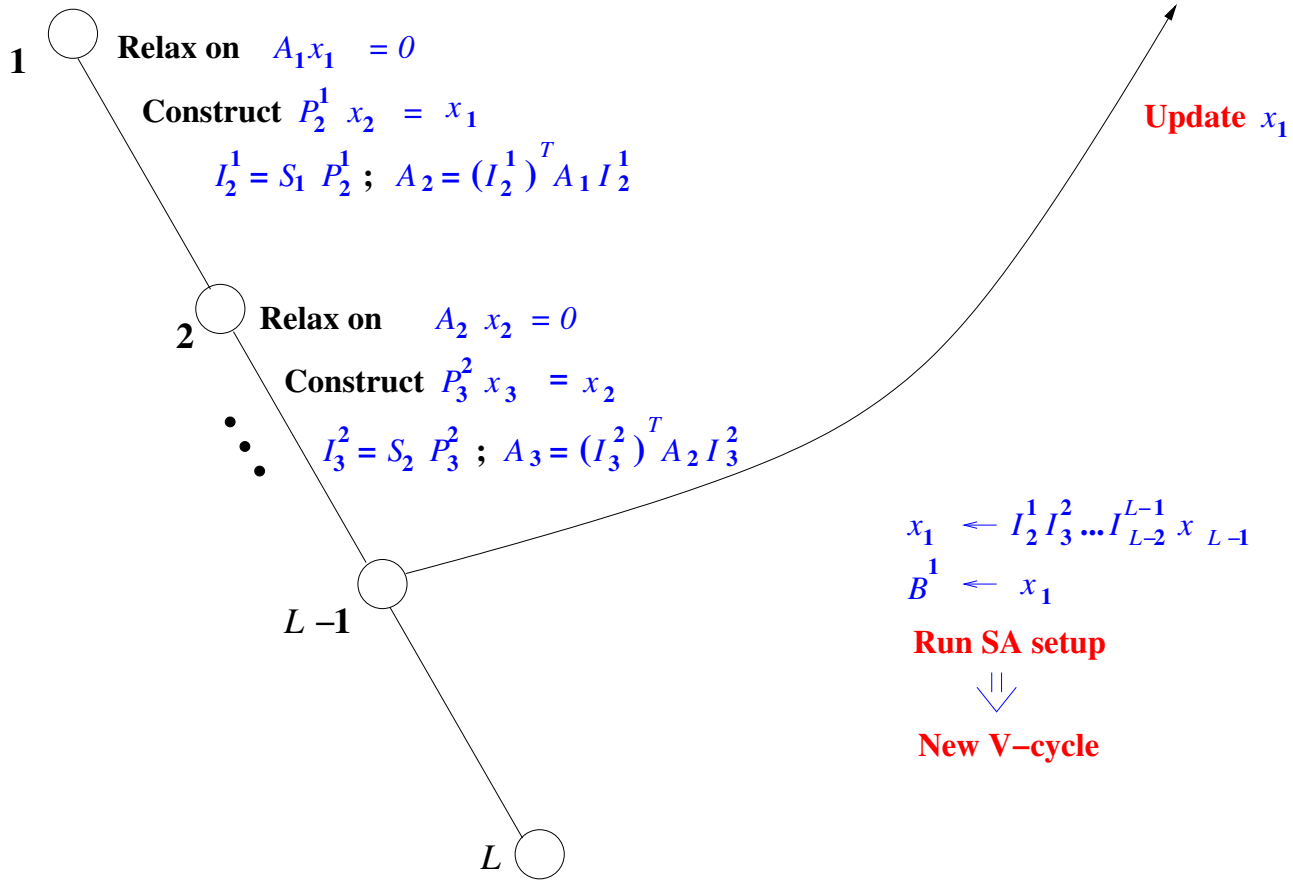
To guarantee improved solver quality after every adaptation step, one needs efficient algorithms for building high–quality updates P_{new} of P

Today we consider the performance of a complex valued SA-based adaptive MG algorithm

* Brezina, et. al., "Adaptive smoothed aggregation", 2004

* Brannick, et. al., "Adaptive smoothed aggregation in lattice QCD", 2006

Adaptive SA Setup



Relation to PCG

* A simple version of the adpative procedure mimics PCG
* Given e_0 relax on $Ae = 0$ such that $e_1 = Se_0$
* Define $P = [e_1]$ and perform two-level MG correction:

$$e_1 \leftarrow (I - \pi_1)Se_0, \quad \pi_1 = P_1(P_1^t A P_1)^{-1} P_1^t A$$

* At kth step define $P_k = [P_{k-1}, e_k]$: $e_k = (I - \pi_k)Se_0$. Then, π_k is the A-orthogonal projector onto:

$$\mathcal{K}_k = \{Se_0, S^2 e_0, ..., S^k e_0\}$$

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Complex valued adaptive SA solver (M. Clark)

* Variational MG: $A_c = (P_c^f)^t A P_c^f$, $P_c^f = S_f \tilde{P}_c^f$
* Partition fine–level dofs into aggregates
* Given B_f, construct $\tilde{P}_c^f$ and B_c such that $\tilde{P}_c^f B_c = B_f$
* B_f is computed using a multilevel power method based on error propagation operator
* Rely on SA framework to use B_f: in contrast to CG, representative vectors are localized over the aggregates to approximate much larger subspace

Solver components / performance measures

* For all tests we use a point source as rhs and report iteration counts needed to reduce relative residual by 10^8

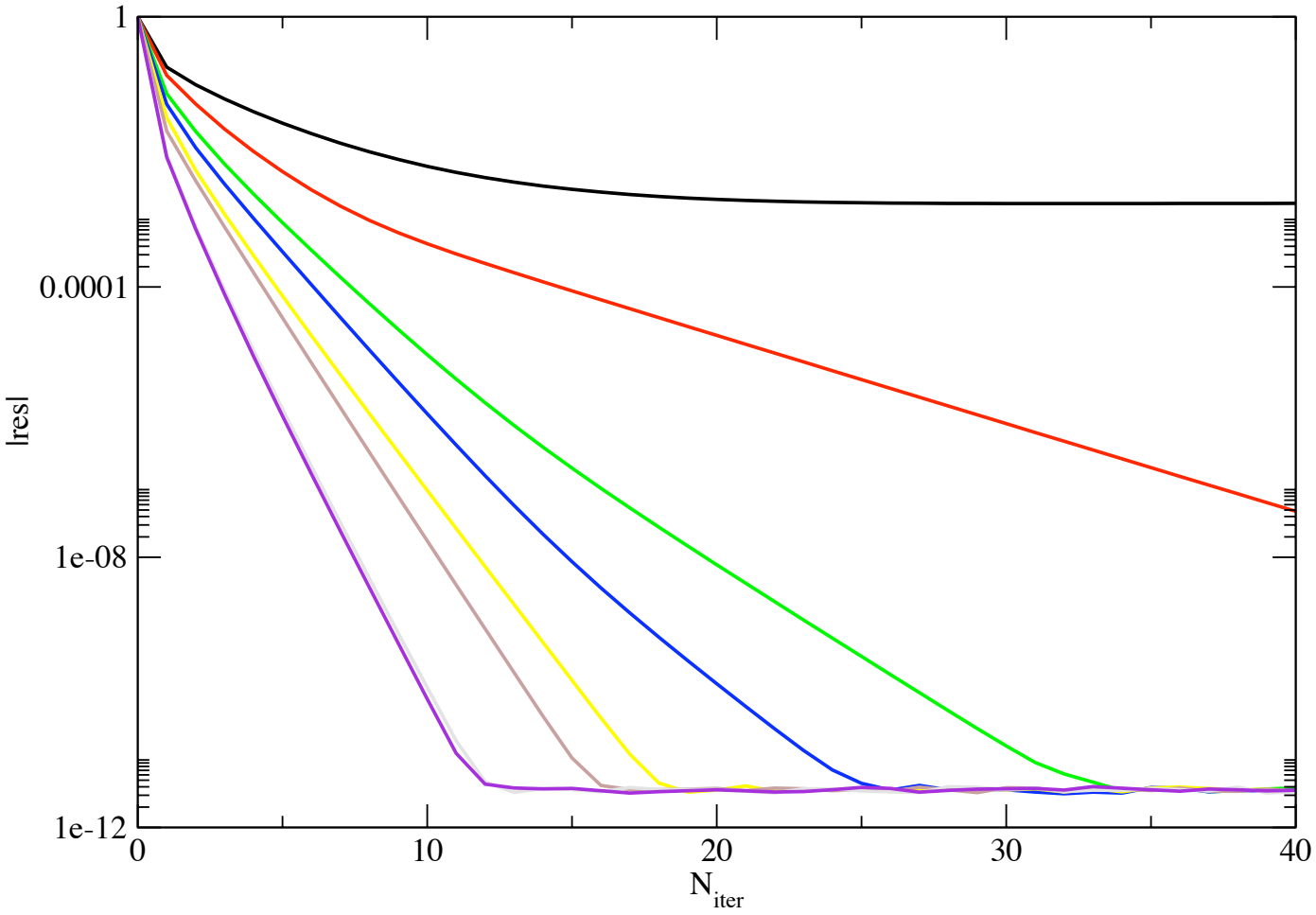
* Smoothers: SOR with $\omega = 1.05$ and ω-Jacobi with $\omega = .6$

* The cost of a single $V(\nu, \mu)$-cycle is approximately $\nu \cdot \mu \cdot GC \cdot OC$ CG iterations, where

$$GC := \frac{\sum_{i=1}^{J} n_{c,i}}{n} \quad \text{and} \quad OC := \frac{\sum_{i=1}^{J} nnz(A_i)}{nnz(A)}$$

3 level, exact coarse solve

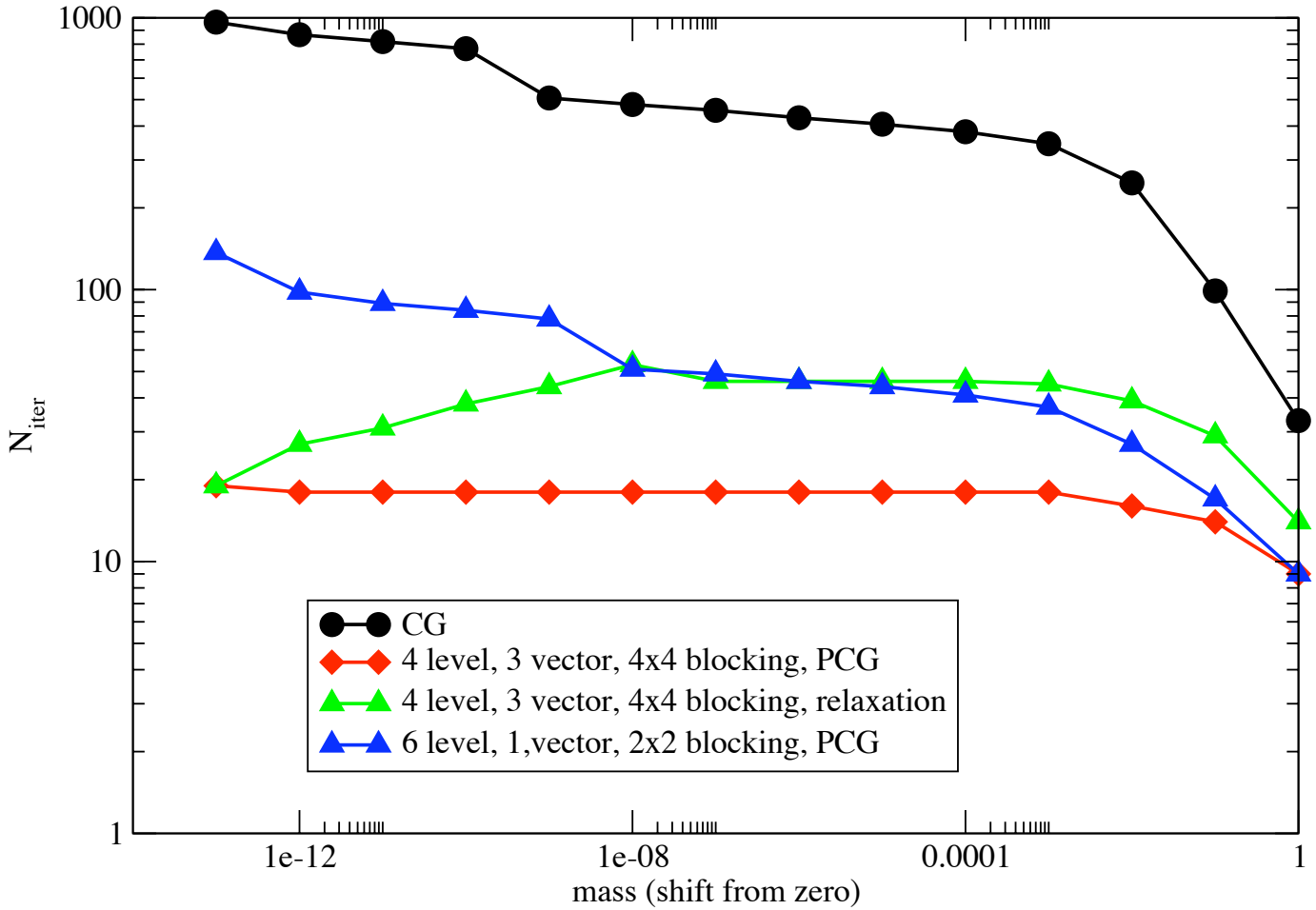
128^2, m=10^{-7}, β=1, 4x4 blocking



Gauge Laplacian: ω-Jacobi ($\omega = .75$), $GC = 1.1$ $OC = 1.1, 1.5, 2.1$

Mass scaling of Gauged Laplacian

V=128^2, β=1.0



ω-Jacobi ($\omega = .75$), $GC = 1.2(1.3)$, $OC = 2.1(2.5)$

Gauge Laplacian

* Ritz values for $N = 128$, $\beta = 1$, and $m = 0$

$$\lambda_1 = 2.1645416870664e-01$$
$$\lambda_2 = 2.2349797163528e-01$$
$$\lambda_3 = 2.2360679843404e-01$$
$$\lambda_4 = 2.3001814768025e-01$$

* Iteration counts needed to reduce relative residual by 10^8 for aSA-PCG, $V(2,2)$-cycles with SOR, $nvec = 1$, 2×2 blocking, $GC = 1.3$, $OC = 2.4$

N/m_0	$1.0e-08$	$1.0e-04$	$1.0e-02$	$1.0e-01$
32	8	7	6	5
64	13	13	10	7
128	14 (425)	13 (343)	11 (232)	8 (107)
256	15	15	13	8
512	15	15	13	9

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$$\lambda_4 = 2.3001814768025e-01$$

* Iteration counts needed to reduce relative residual by 10^8 for aSA-PCG, $V(1,1)$-cycles with SOR, $nvec = 1$, 4×4 blocking, $GC = 1.1$, $OC = 1.1$

N/m_0	$1.0e-08$	$1.0e-04$	$1.0e-02$	$1.0e-01$
32	8	7	6	5
64	13	13	10	7
128	35 (425)	27 (343)	23 (232)	17 (107)
256	15	15	13	8
512	15	15	13	9

Gauge Laplacian

* Iteration counts needed to reduce relative residual by 10^8 for aSA-PCG, $V(1,1)$-cycles with SOR, $nvec = 1$, 4×4 blocking, $GC = 1.1$, $OC = 1.1$

m_0	$1.0e-08$	$1.0e-04$	$1.0e-02$	$1.0e-01$
cg its	435	343	232	107
setup - MVs	277	186	92	15
aSA-PCG its	32	24	18	10

* Approximate setup costs for $m_0 = 1.0e-08$

setup - MVs	411	277	167	123	84
aSA-PCG its	26	32	36	49	51
aSA its	31	38	59	65	78

Schwinger model

* Ritz values for $N = 64$, $\beta = 1$, $m = 0$, top. charge = 1

λ_1	$2.4072960956544e-01$	$7.4457724811804e-17$
λ_2	$2.7543643782929e-01$	$-1.1102230246252e-16$
λ_3	$2.7644821995514e-01$	$6.0828034281699e-03$
λ_4	$2.7644821995513e-01$	$-6.0828034281690e-03$

* Iteration counts needed to reduce relative residual by 10^8 for aSA-PCG applied to H^2, $V(2,2)$-cycles, $nvec = 1$, 2×2 blocking, $GC = 1.2$, $OC = 2.7$

setup / m_0	$1.0e-04$	$1.0e-03$	$1.0e-02$	$1.0e-01$
917	34	32	20	12
1361	28	27	16	7
1654	23 (2113)	20 (1058)	17 (336)	5 (106)

Schwinger model

* Ritz values for $N = 64$, $\beta = 10$, $m = 0$, top. charge = 0

λ_1	$5.2306384031557e-02$	$-2.3671180635050e-02$
λ_2	$5.2306384031563e-02$	$2.3671180635057e-02$
λ_3	$5.2574243587467e-02$	$-7.9255143077699e-03$
λ_4	$5.2574243587460e-02$	$7.9255143077641e-03$

* Iteration counts needed to reduce relative residual by 10^8 for aSA-PCG applied to H^2, $V(2,2)$-cycles, $nvec = 1$, 2×2 blocking, $GC = 1.2$, $OC = 2.7$

setup / m_0	$1.0e-04$	$1.0e-03$	$1.0e-02$	$1.0e-01$
316	34	23	14	10
504	32	23	15	10
1114	22 (1305)	22 (968)	15 (329)	10 (112)

Concluding Remarks

* Several difficulties must be addressed in designing an AMG method for QCD systems
* Adaptive MG methodology naturally handles these difficulties
  * The adaptive setup is designed to expose the *oscillatory* low energy modes
  * Construction of the sequence of coarse problems is based on these computed low energy modes
  * Key issue now is complexity

Current and future works

* Various complex-valued adaptive AMG test codes
  * In the Classical AMG setting by MacLachlan and Osterlee
  * In SA setting by M. Clark in serial and by A. Bessen in parallel
* Systems MG: block smoothers
* MG for $H f = \phi$
* Preconditioners based on Gauge Laplacian
* Parallel implementation

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"Ideal" interpolation operator

Given R, let

$$K_* = \inf_P \sup_v \frac{\|(I - PR)v\|_{\bar{M}}^2}{\|v\|_A^2}$$

The minimum and minimizer are given by

$$K_* = \frac{1}{\lambda_{\min}(\bar{M}_{ff}^{-1} A_{ff})} \quad \text{and} \quad P_* = \begin{bmatrix} -A_{ff}^{-1} A_{fc} \\ I_c \end{bmatrix}$$

Thus, if K_* is uniformly bounded, then there exists a P, namely P_*, such that the two-level method is uniformly convergent

Trace minimization

* Assume $\mathcal{N}_c$ and $\{\Omega_i\}_{i=1}^{n_c}$ are given. Then

  Each Ω_i contains exactly one index from $\mathcal{N}_c$

* Consider the following affine subspaces of $\mathbb{R}^{n \times n_c}$:

$$\mathcal{X} = \{Q : Q = \begin{bmatrix} W \\ I_c \end{bmatrix}, W \in \mathbb{R}^{n_f \times n_c}\},$$

$$\mathcal{X}_H = \{Q : Q \in \mathcal{X}, \ Q_{ji} = 0 \text{ for all } j \notin \Omega_i, Q\mathbf{1}_c = e\}$$

Here, e is an arbitrary nonzero element of $\mathbb{R}^n : e = \begin{bmatrix} * \\ \mathbf{1}_c \end{bmatrix}$

Definition of P

* Let $I_i \in \mathbb{R}^{n \times n_i}$ be the characteristic function over Ω_i and define $A_i = I_i^T A I_i$.

* Consider

$$P = \arg\min J(Q) := \arg\min \text{trace}(Q^T A Q), \quad Q \in \mathcal{X}_H$$

* The i-th column of the **unique** solution to the minimization problem is given by

$$[P]_i = I_i A_i^{-1} I_i^T M_a e, \quad M_a^{-1} = \sum_{i=1}^{n_c} I_i A_i^{-1} I_i^T$$

On the best approximation to P_* in the trace norm

The matrix M_a^{-1} is the standard additive Schwarz preconditioner for A where the n_c blocks are defined in terms of $\{\Omega_i\}_{i=1}^{n_c}$. Letting each $\Omega_i = \{1 : n_f\}$ and $e = P_* \mathbf{1}_c$ we have that

$J(P_*) = \text{trace}(\mathcal{S}(A))$ and

$$\begin{aligned} \text{trace}(\mathcal{S}(A)) = \sum_{i=1}^{n_c} (\mathcal{S}(A)e_i, e_i) &= \sum_{i=1}^{n_c} \inf_{v: v_c = e_i} (Av, v) \\ \leq \sum_{i=1}^{n_c} (APe_i, Pe_i) &= \text{trace}(P^T AP) \end{aligned}$$

The best approximation property

Theorem. Let $J(\cdot) = |||\cdot|||_A$ and P be the unique solution of the trace-minimization problem. Then

$$|||P_* - P|||_A = \min_{Q \in \mathcal{X}_H} |||P_* - Q|||_A$$

Proof. Let $Q \in \mathcal{X}_H$ be arbitrary. Since, $P_*^T A(Q - P_*) = 0$, we have

$$J(Q) = J(P_* + (Q - P_*)) = \text{trace}(\mathcal{S}(A)) + |||P_* - Q|||_A^2$$

The optimal choice of e

* By direct computation we have that $J(P) = (M_a e, e)$, implying

$$|||P_* - P|||_A^2 = (M_a e, e) - \text{trace}(\mathcal{S}(A))$$

* We can now take the minimum with respect to e on both sides and arrive at

$$|||P_* - P|||_A^2 = \text{trace}[\mathcal{S}(M_a) - \mathcal{S}(A)]$$

where the minimizer is $e = \begin{bmatrix} -M_{a,ff}^{-1} M_{a,fc} \mathbf{1}_c \\ \mathbf{1}_c \end{bmatrix}$