Multigrid solvers for quantum dynamics - a first look

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Support

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What is QCD?

Quantum Chromodynamics is the theory of the strong interaction

- Part of the Standard model of particle physics
- Describes interactions between quarks and gluons
- Consistent with particle accelerator experiments

We generally believe QCD to be true, but look to make consistent predictions to check it.
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We generally believe QCD to be true, but look to make consistent predictions to check it

- Accelerators measure particle masses, decay rates, . . .
- Use QCD theory to make predictions
- QCD not amenable to asymptotic analysis
- Need high-precision numerical simulations
What’s a Quark?

Quarks are elementary particles

- Protons/Neutron composed of three quarks
- Each quark has a flavour
  - Up, Down, Strange, Charm, Top, Bottom
- Quarks bound together by strong force
  - Force between quarks grows as they move apart

We characterize quarks by their

- Spin (4 degrees of freedom)
- Colour (3 degrees of freedom)
QCD Resources

Accelerators:
- Fermilab Tevatron: $120 million (in 1983)
- Large Hadron Collider: €2 billion (in 2007)
- International Linear Collider: est’d $6.65 billion

Computational:
- QCDOC: 3 systems at 10 Teraflops each
- APEnext: 7 TeraFlops
- Commodity clusters in USQCD: ~ 10 Teraflops
- Blue Gene, Cray XT3

Multigrid solvers for quantum dynamics - a first look- p.5
The Continuum Challenge

Compute:

$$\langle \mathcal{O}(A, \psi, \bar{\psi}) \rangle = \frac{1}{Z} \int \mathcal{O}(A, \psi, \bar{\psi}) e^{-S_{pg} - S_F} d\psi d\bar{\psi} dA$$

where

- $\langle \mathcal{O} \rangle$ is the expected value of $\mathcal{O}$
- $A = A_\mu(x) \in \mathbb{C}^{3 \times 3}$ is the gauge potential
- $\psi(x), \bar{\psi}(x)$ are Grassman-valued fermion fields
- $Z = \int e^{-S_{pg} - S_F} d\psi d\bar{\psi} dA$
- $S_{pg} = S_{pg}(A)$ is the “pure gauge” action
- $S_F = \int_{x,y} \bar{\psi}(x) M(A) \psi(y)$ is the fermionic action
The Dirac Operator

$M$ is block-structured in colour-spin

$$M(A) = \sum_{\mu=1}^{4} \left( \gamma_\mu \otimes \left( I_3 \partial_\mu - \imath A_\mu \right) \right) - m I_{12}$$

where

- $\mu = 1, \ldots, 4$ represent space-time directions
- $\gamma_\mu$ are unitary $4 \times 4$ matrices
- $I_3$ and $I_{12}$ are the $3 \times 3$ and $12 \times 12$ identities
- $\partial_\mu$ is a regular partial derivative
- $A_\mu(x) \in \mathbb{C}^{3 \times 3}$ is the gauge potential
- $m$ is a mass term
Block Form

Writing \( D_\mu = l_3 \partial_\mu - iA_\mu \),

\[
M = \begin{pmatrix}
-ml_3 & 0 & \nu D_3 - D_4 & \nu D_1 - D_2 \\
0 & -ml_3 & \nu D_1 + D_2 & -\nu D_3 - D_4 \\
-\nu D_3 - D_4 & -\nu D_1 + D_2 & -ml_3 & 0 \\
-\nu D_1 - D_2 & \nu D_3 - D_4 & 0 & -ml_3
\end{pmatrix}
\]

Notice that \( D_\mu^* = -D_\mu \), so

\[
\begin{pmatrix}
l_3 & 0 & 0 & 0 \\
0 & l_3 & 0 & 0 \\
0 & 0 & -l_3 & 0 \\
0 & 0 & 0 & -l_3
\end{pmatrix} M \text{ is a Hermitian operator}
\]
Perturbative Methods

Early success in quantum field theory came from asymptotic analysis.

Quantum Electrodynamics (QED)
- Predictions accurate to 13 digits!

QCD resists this approach.
Perturbative Methods

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QCD resists this approach

Discretize
- Space-time becomes discrete lattice
- Gauge potential, $A_\mu$, integrated over lattice links

$$A_\mu(x) \rightarrow U(x, \mu) = e^{-i g A_\mu(x_j)}$$
The Discrete Challenge

Compute:

\[ \langle O(U, \psi, \overline{\psi}) \rangle = \frac{1}{Z} \int O(U, \psi, \overline{\psi}) e^{-S_{pg} - S_F} \, d\psi \, d\overline{\psi} \, dU \]

where

- \( \langle O \rangle \) is the expected value of \( O \)
- \( U(x, \mu) = e^{-i g A_\mu(x)} \) is the lattice gauge field
- \( \psi(x), \overline{\psi}(x) \) are Grassman-valued fermion fields
- \( Z = \int e^{-S_{pg} - S_F} \, d\psi \, d\overline{\psi} \, dU \)
- \( S_{pg} = S_{pg}(U) \) is the “pure gauge” action
- \( S_F = \sum_{x,y} \overline{\psi}(x) M(U) \psi(y) \) is the fermionic action
Simplifying the integrals

“Easy” to simplify $Z$: \[ \int e^{-S_F} d\psi d\bar{\psi} = \det(M) \]

\[
Z = \int \det(M(U)) e^{-S_{pg}(U)} dU = \int e^{-S_{pg}^{\text{eff}}(U)} dU
\]

for $S_{pg}^{\text{eff}} = S_{pg}(U) + \text{Tr}(\log(M(U)))$
Simplifying the integrals

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\]

for $S_{pg}^{\text{eff}} = S_{pg}(U) + \text{Tr}(\log(M(U)))$

Similar simplification for certain $\mathcal{O}(U, \psi, \bar{\psi})$:

\[
\langle \psi(y) \bar{\psi}(x) f(U) \rangle = \frac{1}{Z} \int e^{-S_{pg}^{\text{eff}}(U)} f(U) M^{-1}(y, x) dU
\]

In general, integrate out fermion fields:

\[
\langle \mathcal{O}(U, \psi, \bar{\psi}) \rangle = \frac{1}{Z} \int e^{-S_{pg}^{\text{eff}}} \mathcal{O}_{\text{eff}}^{\text{eff}}(U, M^{-1}(U)) dU
\]
Integrating over $U$

Use Monte-Carlo to integrate over $U$:

- **Assume** we can generate gauge fields with given probability

  $$P(U_k) = \frac{1}{Z} e^{-S_{pg}(U_k)}$$

Then,

$$\langle O(U, \psi, \bar{\psi}) \rangle \approx \frac{1}{N} \sum_{k=1}^{N} O^{\text{eff}}(U_k, M^{-1}(U_k))$$

Two challenges:

- How do we pick $\{U_k\}_{k=1}^{N}$?
- How do we evaluate $O^{\text{eff}}(U_k, M^{-1}(U_k))$?
Discretization

Discretization of $M$ must preserve several properties for consistency within Monte-Carlo scheme

Several choices for $D_\mu = I_3 \partial_\mu - \imath A_\mu$:

$$D_\mu \psi^\nu(x) \approx \frac{1}{h} (U(x, \mu) \psi^\nu(x + h \hat{\mu}) - \psi^\nu(x))$$

$$\approx \frac{1}{h} (\psi^\nu(x) - U^*(x - h \hat{\mu}, \mu) \psi^\nu(x - h \hat{\mu}))$$

$$\approx \frac{1}{2h} (U(x, \mu) \psi^\nu(x + h \hat{\mu}) - U^*(x - h \hat{\mu}, \mu) \psi^\nu(x - h \hat{\mu}))$$

where $\hat{\mu}$ is the unit-vector in the $\mu$-direction
Choosing central differences for $D_\mu \psi^\nu(x)$ leads to instability (Analogy: Nodal vs. staggered discretizations of Stokes)

Modify $M$ by adding

$$\frac{-h}{2} \sum_\mu D^2_\mu \psi^\nu(x) \approx \frac{1}{2h} \sum_\mu (-U(x + h\mu, \mu)\psi^\nu(x + h\mu) + 2\psi^\nu(x) - U^*(x - h\mu, \mu)\psi^\nu(x - h\mu))$$

to its diagonal, $M \rightarrow \tilde{M}$

Stabilized matrix, $\tilde{M}$, is known as the Dirac-Wilson operator
$M^{-1}$ is called a quark propagator

Typically, approximating $O^{\text{eff}}(U_k, M^{-1}(U_k))$ requires computing several/many entries in $\tilde{M}^{-1}(U_k)$. 
$M^{-1}$ is called a quark propagator

Typically, approximating $\mathcal{O}^{\text{eff}}(U_k, M^{-1}(U_k))$ requires computing several/many entries in $\tilde{M}^{-1}(U_k)$

After discretization, $\tilde{M}$ has dimension $12n_x^3n_t$

- $n_x \times n_x \times n_x$ spatial lattice
- $n_t$ points in time (4th space dimension)
- 3 colour indices per lattice point
- 4 spin indices per colour/lattice point
Solve $\tilde{M}\psi_j = \eta_j$ for some collection, $\{\eta_j\}$

Size of $\{\eta_j\}$ varies with application

- May be only a few RHS
- May want all (or most) of $\tilde{M}^{-1}$

Our interest: when $\{\eta_j\}$ is small enough that iterative methods are appropriate, but large enough that multigrid setup costs may be amortized
Challenges in Lattice QCD

Numerical challenges arise because

- Need large $n_x, n_t$ for physical accuracy
- $\tilde{M}$ is large, $12n_x^3n_t$ degrees of freedom
- Gauge field, $U$, is very disordered
Challenges in Lattice QCD

Numerical challenges arise because

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Assets in Lattice QCD

Opportunity for fast solvers exists because

- $\tilde{M}$ is sparse, 108 nonzeros per row
- $\tilde{M}$ is easily permuted to be Hermitian
- Many right-hand sides for each realization of $U$
Extreme Simplification

Consider

- 2D spatial lattice, instead of 4D space-time
- Single colour/spin per lattice site ($\Rightarrow$ scalar $U$)
- "Cold" Gauge field, $U(x, \mu) \equiv 1$
- Mass term, $m = 0$
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Result:

2D Poisson equation:

\[
\tilde{M} \rightarrow \begin{bmatrix}
\frac{-1}{h^2} & \frac{-1}{h^2} & \frac{-1}{h^2} \\
\frac{-1}{h^2} & \frac{4}{h^2} & \frac{-1}{h^2} \\
\frac{-1}{h^2} & \frac{-1}{h^2} & \frac{4}{h^2}
\end{bmatrix}
\]

Start search for good QCD solver with good Poisson solver.
Extreme Simplification

Consider

- 2D spatial lattice, instead of 4D space-time
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Start search for good QCD solver with good Poisson solver
Scalability

Problem Size

Estimated Required Solution Time (s)

- one minute
- 60 years
- age of the universe

Cholesky
Jacobi
GS
Band Cholesky
CG–MIC(0)
Optimal

Multigrid solvers for quantum dynamics - a first look- p.19
Stationary Iterative Methods

- Want to improve approximation, $x^{(0)}$, to $x = A^{-1}b$
- Residual, $r^{(0)}$, is a measure of the error

$$r^{(0)} = b - Ax^{(0)} = Ax - Ax^{(0)} = A(x - x^{(0)})$$

- Choose $B^{-1} \approx A^{-1}$
- Take $x^{(1)} = x^{(0)} + B^{-1}r^{(0)}$

Error propagation form: $e^{(1)} = (I - B^{-1}A)e^{(0)}$
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Error propagation form:  
\[
\begin{align*}
  e^{(1)} &= (I - B^{-1}A)e^{(0)} \\
  e^{(2)} &= (I - B^{-1}A)e^{(1)}
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Stationary Iterative Methods

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Stationary Iterative Methods

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Error propagation form:

$$e^{(1)} = (I - B^{-1}A)e^{(0)}$$
$$e^{(2)} = (I - B^{-1}A)^2e^{(0)}$$
$$\vdots$$
$$e^{(n)} = (I - B^{-1}A)^ne^{(0)}$$
Convergence of Stationary Iterations

Convergence depends on spectrum of $I - B^{-1}A$

Weighted Jacobi Iteration: $e^{(n)} = (I - \frac{3}{4}D^{-1}A)^n e^{(0)}$
Convergence of Stationary Iterations

Convergence depends on spectrum of $I - B^{-1}A$

Gauss-Seidel Iteration: $e^{(n)} = (I - L^{-1}A)^n e^{(0)}$
Smoothing Property

Error after 1 weighted Jacobi iteration
Smoothing Property

Error after 2 weighted Jacobi iterations

Error after 2 weighted Jacobi iterations
Smoothing Property

Error after 3 weighted Jacobi iterations

Multigrid solvers for quantum dynamics - a first look - p.22
Smoothing Property

Error after 4 weighted Jacobi iterations
Smoothing Property

Error after 5 weighted Jacobi iterations

Error after 5 weighted Jacobi iterations
Smoothing Property

Error after 6 weighted Jacobi iterations

Error after 6 weighted Jacobi iterations
Error after 7 weighted Jacobi iterations
Smoothing Property

Error after 8 weighted Jacobi iterations
Smoothing Property

Error after 9 weighted Jacobi iterations
Smoothing Property

Error after 10 weighted Jacobi iterations
Complementarity

- Error after a few weighted Jacobi iterations has structure
- Instead of throwing out the method, look to complement its failings

How can we best correct error modes that are slow to be reduced by relaxation?
Complementarity

- Error after a few weighted Jacobi iterations has structure
- Instead of throwing out the method, look to complement its failings

How can we best correct error modes that are slow to be reduced by relaxation?

- Slow-to-converge errors are smooth
- Smooth vectors can be easily represented using fewer degrees of freedom
Coarse-Grid Correction

- Smooth vectors can be accurately represented using fewer degrees of freedom
- Idea: transfer job of resolving smooth components to a coarser grid version of the problem
- Need:
  - Complementary process for resolving smooth components of the error on the coarse grid
  - Way to combine the results of the two processes
Variational Coarsening

- Correct the approximation after relaxation, \( x^{(1)} \), from an auxiliary (coarse-grid) problem
- Need interpolation map, \( P \), from coarse grid to fine grid
- Corrected approximation will be \( x^{(2)} = x^{(1)} + Px_c \)

What is the best \( x_c \) for correction?
A-norm and A-inner product

- Asking for the best solution implies a metric
- Hermitian and positive-definite matrix, $A$, defines an inner product and a norm:

$$\langle x, y \rangle_A = y^*Ax \quad \text{and} \quad \|x\|^2_A = x^*Ax$$

- Best then means closest to the exact solution in norm

$$y^{opt} = \arg\min_y \|x - y\|_A$$
Variational Coarsening

- Want to correct the approximation after relaxation, $x^{(1)}$, from a coarse-grid version of the problem.
- Need interpolation map, $P$, from coarse grid to fine grid.
- Corrected approximation will be $x^{(2)} = x^{(1)} + P x_c$

What is the best $x_c$ for correction?

- Best means closest to the exact solution in norm

$$x_c = \arg\min_{y_c} \| x - (x^{(1)} + P y_c) \|_A$$

- Best $x_c$ satisfies $(P^* A P)x_c = P^* A(x - x^{(1)}) = P^* r^{(1)}$
Multigrid

Multigrid Components

- Relaxation

\[ \text{Relax: } x^{(1)} = x^{(0)} + D^{-1}r^{(0)} \]

- Use a smoothing process (such as Jacobi or Gauss-Seidel) to eliminate oscillatory errors

- Remaining error satisfies \( Ae^{(1)} = r^{(1)} = b - Ax^{(1)} \)
Multigrid

Multigrid Components

- Relaxation
- Restriction

\[
\text{Relax: } x^{(1)} = x^{(0)} + D^{-1} r^{(0)}
\]

- Transfer residual to coarse grid
- Compute \( P^* r^{(1)} \)
Multigrid Components

- Relaxation
- Restriction
- Coarse-Grid Correction

Use coarse-grid correction to eliminate smooth errors

Best correction, $x_c$, in terms of $A$-norm satisfies

$$ P^* A P x_c = P^* r^{(1)} $$
Multigrid Components

- Relaxation
- Restriction
- Coarse-Grid Correction
- Interpolation

Transfer correction to fine grid
Compute $x^{(2)} = x^{(1)} + Px_c$

Relax: $x^{(1)} = x^{(0)} + D^{-1}r^{(0)}$

Solve: $P^*APx_c = P^*r^{(1)}$
Multigrid Components

- Relaxation
- Restriction
- Coarse-Grid Correction
- Interpolation
- Relaxation

- Relax once again to remove oscillatory error introduced in coarse-grid correction
Direct solution of coarse-grid problem isn’t practical

Recursion!

Apply same methodology to solve coarse-grid problem
Performance

- Uniform grid coarsening
- Bilinear Interpolation
- $V(2,2)$ cycles, with under-relaxed Jacobi

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<tr>
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<td>$\rho_{MG}$</td>
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Performance

- Uniform grid coarsening
- Bilinear Interpolation
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Now relax simplifications:

- Allow $U(x, \mu)$ to take physical (scalar) values
  - “Gauge Laplacian”

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Accounting for Heterogeneity

Poor performance results from ignoring heterogeneity

Error after relaxation on Poisson’s equation is smooth
  • Low-order geometric interpolation is accurate
Accounting for Heterogeneity

Poor performance results from ignoring heterogeneity.

Error after relaxation on Poisson’s equation is smooth:
- Low-order geometric interpolation is accurate.

Geometric multigrid defines interpolation based on:
- grid geometry
- assumptions on performance of relaxation

*Heterogeneity* strongly influences performance of relaxation.
“Smooth” Errors

- Linear interpolation can make $O(1)$ errors for problems with non-smooth coefficients.

Slowest to converge error for $\frac{d}{dx} \left( \sigma \frac{du}{dx} \right)$, for

$$\sigma = \begin{cases} 
10^{-8} & x \leq \frac{3}{8} \\
1 & x > \frac{3}{8}
\end{cases}$$
“Smooth” Errors

- Linear interpolation can make $O(1)$ errors for problems with non-smooth coefficients

Slowest to converge error for $\frac{d}{dx} \left( \sigma \frac{du}{dx} \right)$, for

$$\sigma = \begin{cases} 
10^{-8} & x \leq \frac{3}{8} \\
1 & x > \frac{3}{8}
\end{cases}$$

and linear interpolant from coarse grid.
“Smooth” Errors

- Linear interpolation can make $O(1)$ errors for problems with non-smooth coefficients
- The abrupt change in character of slow-to-converge errors is reflected in matrix entries

$$A = \frac{1}{h^2} \begin{bmatrix}
2 \times 10^{-8} & -10^{-8} & -10^{-8} & -10^{-8} \\
-10^{-8} & 2 \times 10^{-8} & -10^{-8} & -10^{-8} \\
-10^{-8} & 1 + 10^{-8} & -1 & -1 \\
-1 & 2 & -1 & -1 \\
-1 & 2 & -1 & -1 \\
-1 & 2 & 2 & 2
\end{bmatrix}$$
“Smooth” Errors

- Linear interpolation can make $O(1)$ errors for problems with non-smooth coefficients.
- The abrupt change in character of slow-to-converge errors is reflected in matrix entries.
- Idea: Use the entries in the matrix operator to help define interpolation.
Algebraic Multigrid Interpolation

- Assume a partition into fine ($F$) and coarse ($C$) grid sets
- Define interpolation based only on entries in $A$
- Start with assumption that errors left after relaxation have small residuals: for $i \in F$,
  \[(Ae)_i \approx 0\]
  \[a_{ii}e_i = -\sum_{j \in F} a_{ij}e_j - \sum_{k \in C} a_{ik}e_k\]

- Use assumptions about slow-to-converge error to collapse connections to $j \in F$ onto $k \in C \cap \{k : a_{ik} \neq 0\}$

---

J. Ruge and K. Stüben, in Multigrid Methods, 1987
Complex-Valued AMG

Gauge Laplacian is a Hermitian H-matrix

- $A$ is an H-matrix if $\mathcal{M}(A)$ is an M-matrix,

$$(\mathcal{M}(A))_{ij} = \begin{cases} 
|a_{ii}| & \text{if } i = j \\
-|a_{ij}| & \text{if } i \neq j
\end{cases}$$

- Jacobi/Gauss-Seidel converge for H-matrices
- Fourier analysis confirms (algebraic) smoothing properties
- Interpolation based on classical AMG
- Restriction as adjoint of interpolation
- Galerkin coarse-grid operators

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Varga, Linear Algebra and Appl. 1976, **13**:1-9
## Solving the Gauge Laplacian

### Convergence Factors

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### Operator Complexities

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<td>2.59</td>
<td>2.55</td>
<td>2.52</td>
</tr>
</tbody>
</table>
Solving the Gauge Laplacian

### Convergence Factors

<table>
<thead>
<tr>
<th>grid</th>
<th>$64^2$</th>
<th>$128^2$</th>
<th>$256^2$</th>
<th>$512^2$</th>
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<tbody>
<tr>
<td>$\rho_{MG}$</td>
<td>0.689</td>
<td>0.762</td>
<td>0.776</td>
<td>0.736</td>
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<tr>
<td>$\rho_{AMG}$</td>
<td>0.277</td>
<td>0.378</td>
<td>0.404</td>
<td>0.390</td>
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</table>

### Operator Complexities

<table>
<thead>
<tr>
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<th>$512^2$</th>
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</thead>
<tbody>
<tr>
<td>$C_{MG}$</td>
<td>1.63</td>
<td>1.62</td>
<td>1.61</td>
<td>1.60</td>
</tr>
<tr>
<td>$C_{AMG}$</td>
<td>2.68</td>
<td>2.59</td>
<td>2.55</td>
<td>2.52</td>
</tr>
</tbody>
</table>

### Convergence factor per matvec equivalent

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>$\rho_{MG}^{eff}$</td>
<td>0.944</td>
<td>0.959</td>
<td>0.961</td>
<td>0.953</td>
</tr>
<tr>
<td>$\rho_{AMG}^{eff}$</td>
<td>0.887</td>
<td>0.910</td>
<td>0.915</td>
<td>0.911</td>
</tr>
</tbody>
</table>

Multigrid solvers for quantum dynamics - a first look - p.34
Now take realistic values of $U(x, \mu)$ and $m$

$$\tilde{M} \rightarrow \begin{bmatrix}
-U^*(x - (h, 0), (1, 0)) & -U(x, (0, 1)) & 4 - m & -U(x, (1, 0)) \\
-U^*(x - (0, h), (0, 1)) & -U(x - (0, h), (0, 1)) & -U^*(x - (h, 0), (1, 0)) & -U(x, (0, 1))
\end{bmatrix}$$

- $|U(x, \mu)| = 1$ for all $x, \mu$
- For “physical” fields $U(x, \mu)$ and $m = 0$, $\lambda_{\text{min}}(\tilde{M}) > 0$.
- Choose $m > 0$ so that $\lambda_{\text{min}}(\tilde{M}) \to 0$
**Effect of Shifting**

### AMG Convergence Factors

<table>
<thead>
<tr>
<th>$\lambda_{\text{min}}(\tilde{M})$</th>
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<th>$512^2$</th>
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<tr>
<td>1.0</td>
<td>0.040</td>
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<td>$10^{-1}$</td>
<td>0.475</td>
<td>0.598</td>
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<tr>
<td>$10^{-2}$</td>
<td>0.893</td>
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<tr>
<td>$10^{-3}$</td>
<td>0.988</td>
<td>0.993</td>
<td>0.993</td>
<td>0.990</td>
</tr>
<tr>
<td>$10^{-4}$</td>
<td>0.9988</td>
<td>0.9993</td>
<td>0.9993</td>
<td>0.9990</td>
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</tbody>
</table>
Algebraically Smooth Error

Slow-to-converge errors must be in range of interpolation

- AMG treats heterogeneity in coarse-grid correction
- Heterogeneity in $\tilde{M}$ affects performance of relaxation
- As $\lambda_{\text{min}}(\tilde{M}) \to 0$, performance of relaxation degrades
- As $\lambda_{\text{min}}(\tilde{M}) \to 0$, accuracy of interpolation must increase
Algebraically Smooth Error

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- As $\lambda_{\text{min}}(\tilde{M}) \to 0$, accuracy of interpolation must increase

AMG process makes assumptions on relaxation for generality

- AMG assumptions are violated as $\lambda_{\text{min}}(\tilde{M}) \to 0$
If only one bad eigenvalue, then CG acceleration should be effective.

PCG Iterations so that $\frac{\|r^{(k)}\|}{\|r^{(0)}\|} < 10^{-10}$

<table>
<thead>
<tr>
<th>$\lambda_{\text{min}}(\tilde{M})$</th>
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If only one bad eigenvalue, then CG acceleration should be effective.

PCG Iterations so that $\|r^{(k)}\|/\|r^{(0)}\| < 10^{-10}$

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<td>12</td>
<td>14</td>
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</table>
Krylov Acceleration

If only one bad eigenvalue, then CG acceleration should be effective

PCG Iterations so that \( \| r^{(k)} \| / \| r^{(0)} \| < 10^{-10} \)

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<tr>
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<tr>
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May solve 1000+ RHS in each Monte-Carlo step
Can amortize expensive setup, if it pays off in solve phase

Multigrid solvers for quantum dynamics - a first look- p.38
Calibrating Interpolation

AMG based on assumptions about slow-to-converge errors

What if we don’t know what to assume?

A. Brandt and D. Ron, in *Multilevel Optimization in VLSICAD*, 2003
M. Brezina et al., SISC 2004, **25**:1896-1920; SISC 2006, **27**:1261-1286
Calibrating Interpolation

AMG based on assumptions about slow-to-converge errors

What if we don’t know what to assume?

Run relaxation to find out!

- Run relaxation on $Ax = 0$ with a random initial guess
- This exposes the local character of slow-to-converge errors
- Use resulting vector as a prototype of errors to be corrected by interpolation within algebraic multigrid

Adapt AMG interpolation based on true performance of relaxation

A. Brandt and D. Ron, in *Multilevel Optimization in VLSICAD*, 2003
Controlling Adaptation

- Two possible sources of slow adaptive MG convergence
  - Prototype is a bad representative error
  - Prototype is good, but there is distinct slow-to-converge error
- Want a measure to distinguish cause of bad performance

Use estimates of $\|I - B^{-1}A\|$ to measure both performance and quality of prototype sets

- Estimate $\lambda_{\text{min}}(B^{-1}A)$ using Rayleigh Quotients
Adaptive Algorithm

While $\| I - B_{\text{MG}}^{-1} A \|_{\text{est}}$ is large

- if $\| I - B_{\text{rel}}^{-1} A \|_{\text{est}}$ is increasing
  - iterate on $Ax = 0$ with “relaxation”, $x \leftarrow (I - B_{\text{rel}}^{-1} A)x$
  - recalibrate interpolation based on new $x$
  - recompute coarse-grid operator
  - restrict $x$ to coarse grid and cycle there
  - interpolate further improved $x$ after coarse-grid cycle

- else
  - Replace “relaxation” with multigrid cycle: $B_{\text{rel}} \leftarrow B_{\text{MG}}$
## Effect of Adaptivity

### AMG Convergence Factors

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</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>0.024</td>
<td>0.039</td>
<td>0.036</td>
<td>0.034</td>
</tr>
<tr>
<td>$10^{-1}$</td>
<td>0.197</td>
<td>0.311</td>
<td>0.328</td>
<td>0.294</td>
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<tr>
<td>$10^{-2}$</td>
<td>0.414</td>
<td>0.446</td>
<td>0.488</td>
<td>0.550</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>0.587</td>
<td>0.527</td>
<td>0.542</td>
<td>0.630</td>
</tr>
<tr>
<td>$10^{-4}$</td>
<td>0.626</td>
<td>0.557</td>
<td>0.477</td>
<td>0.586</td>
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**Effect of Adaptivity**

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<td>13</td>
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</table>
Cost of Adaptivity

Extra relaxations pay off with multiple RHS

![Graph showing the log of the norm of the residual vs iterations for different methods.](Image)

- **Geometric MG**
- **AMG**
- **Adaptive AMG**
Cost of Adaptivity

Extra relaxations pay off with multiple RHS

![Graph showing the cost of adaptivity with multiple RHS](image)
Optimising Adaptivity

Large parameter space to search

- Relaxation on $Ax = 0$ is cheap
- Constructing coarse grids is expense
- Ability of relaxation to improve prototype diminishes
- Coarse-grid correction significantly improves prototype

Relax until performance slows, then coarsen
Optimising Adaptivity

Large parameter space to search

- Relaxation on $Ax = 0$ is cheap
- Constructing coarse grids is expense
- Ability of relaxation to improve prototype diminishes
- Coarse-grid correction significantly improves prototype

Relax until performance slows, then coarsen

Difficult to optimise due to problem-dependent behaviour
Final challenge: attack full 4D system

\[
\begin{pmatrix}
-\frac{1}{2h} D^2 - ml_3 & 0 & \imath D_3 - D_4 & \imath D_1 - D_2 \\
0 & -\frac{1}{2h} D^2 - ml_3 & \imath D_1 + D_2 & -\imath D_3 - D_4 \\
-\imath D_3 - D_4 & -\imath D_1 + D_2 & -\frac{1}{2h} D^2 - ml_3 & 0 \\
-\imath D_1 - D_2 & \imath D_3 - D_4 & 0 & -\frac{1}{2h} D^2 - ml_3
\end{pmatrix}
\]

where \( D_\mu = l_3 \partial_\mu - iA_\mu \), \( D^2 = \sum_\mu D_\mu^2 \)
Full Physics

Final challenge: attack full 4D system

\[
\begin{pmatrix}
-\frac{1}{2h}D^2 - ml_3 & 0 & \imath D_3 - D_4 & \imath D_1 - D_2 \\
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-\imath D_1 - D_2 & \imath D_3 - D_4 & 0 & -\frac{1}{2h}D^2 - ml_3
\end{pmatrix}
\]

where \( D_\mu = l_3 \partial_\mu - iA_\mu \), \( D^2 = \sum_\mu D_\mu^2 \)

Half step: 2D System:

\[
\begin{pmatrix}
-\frac{1}{2h}D^2 - ml_3 & \imath D_1 - D_2 \\
-\imath D_1 - D_2 & -\frac{1}{2h}D^2 - ml_3
\end{pmatrix}
\]
**Brute Force Approach**

- Adaptive smoothed aggregation multigrid
- Solve equivalent real form of $\tilde{M}^*\tilde{M}$
- $128 \times 128$ periodic lattice

### Average residual reduction per iteration

<table>
<thead>
<tr>
<th>$\lambda_{\min}(\tilde{M})$</th>
<th>Diagonal-PCG</th>
<th>AdaptiveMG-PCG</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>0.1</td>
<td>0.05</td>
</tr>
<tr>
<td>0.3</td>
<td>0.1</td>
<td>0.05</td>
</tr>
<tr>
<td>0.2</td>
<td>0.83</td>
<td>0.92</td>
</tr>
<tr>
<td>0.3</td>
<td>0.96</td>
<td>0.99</td>
</tr>
<tr>
<td>0.5</td>
<td>0.94</td>
<td>0.99</td>
</tr>
</tbody>
</table>

Adaptive MG setup time: 13.7 seconds
Adaptive MG-PCG solve time: 0.8 seconds
Diagonal-PCG solve time: 4.7 seconds

J. Brannick et al., to appear in *Proc. DD16*, 2007
Brute Force Approach

- Adaptive smoothed aggregation multigrid
- Solve equivalent real form of $\tilde{M}^*\tilde{M}$
- $128 \times 128$ periodic lattice

Average residual reduction per iteration

| $\lambda_{\text{min}}(\tilde{M})$ | Diagonal-PCG | | | | | AdaptiveMG-PCG | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 0.3 | 0.1 | 0.05 | 0.01 | 0.3 | 0.1 | 0.05 | 0.01 |
| $\beta \approx 0.2$ | 0.83 | 0.92 | 0.96 | 0.99 | 0.28 | 0.29 | 0.31 | 0.31 |
| $\beta \approx 0.3$ | 0.86 | 0.93 | 0.97 | 0.98 | 0.31 | 0.40 | 0.42 | 0.42 |
| $\beta \approx 0.5$ | 0.85 | 0.94 | 0.96 | 0.99 | 0.31 | 0.31 | 0.31 | 0.33 |

Adaptive MG setup time: 13.7 seconds
Adaptive MG-PCG solve time: 0.8 seconds
Diagonal-PCG solve time: 4.7 seconds

J. Brannick et al., to appear in *Proc. DD16, 2007*
Relaxation on $MM^*$

Equivalent real form of $M^*M$ expensive:

- Real form doubles needed storage
- Real form hides complex structure
- $M^*M$ (or $MM^*$) much denser than $M$

**Advantage:** Structure of $MM^*$ more amenable to multigrid

\[
(MM^*)_{jj} = -D^2 + \left(-\frac{1}{2h}D^2 - ml_3 \right)^2
\]

\[
(MM^*)_{jk} \rightarrow \text{lower-order terms for } j \neq k
\]
Hybrid approach

Implicitly relax on $MM^*$, but coarsen based on $M$

- Kaczmarz relaxation on $M$
- No need to compute or store $MM^*$
- Slow to converge components dominated by $D^2$
- Use adaptive AMG to design effective coarse-grid correction
Summary

- QCD attempts to explain strong force
- Numerical simulation requires many matrix solves
- Matrices are heterogeneous, but structured
- MG/AMG naturally handles some challenges
- Adaptive AMG key to addressing mass shift
- **Key Question**: most efficient setup approach
- Generalization to full physics underway