Algebraic Multigrid Methods for Complex-Valued Systems

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Complex-Valued Systems

Many applications lead to complex-valued linear systems

- Fourier-domain wave propagation

$$u_{tt} + \alpha u_t = c^2 \Delta u \Rightarrow -c^2 \Delta \hat{u} + \imath \alpha k \hat{u} - k^2 \hat{u} = 0$$

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- Schrödinger equation
- Quantum dynamics
- Maxwell equations
- Conformal mapping
- Structural dynamics

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How do we solve these problems efficiently?

Krylov Techniques

Core numerical linear algebra easily extends to complex case

- Orthogonality conditions still apply
- Hermitian PD matrices give inner products and norms

Major Krylov methods extend trivially

- GMRES
- BiCG/CGS/BiCGStab
- CG (for Hermitian PD systems)

Other techniques specifically aimed at complex systems

- QMR

Freund, SISC 1992, **13**:425:448

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Simple preconditioners extend easily

- Diagonal Scaling
- ILU

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- MG & DD for Helmholtz equation
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What about AMG?

Equivalent Real Forms

Rewrite the complex system $A\mathbf{u} = \mathbf{b}$ as

$$\begin{bmatrix} A^{(R)} & -A^{(I)} \\ A^{(I)} & A^{(R)} \end{bmatrix} \begin{bmatrix} \mathbf{u}^{(R)} \\ \mathbf{u}^{(I)} \end{bmatrix} = \begin{bmatrix} \mathbf{b}^{(R)} \\ \mathbf{b}^{(I)} \end{bmatrix}.$$

Now apply standard algebraic preconditioner to real form

- ILU
- Smoothed Aggregation

Day & Heroux, SISC 2001, **23**:480-498
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Disadvantages:

- Extra cost (double dimension and *nnz*)
- Lose structure

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Real AMG For Complex-Valued Problems

For many problems, real-valued part is dominant

$$-\Delta u + \imath k^2 u = f$$

Question: Why not ignore complex part?

- Apply AMG coarsening to $\Re(A)$
- Build interpolation based on $\Re(A)$
- Coarsen A as before, $A_c = P^T A P$

If a dominating real operator can be found, then preconditioning can be effective

Lahaye et al., IEEE Trans. Magn. 2000, **36**:1535-1538
Lahaye Ph.D. Thesis, KU-Leuven, 2001
Reitzinger et al., J. Comput. Appl. Math. 2003, **155**:405-421

Inherently Complex Operators

What if no dominating real matrix can be found?

Covariant Derivatives:

$$D_\mu \psi(\mathbf{x}) = e^{i\omega(\mathbf{x})} \partial_\mu \left(e^{-i\omega(\mathbf{x})} \psi(\mathbf{x}) \right)$$
$$D_\mu^2 \psi(\mathbf{x}) = e^{i\omega(\mathbf{x})} \partial_\mu^2 \left(e^{-i\omega(\mathbf{x})} \psi(\mathbf{x}) \right)$$

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Extend individual AMG components to naturally handle complex-valued systems

Interpolation

Expanding $A\mathbf{u} = \mathbf{b}$,

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Apply heuristic for real matrices:

Choose P based on symmetric part of $\hat{A}$

- If A is Hermitian, $\hat{A}$ is symmetric
- If A is complex-symmetric, base P on $A^{(R)}$

Dendy, Appl. Math. Comp. 1983 **13**:261-283

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- If A is complex-symmetric, base P on $A^{(R)}$
- If $B = \imath A$, interpolate differently for A and B

Dendy, Appl. Math. Comp. 1983 **13**:261-283

Another Point of View

Form of coarse-grid correction doesn't change

$$\mathbf{e}^{(\text{new})} = (I - PB_c^{-1}RA)\mathbf{e}^{(\text{old})}$$

Still need

- Complementary relaxation and coarse-grid correction
- Algebraically smooth errors in Range(P)

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Use classical AMG interpolation, just with complex values

Restriction

Choice of $R = P^T$ (or $R = P^\star$) no longer automatic

- Hermitian problems $\Rightarrow R = P^\star$
- Complex-symmetric problems $\Rightarrow R = P^T$
- Complex non-symmetric problems $\Rightarrow R =$???

Can justify many things...

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Can justify many things...
But don't want to stray too far from AMG

Adjoints

A may not define a norm, but $A^\star A$ does

Take $T = (I - M_2^{-1}A)(I - PB_c^{-1}RA)(I - M_1^{-1}A)$, then

$$\|T\|_{A^\star A} = \|(A^\star A)^{-1} T^\star (A^\star A)\|_{A^\star A}$$

Define the cycle for $A^\star$ by

$$\begin{aligned}\overline{T} &= \left(I - (M_1^{-1})^\star A^\star\right)\left(I - R^\star (B_c^{-1})^\star P^\star A^\star\right)\left(I - (M_2^{-1})^\star A^\star\right)\\ &= (A^\star)^{-1}\, T^\star A^\star\end{aligned}$$

Then $\|T\|_{A^\star A} = \|\overline{T}\|_2$

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$R^\star$ must be an effective interpolation operator for $A^\star$

Special Cases

- If $A = A^\star$, then can choose $R = P^\star$

$$\Rightarrow \text{ Variational Condition}$$

- If $A = A^T$, and interpolation preserves complex conjugation

$$\Rightarrow R = P^T, \text{ also Variational}$$

Otherwise, compute restriction separately from interpolation

We always use $R = P^\star(A^\star)$

Coarse-Grid Selection

Still use strength-of-connection measure

$$S_i = \{j : |a_{ij}| \geq \theta \max_{k \neq i} |a_{ik}|\}$$

Then

- Independent set over graph of strong connections
- Second pass to ensure good AMG interpolation possible

Easy to extend many coarsening schemes, but what makes most sense?

Relaxation

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

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

If A is an H-matrix, then

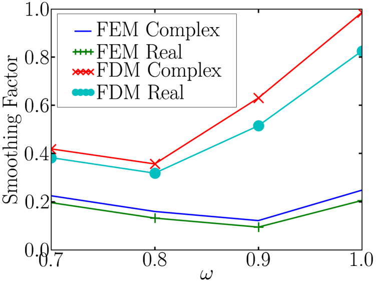
- Jacobi converges for A at least as fast as for $\mathcal{M}(A)$
- Weighted Jacobi converges for all $\omega \leq 1$
- SOR converges for all $\omega \leq 1$

Varga, Linear Algebra and Appl. 1976, **13**:1-9

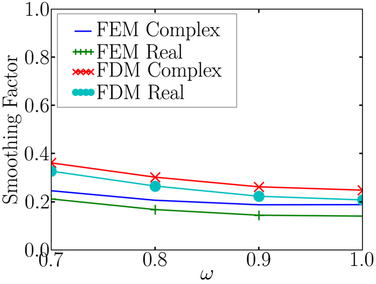
What About Smoothing?

Convergence theory says nothing about smoothing properties

Use local Fourier analysis (LFA) for $-\Delta u + \alpha u$, $\alpha = k^2, k^2\imath$



Jacobi



Gauss-Seidel

Time-Harmonic Maxwell Equations

Reduce Maxwell's equations by assuming:

- linear constitutive laws
- low-frequency excitation
- 2D cross-section

$$\Rightarrow -\nabla \cdot \left(\frac{1}{\mu} \nabla \hat{A}_z \right) + \imath\omega\sigma\hat{A}_z = \hat{J}_{s,z}$$

for Fourier-domain potential, $\hat{A} = (0, 0, \hat{A}_z)^T$

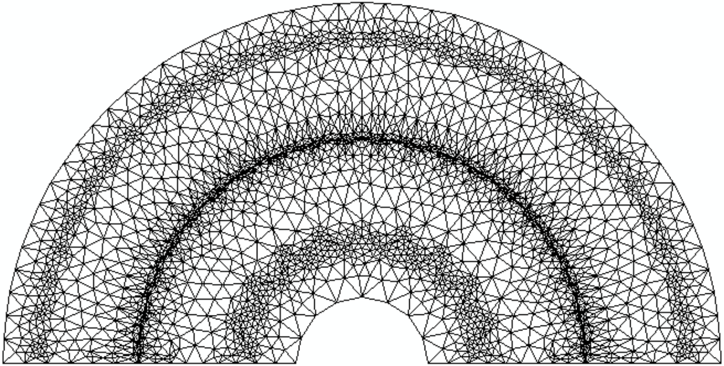
Lahaye et al., IEEE Trans. Magn. 2000, **36**:1535-1538

Induction Motor

Solve

$$-\nabla \cdot \left(\frac{1}{\mu} \nabla \hat{A}_z \right) + \imath \omega \sigma \hat{A}_z = \hat{J}_{s,z}$$

on annular geometry



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AMG Performance

Problem	Solver	c_A	t_{setup}	t_{solve}	# Iters.
15302 nodes $nnz = 104926$	real AMG	2.86	0.1	0.6	29
	complex AMG	2.85	0.2	0.7	32
	AMG-BiCGStab	2.86	0.1	0.4	9
	cAMG-BiCGStab	2.85	0.2	0.3	8
34555 nodes $nnz = 239661$	real AMG	2.91	0.4	1.7	31
	complex AMG	2.91	0.4	1.7	30
	AMG-BiCGStab	2.91	0.4	1.0	8.5
	cAMG-BiCGStab	2.91	0.4	1.0	8.5
75951 nodes $nnz = 529317$	real AMG	2.87	1.0	4.5	31
	complex AMG	2.87	1.1	4.2	29
	AMG-BiCGStab	2.87	1.0	2.6	8.5
	cAMG-BiCGStab	2.87	1.1	2.5	8

Lattice Gauge Theory

Gauge theories model physics at quantum scales

Lattice gauge theory is discrete form of standard model

- Model of interactions between elementary particles
- Includes electromagnetism, weak force, strong force
- Consistent with known particle accelerator experiments

Goal: Use simulation to predict behavior out of reach of experiment

Covariant Laplacian

Conservation laws play important role in gauge theory

- Derivatives are always covariant

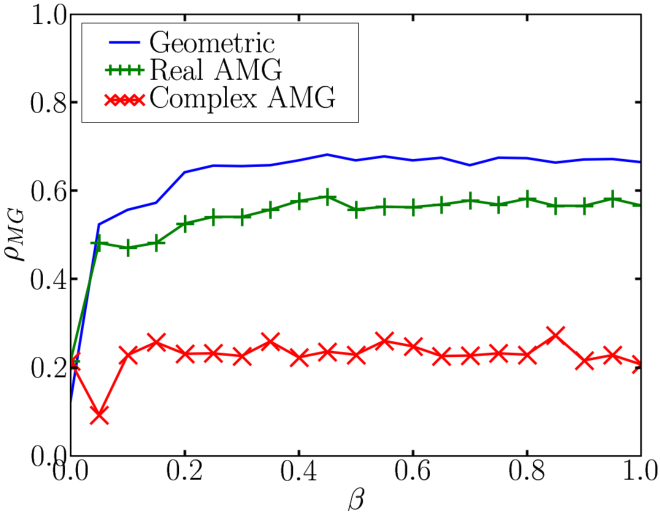
$$D_\mu \psi(\mathbf{x}) = e^{i\omega(\mathbf{x})} \partial_\mu \left(e^{-i\omega(\mathbf{x})} \psi(\mathbf{x}) \right)$$

- Discretizations are always consistent

Model Problem: Covariant Laplacian

$$\sum_\mu D_\mu^2 \psi(\mathbf{x}) \Rightarrow \begin{bmatrix} & -e^{i\beta\phi(\mathbf{x})} & \\ -e^{-i\beta\theta(\mathbf{x}-\binom{1}{0})} & 4 & -e^{i\beta\theta(\mathbf{x})} \\ & -e^{-i\beta\phi(\mathbf{x}-\binom{0}{1})} & \end{bmatrix}$$

Convergence



Shifted Covariant Laplacian

Two reasons to consider shifting

- As β increases, discrete problem becomes better conditioned
- Physical operators always appear with negative-definite shift

$$\sum_{\mu} D_{\mu}^2\psi - m^2\psi \Rightarrow \begin{bmatrix} & -e^{i\beta\phi(\mathbf{x})} & \\ -e^{-i\beta\theta(\mathbf{x}-\left(\begin{smallmatrix}1\\0\end{smallmatrix}\right))} & 4-m^2 & -e^{i\beta\theta(\mathbf{x})} \\ & -e^{-i\beta\phi(\mathbf{x}-\left(\begin{smallmatrix}0\\1\end{smallmatrix}\right))} & \end{bmatrix}$$

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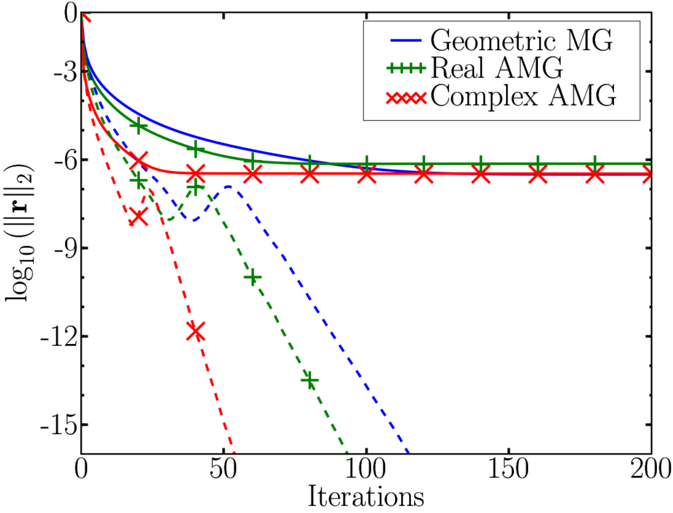
Shifting changes energy but not form of algebraically smooth errors

Convergence histories



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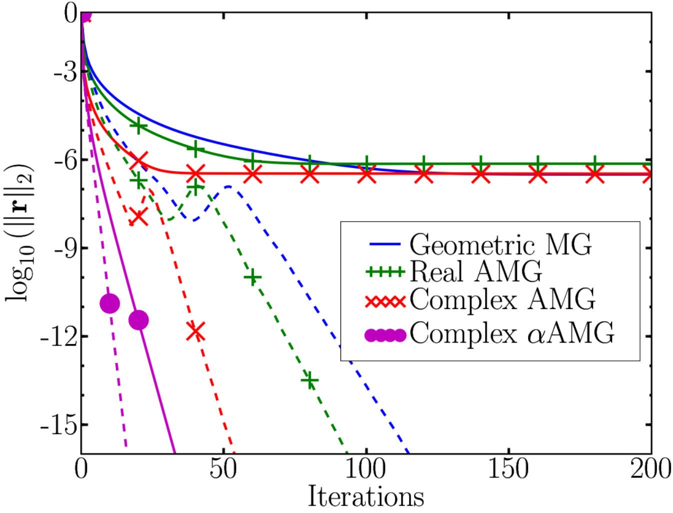

Summary

- Natural extension of AMG to complex arithmetic
- Consistent choice of restriction for special cases
- Local Fourier analysis confirms algorithmic choices
- Performance similar to real AMG for complex problems

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Future Work

- Better understand coarse-grid selection (real and complex)
- Extend to systems, distributed relaxation
- Provide solvers for quantum dynamical simulation