A new level-dependent coarsegrid correction scheme for indefinite Helmholtz problems

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European Multigrid Conference, Leuven, 8-12 September 2014

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Outline

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Introducing the Helmholtz equation

Story of a Helmholtz preconditioner

A level-dependent coarse grid correction scheme

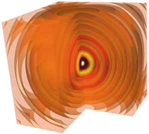
Numerical results and scalability

The Helmholtz equation

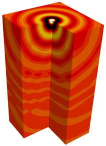
$$-\left[\triangle + k(\vec{x})^2\right]\psi(\vec{x}) = \chi(\vec{x}) \; in \; \Omega \subseteq \mathbb{R}^d. \qquad (1)$$

Application area:

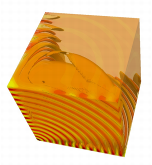
- Numerical solution of scattering models
- Usually solved for inverse problems (forward problem)
- E.g. radars, seismic exploration, quantum-mechanical break-up problems (cf. Schrödinger equation), ...



Homogeneous medium



Wedge problem

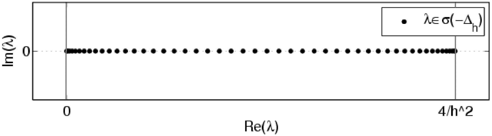


Coulomb problem

The Helmholtz equation

$$-\left[\Delta + k(\vec{x})^2\right]\psi(\vec{x}) = \chi(\vec{x}) \textit{ in } \Omega \subseteq \mathbb{R}^d. \quad (1)$$

If $k = 0$ then (1) reduces to a positive definite Poisson problem.



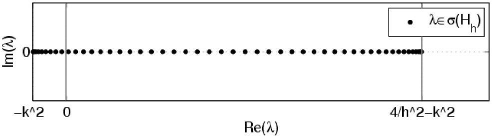
Easy to solve with most numerical methods e.g.

- Krylov subspace methods
- ILU factorization
- Geometric/algebraic multigrid
- Domain decomposition

The Helmholtz equation

$$-\left[\triangle + k(\vec{x})^2\right]\psi(\vec{x}) = \chi(\vec{x}) \text{ in } \Omega \subseteq \mathbb{R}^d. \qquad (1)$$

If $k \neq 0$ then (1) can become indefinite.



Hard to solve with most numerical methods e.g.

- Krylov subspace methods [Elman Ernst O'Leary 2001]
- ILU factorization [Gander Nataf 2005]
- Geometric/algebraic multigrid [Erlangga Vuik Oosterlee 2006]
- Domain decomposition [Engquist Ying 2011]

Outline

Preconditioned Krylov methods

Solve (1) *using Krylov methods, with preconditioner*

$$\mathcal{M} = -\triangle - \gamma k(\vec{x})^2$$

for $\mathcal{H} = -\triangle - k(\vec{x})^2$, *with* $\mathcal{M}u = f$ *easily solvable iteratively.*

- $\gamma = 1$: original Helmholtz operator
  [von Helmholtz 19th century]
- $\gamma = 0$: Laplacian
  [Bayliss Goldstein Turkel 1983]
- $\gamma < 0$: shifted Laplacian or screened Poisson operator
  [Laird 2001]
- $\gamma \in \mathbb{C}$: complex shifted Laplacian (CSL): $\gamma = \alpha + \beta i$
  [Erlangga Vuik Oosterlee 2004]

Complex shifted Laplacian (CSL)

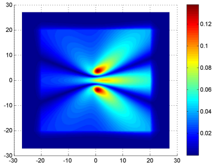
Physical interpretation. Complex shift β induces damping

$\rightarrow$ smooth modes of $\mathcal{H}$ represented accurately by $\mathcal{M}_{CSL}$,

$\rightarrow$ oscillatory modes of $\mathcal{H}$ damped in $\mathcal{M}_{CSL}$.

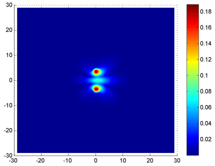
Original Helmholtz operator

$$\mathcal{H} = -\triangle - k(\vec{x})^2$$



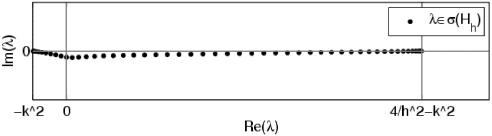
Complex shifted Laplacian

$$\mathcal{M}_{CSL} = -\triangle - \gamma k(\vec{x})^2$$

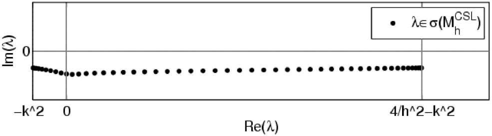


Complex shifted Laplacian (CSL)

Spectral interpretation. Let L^h be the discretization matrix of the *negative* Laplacian $-\Delta$ with eigenvalues λ_L^h. If $k(\vec{x}) = k$ constant then the eigenvalues of M_{CSL}^h and H^h are:



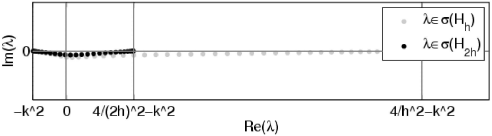
Helmholtz $\lambda^h = \lambda_L^h - k^2$



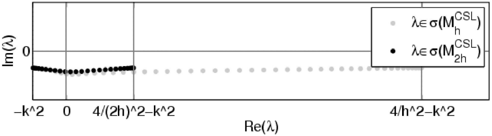
Complex shifted Laplacian $\lambda^h = \lambda_L^h - \gamma k^2$

Complex shifted Laplacian (CSL)

Spectral interpretation. Let L^{2h} be the discretization matrix of the *negative* Laplacian $-\Delta$ with eigenvalues λ_L^{2h}. If $k(\vec{x}) = k$ constant then the eigenvalues of M_{CSL}^{2h} and H^{2h} are:



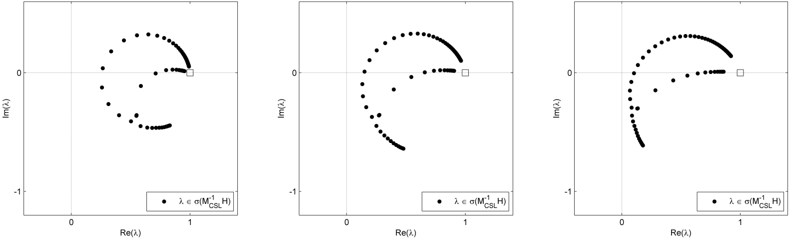
Helmholtz $\lambda^{2h} = \lambda_L^{2h} - k^2$



Complex shifted Laplacian $\lambda^{2h} = \lambda_L^{2h} - \gamma k^2$

Complex shifted Laplacian (CSL)

Spectral interpretation. Let L^h be the discretization matrix of the *negative* Laplacian $-\Delta$ with eigenvalues λ_L^h. If $k(\vec{x}) = k$ constant then the eigenvalues of M_{CSL}^h and H^h are related as:



$\beta = 0.25$ $\beta = 0.50$ $\beta = 0.75$

Preconditioned system $\lambda^h = \frac{\lambda_L^h - k^2}{\lambda_L^h - \gamma k^2}$

Complex shifted Laplacian (CSL)

The Helmholtz equation (1) can be solved numerically with a M_{CSL}-preconditioned Krylov subspace method

Observation 1. *MG preconditioner*

The larger the shift β the better the MG convergence.

Observation 2. *Krylov solver*

The smaller the shift β the better $\kappa(M_{CSL}^{-1}H)$.

Choice of the shift parameter is compromise between 1. and 2.

$\gamma \approx 1 + 0.5i$ optimal for both MG [Erlangga et al. 2006] [Cools Vanroose 2013] and DDM [Kimn Sarkis 2011] [Shanks et al. 2013].

Outline

Two-grid analysis

Two-grid analysis for coarsegrid correction scheme:

$$\mathbf{e}^h - P\mathbf{e}^{2h} \approx \mathbf{v}^h - \frac{\lambda^h}{\lambda^{2h}} PR\mathbf{v}^h = \left(1 - \frac{\lambda^h}{\lambda^{2h}}\right)\mathbf{v}^h$$

with $\lambda^h \in \sigma(A^h)$ and $\mathbf{v}^h$ a smooth eigenvector.

[Brandt 1986] [Elman Ernst O'Leary 2001]

Coarsegrid correction cancels out smooth modes if

$$\left|1 - \frac{\lambda_L^h - k^2}{\lambda_L^{2h} - k^2}\right| < 1,$$

for indefinite Helmholtz, with $\lambda_L > 0$.

Two-grid analysis

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$$\left|1 - \frac{\lambda_L^h - \gamma k^2}{\lambda_L^{2h} - \gamma k^2}\right| < 1,$$

for complex shifted Laplacian, with $\lambda_L > 0$.

Two-grid analysis

When exactly do we violate

$$\left| 1 - \frac{\lambda_L^h - k^2}{\lambda_L^{2h} - k^2} \right| < 1$$

for the indefinite Helmholtz operator?

- Most problematic when $\lambda_L^{2h} - k^2 \approx 0$.
- Instability only occurs on few intermediate levels, so replace standard smoother on those levels by GMRES(m), damping a broader range of eigenmodes.

  [Elman et al. 2001] [Calandra et al. 2011] [Reps et al. 2013].
- Use MG on complex shifted Laplace system on all levels, s.t. $\lambda_L^{lh} - \gamma k^2 \neq 0$ $(\forall l)$.

  [Erlangga et al. 2006]

Motivation

Observations:

(1) MG works like a charm on the CSL system (all levels), but does not solve the original Helmholtz equation.

MG as preconditioner only

(2) MG instability occurs only on some intermediate levels, i.e. where $\lambda_L^{lh} - k^2 \approx 0$.

$\Downarrow$

Key idea:

Level-dependent MG scheme, with gradually increasing complex shift throughout the level hierarchy.

A level-dependent shift

Assume a level-dependent complex shift (*)

$$\gamma_h = e^{i\theta_h},$$

with $\theta_h \in [0, 2\pi]$, thus
$$H^h = L^h - e^{i\theta_h} k^2$$
$$H^{2h} = L^{2h} - e^{i\theta_{2h}} k^2$$

Analogue two-grid analysis leads to the requirement

$$\left| 1 - \frac{\lambda_L^h - e^{i\theta_h} k^2}{\lambda_L^{2h} - e^{i\theta_{2h}} k^2} \right| < 1.$$

$$\Big\downarrow \text{ smooth modes } \lambda_L \ll k^2$$

$$\left| 1 - e^{i(\theta_h - \theta_{2h})} \right|$$

(*) Other choices possible, e.g. $\gamma_h = 1 + \beta_h i$ with $\beta_h \in \mathbb{R}$.

A level-dependent shift

Coarsegrid correction scheme:

$$\left|1 - \frac{\lambda_L^h - e^{i\theta_h}k^2}{\lambda_L^{2h} - e^{i\theta_{2h}}k^2}\right| \approx \underbrace{\left|1 - e^{i(\theta_h - \theta_{2h})}\right| \approx 0}_{(\text{if } \theta_h \approx \theta_{2h})}$$

- If $\theta_h = \theta_{2h}$ then classical complex shifted Laplacian.
- If $0 < \theta_h - \theta_{2h} < \delta$ then an additional error is introduced, yet arbitrary small and oscillatory (see next slide).
- If $\theta_h = 0$ then original Helmholtz eqn. is solved on fine grid

MG as Helmholtz solver

E.g. choose $\gamma_h = e^{i\theta_h} = e^{i\, level\, d\theta}$, with uniform shift increment $d\theta$.

A level-dependent shift

Correction step: $\mathbf{x}^h = \mathbf{x}^h + P\tilde{\mathbf{e}}^{2h}$

$\swarrow$ $\searrow$

Solution to $A^h \mathbf{x}^h = \mathbf{f}^h$ with $\lambda^h = \lambda_L^h - e^{i\theta_h} k^2$	Solution to $\tilde{A}^{2h} \tilde{\mathbf{e}}^{2h} = \mathbf{r}^{2h}$ with $\lambda^{2h} = \lambda_L^{2h} - e^{i\theta_{2h}} k^2$

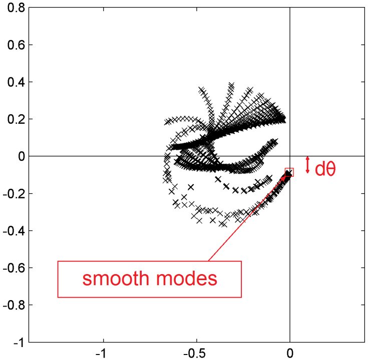
Characterization:

$$\begin{aligned}\tilde{\mathbf{e}}^{2h} &= \mathbf{e}^{2h} + (\tilde{A}^{2h})^{-1}(A^{2h} - \tilde{A}^{2h})\,\mathbf{e}^{2h} \\ &= \mathbf{e}^{2h} + \mathbf{q}^{2h} \rightarrow \text{unwanted error!}\end{aligned}$$

Writing $\mathbf{e}^{2h} = \sum_i a_i \, \mathbf{v}_i^{2h}$ (with $\mathbf{v}_i^{2h}$ eigenmodes), we obtain

$$\mathbf{q}^{2h} = \sum_i a_i \left(\frac{\lambda_i^{2h} - \tilde{\lambda}_i^{2h}}{\tilde{\lambda}_i^{2h}} \right) \mathbf{v}_i^{2h}.$$

A level-dependent shift



$$\frac{\lambda^{2h} - \tilde{\lambda}^{2h}}{\tilde{\lambda}^{2h}} = \frac{k^2(e^{id\theta} - 1)}{\lambda_L^{2h} - k^2 e^{id\theta}}$$

$$\mathbf{q}^{2h} = \sum_i a_i \left(\frac{\lambda^{2h} - \tilde{\lambda}^{2h}}{\tilde{\lambda}^{2h}} \right)_i \mathbf{v}_i^{2h}$$

Only oscillatory eigenmodes contribute to the unwanted error $\mathbf{q}^{2h}$!

$\Downarrow$ V(1,1)-cycle

The correction step error $\mathbf{q}^{2h}$ is eliminated by post-smoothing.

Denote $d\theta = |\theta^h - \theta^{2h}|$.

Outline

Numerical results

N-scalability

$n_x \times n_y$	128^2	256^2	512^2	1024^2	2048^2
L-MG iter	57	39	40	40	43
CPU total	6.26	19.99	86.45	357.2	1552
CPU/1000 pts	0.38	0.31	0.33	0.34	0.37

Number of iterations and CPU timings (in s.).

- 2D constant-k problem: $k(\vec{x}) = k_0 = 80$
- Sommerfeld BCs [Sommerfeld 1949]
- GMRES(3) as smoother substitute

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Numerical results

k_0	20	40	80	160	320
$n_x \times n_y$	32^2	64^2	128^2	256^2	512^2
MG-FGMRES	19 (0.37)	29 (1.20)	53 (8.09)	106 (125)	204 (**1605**)
MG-FGMRES(10)	21 (0.38)	30 (1.13)	62 (7.48)	125 (73)	249 (**625**)
L-MG-FGMRES	19 (0.25)	30 (1.11)	52 (7.73)	97 (112)	196 (1541)
L-MG-FGMRES(10)	20 (0.25)	31 (1.04)	58 (6.88)	117 (69)	220 (586)
L-MG	22 (0.37)	33 (1.12)	57 (6.26)	111 (57)	224 (**488**)

Number of iterations and CPU timings (in s.).

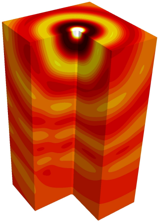
- 2D constant-k problem: $k(\vec{x}) = k_0$
- ECS BCs [Aguilar et al. 1971] cf. PML [Berenger 1994]
- GMRES(3) as smoother substitute

Numerical results

f	12	14	16	18	20
$n_x \times n_y \times n_z$			$64 \times 128 \times 64$		
MG-FGMRES	34 (294)	39 (354)	45 (430)	53 (541)	60 (**645**)
MG-FGMRES(10)	35 (234)	40 (269)	47 (315)	55 (369)	62 (**416**)
L-MG	38 (191)	46 (232)	50 (252)	58 (293)	71 (**356**)

Number of iterations and CPU timings (in s.).

- 3D wedge problem: $k(\vec{x}) = (2\pi f)/c(\vec{x})$
- ECS BCs
- GMRES(3) as smoother substitute

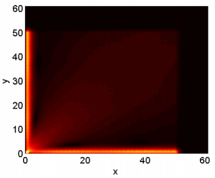


Numerical results

k_0 $n_x \times n_y$	1 128^2	2 256^2	3 256^2	4 512^2	5 512^2
MG-FGMRES	51 (5.40)	92 (46.8)	191 (137)	174 (813)	306 (**2185**)
MG-FGMRES(10)	66 (5.52)	140 (46.7)	245 (81.3)	250 (421)	393 (**661**)
MG-FGMRES(30)	52 (4.86)	93 (34.7)	226 (83.2)	278 (565)	426 (**867**)
L-MG	44 (3.42)	83 (25.3)	208 (63.5)	149 (215)	289 (**418**)

Number of iterations and CPU timings (in s.).

- 2D ionization: $k^2(\vec{x}) = e^{-x^2} + e^{-y^2} + k_0^2$
- Dirichlet (S-W) & ECS (N-E) BCs
- GMRES(3) as smoother substitute



Conclusions

- Complex shifted Laplacian (CSL) is useful preconditioner
  - choice of shift parameter γ is trade-off between preconditioning quality and efficient inversion
- Proposed a new level-dependent coarsegrid correction
  - solve original Helmholtz equation on finest grid
  - gradually increasing shift allows smaller shift on finer levels
  - use sufficiently large shift on problematic levels
- Two-grid analysis
  - level-dependent correction introduces additional error
    $\Rightarrow$ can be tuned arbitrary small and is oscillatory
    $\Rightarrow$ removed by (post-)smoother
  - naive level-dependency scheme could be improved with deeper analysis (future work)

References

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Key publication for this talk:

[1] Cools, Reps, Vanroose. *A new level-dependent coarse grid correction scheme for indefinite Helmholtz problems.* Num. Lin. Alg. with Applications (2014).

Related literature:

[2] Erlangga, Oosterlee, Vuik. *On a class of preconditioners for solving the Helmholtz equation.* Applied Numerical Mathematics (2004).

[3] Elman, Ernst, O'Leary. *A multigrid method enhanced by Krylov subspace iteration for discrete Helmholtz equations.* SIAM J. Sci. Comput. (2002).

[4] Ernst, Gander. *Why it is difficult to solve Helmholtz problems with classical iterative methods.* Lecture Notes in Comput. Sci. and Engineering (2012).

[5] Reps, Vanroose, bin Zubair. *On the indefinite Helmholtz equation: Complex stretched absorbing boundary layers, iterative analysis, and preconditioning.* J. Comput. Physics (2010).