Multigrid methods for wave scattering problems governed by the Helmholtz and Schrödinger equation

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What's in a name (or PhD title) ?

"If people do not believe that mathematics is simple, it is only because they do not realize how complicated life is."

John Louis von Neumann, 20th century

Multigrid methods . . .

for wave scattering problems . . .

governed by the Helmholtz . . .

and Schrödinger equation.

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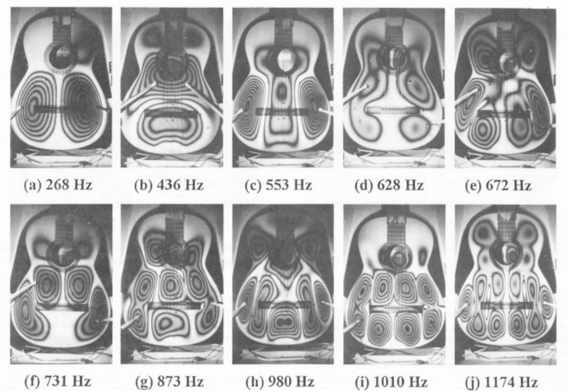
and Schrödinger equation.

The wave equation

Some examples from everyday life

Acoustics: vibrations in a guitar sound box.

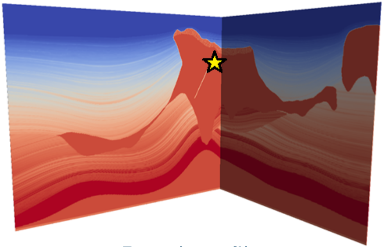


Source: *Music, Physics and Engineering*, H.F. Olson (1967)

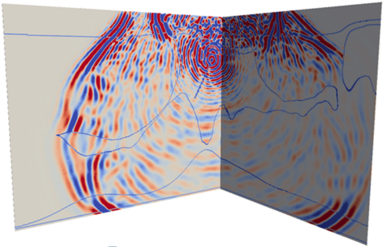
The wave equation

Some examples from everyday life

Seismics: propagation of waves through the subsurface.



3D soil profile



3D wave pattern

Source: *Seismic Wave Propagation and Scattering in the Heterogeneous Earth*, H. Sato, M.C. Fehler & T. Maeda (2008)

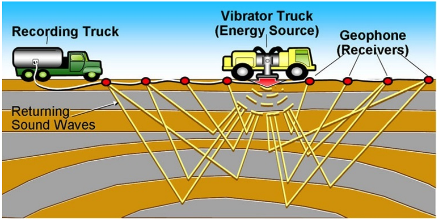
Practical use: earthquake prediction.

The wave equation

Some examples from everyday life

Seismics: exploration of the subsurface.

Vibrator truck



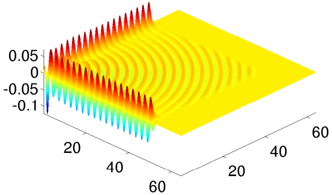
Seismic exploration

Source: Gallego Technic Geophysics & Chesapeake Energy Corporation.

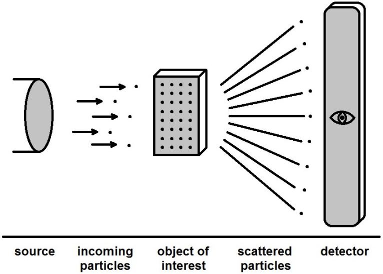
Practical use:

The wave equation
Some examples from everyday life

Quantum mechanics: molecular break-up reactions.



Electron wave character

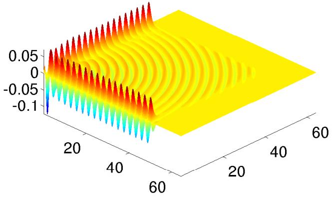


Schematic representation

Practical use: determine material composition & structure.

The wave equation
Some examples from everyday life

Quantum mechanics: molecular break-up reactions.



Electron wave character

CERN Large Hadron Collider

Practical use: determine material composition & structure.

What's in a name (or PhD title) ?

"Mathematics is the most beautiful and most powerful creation of the human spirit."

Stefan Banach, 20th century

Multigrid methods . . .

for wave scattering problems . . .

governed by the Helmholtz . . .

and Schrödinger equation.

The Helmholtz equation

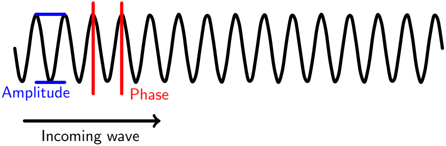
Mathematical description of waves

$$-\left[\triangle + k(\vec{x})^2\right] u(\vec{x}) = f(\vec{x}), \qquad \vec{x} \in \Omega \subseteq \mathbb{R}^d.$$

wavenumber *wave* *source*

Hermann von Helmholtz, 19th century

Partial differential equation (PDE),
time-independent wave eqn. with solution $u(\vec{x})$ of the form:



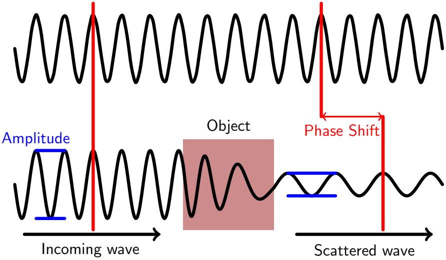
No object, scalar k
(simple wave pattern)

The Helmholtz equation

Mathematical description of waves

$$-\underbrace{\left[\triangle + k(\vec{x})^2\right]}_{\textit{wavenumber}} \underbrace{u(\vec{x})}_{\textit{wave}} = \underbrace{f(\vec{x})}_{\textit{source}}, \qquad \vec{x} \in \Omega \subseteq \mathbb{R}^d.$$

Hermann von Helmholtz, 19th century



Forward problem

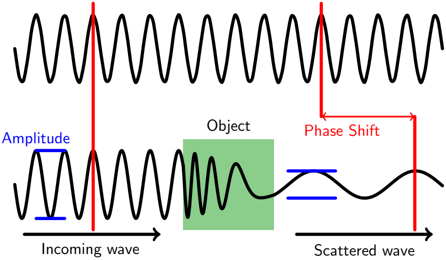
Object properties (materials)
$\Downarrow$ determine
Measurement data (amplitude/phase)

The Helmholtz equation

Mathematical description of waves

$$-\underset{\textit{wavenumber}}{\left[\triangle + k(\vec{x})^2\right]}\ \underset{\textit{wave}}{u(\vec{x})} = \underset{\textit{source}}{f(\vec{x})}, \qquad \vec{x} \in \Omega \subseteq \mathbb{R}^d.$$

Hermann von Helmholtz, 19th century



Inverse problem

Measurement data (amplitude/phase)

$\Downarrow$ determine

Object properties (materials)

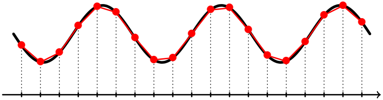
Discretization

From continuous to discrete representation

Computers cannot represent a realistic continuous wave

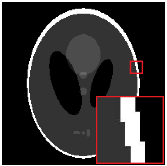
1D "points"

grid points

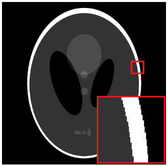


2D "pixels"

picture elements



200×200



1000×1000

3D "voxels"

volume pixels

Very large linear systems!

$(1000 \times 1000 \times 1000 = 1$ billion unknowns$)$

Discretization

From continuous to discrete representation

$$-\left[\triangle + k(\vec{x})^2\right] u(\vec{x}) = f(\vec{x}), \qquad \vec{x} \in \Omega \subseteq \mathbb{R}^d.$$

wavenumber *wave* *source*

Hermann von Helmholtz, 19th century

Discretization: $u = (u(x_1), u(x_2), \ldots, u(x_N))^T$

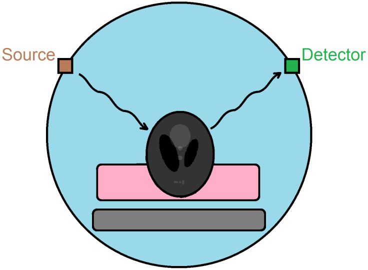
$$u''(x_i) = \frac{u(x_{i-1}) - 2u(x_i) + u(x_{i+1})}{h^2} \qquad (i = 1, \ldots, N)$$

System of linear equations: e.g.

$$\begin{pmatrix} -\frac{2}{h^2} + k(x_1)^2 & \frac{1}{h^2} & & \\ \frac{1}{h^2} & -\frac{2}{h^2} + k(x_2)^2 & \frac{1}{h^2} & \\ & \ddots & \ddots & \ddots \\ & & \frac{1}{h^2} & -\frac{2}{h^2} + k(x_N)^2 \end{pmatrix} \begin{pmatrix} u(x_1) \\ u(x_2) \\ \vdots \\ u(x_N) \end{pmatrix} = \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_N) \end{pmatrix} \quad \Leftrightarrow \quad Au = f$$

Helmholtz in medical physics

Computed Tomography (CT) or MRI scan



Waves = X-ray/Röntgen radiation

Object = patient

CT scan cross section

Modern CT devices: many detectors (data) & high resolution

Advanced numerical methods required

Numerical methods

Or why mathematicians are useful

CT scans have been used for years now...
Has this technology not been perfected?

Yes, Method 1

- in present-day hospitals:
  analytical techniques (1970)
  can't handle limited data
- algebraic techniques
  direct methods (LU) (1950)
  $\rightarrow$ slow for large systems
- You are waiting for your scanning results

Numerical methods

Or why mathematicians are useful

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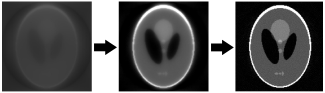
- You are waiting for your scanning results

But, Method 2

- my research area:
  iterative methods (1990)
- step-by-step correction



iteration 1 iteration 50 iteration 200

- Much faster solution possible

Numerical methods

Or why mathematicians are useful

Method 1
Direct methods

Method 2
Iterative methods

physical dimension	unknowns N	algorithm 1 $\mathcal{O}(N^2)$	algorithm 2 $\mathcal{O}(N)$
1D	1000	0.0001 sec.	0.1 sec.
2D	1000×1000	2 min.	2 min.
3D	$1000 \times 1000 \times 1000$	3 years ☹	28 hours ☺

Exemplary computational time required for reconstruction.

Full 3D reconstruction is the future

Roadmap

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[1] Introduction & motivation

[2] Story of a Helmholtz preconditioner

[3] A new level-dependent coarsegrid correction scheme **[Ch4]**

[4] The contour method for far field map calculation **[Ch5]**

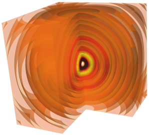
[5] Conclusions

The Helmholtz equation

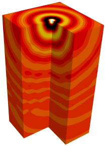
$$\left[-\triangle - k(\vec{x})^2\right] u(\vec{x}) = f(\vec{x}), \quad \vec{x} \in \Omega \subseteq \mathbb{R}^d. \qquad (1)$$

Application areas:

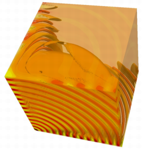
- Numerical simulation of scattering models
- Usually solved for inverse problems (forward problem)
- E.g. radar, seismic exploration, quantum-mechanical break-up problems (cf. Schrödinger equation).



Homogeneous medium



Wedge problem

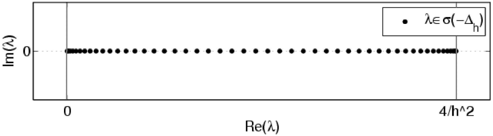


Coulomb problem

The Helmholtz equation

$$\left[-\triangle - k(\vec{x})^2\right] u(\vec{x}) = f(\vec{x}), \quad \vec{x} \in \Omega \subseteq \mathbb{R}^d. \qquad (1)$$

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



1D discretized Poisson operator Dirichlet B.C.

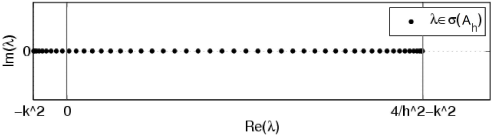
Easy to solve with most numerical methods e.g.

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

The Helmholtz equation

$$\left[-\triangle - k(\vec{x})^2\right] u(\vec{x}) = f(\vec{x}), \quad \vec{x} \in \Omega \subseteq \mathbb{R}^d. \tag{1}$$

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



1D discretized Helmholtz operator Dirichlet B.C.

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]

Preconditioned Krylov methods

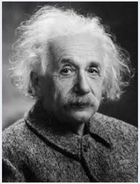
Solve $\mathcal{M}^{-1}\mathcal{A}u = \mathcal{M}^{-1}f$ *using Krylov methods, with*

$$\mathcal{M} = -\triangle - \varrho k(\vec{x})^2 \qquad \textit{(preconditioner)}$$

where $\mathcal{A} = -\triangle - k(\vec{x})^2$ *and* $\mathcal{M}u = f$ *easily solvable iteratively.*

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

What's in a name (or PhD title) ?



"No problem can be solved from the same level of consciousness that created it."

Albert Einstein, 20th century

Multigrid methods . . .

for wave scattering problems . . .

governed by the Helmholtz . . .

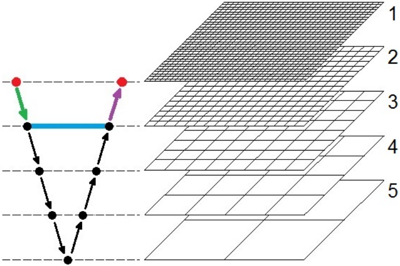
and Schrödinger equation.

The multigrid method

Two-grid correction scheme

- **Smooth** ν_1 times on $A^h v^h = f^h$ (e.g. ω-Jacobi, Gauss-Seidel, ...).
- ↘ **Restrict** $r^{2h} = I_h^{2h} r^h$, where $r^h = f^h - A^h v^h$.
- – **Solve** $A^{2h} e^{2h} = r^{2h}$ for e^{2h}.
- ↗ **Interpolate** $e^h = I_{2h}^h e^{2h}$ and correct $v^h \leftarrow v^h + e^h$.
- **Smooth** ν_2 times on $A^h v^h = f^h$.

Multigrid V-cycle = recursion



> Multigrid cannot solve Helmholtz equation, only CSL systems.
>
> [Ernst Gander 2012]

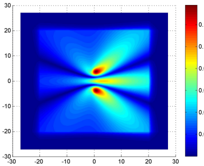
Complex shifted Laplacian

Physical interpretation. Complex shift β induces *damping*, i.e.

- smooth modes of $\mathcal{A}$ represented accurately by $\mathcal{M}_{CSL}$,
- oscillatory modes of $\mathcal{A}$ damped in $\mathcal{M}_{CSL}$.

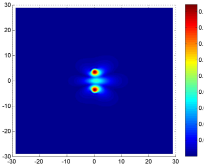
Original Helmholtz operator

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



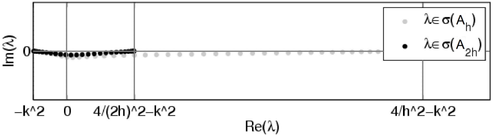
Complex shifted Laplacian

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



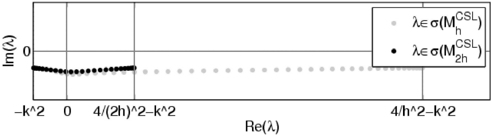
Complex shifted Laplacian

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 A^{2h} are:



1D discretized Helmholtz operator Sommerfeld B.C.

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

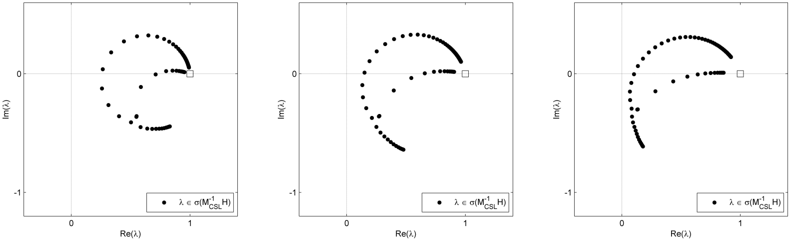


1D discretized CSL operator Sommerfeld B.C.

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

Complex shifted Laplacian

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 A^h are related as:



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

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

Roadmap

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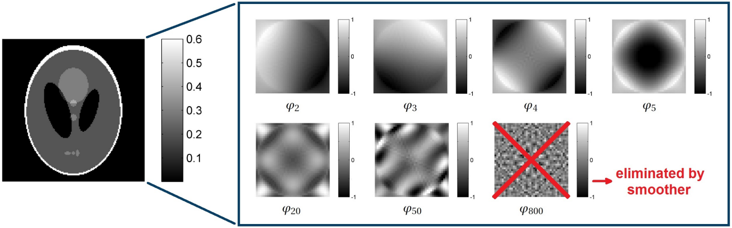
Level-dependent shift

Observation: solution is linear combination of eigenmodes



Two-grid analysis for coarsegrid correction scheme:

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

with $\lambda^h \in \sigma(A^h)$ and φ^h a smooth eigenvector.

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

Level-dependent shift

Stability: coarsegrid correction cancels out smooth modes if

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

When is this condition violated for Helmholtz systems?

- Most problematic when $\lambda_L^{2h} - k^2 \approx 0$.
- Only on some intermediate levels, so replace smoother there by GMRES(m) to damp broader range of modes. [Elman et al. 2001] [Calandra et al. 2011] [Reps et al. 2013]
- Use MG on complex shifted Laplace system on all levels, s.t. $\lambda_L^{2h} - \varrho k^2 \neq 0$ $(\forall h)$. [Erlangga et al. 2006]

MG as preconditioning solver only

Level-dependent shift

Assume level-dependent complex shift $\varrho_h = e^{i\gamma_h}, \quad \gamma_h \in [0, 2\pi]$,

$$A^h = L^h - e^{i\gamma_h} k^2$$

$$A^{2h} = L^{2h} - e^{i\gamma_{2h}} k^2$$

Two-grid analysis for coarsegrid correction scheme:

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

- If $\gamma_h = \gamma_{2h}$ then classical CSL.
- If $0 < |\gamma_h - \gamma_{2h}| < \delta$ then additional error ε^{2h} is introduced.
- If $\gamma_h = 0$ then original Helmholtz eqn. is solved on fine grid.

LVL-MG as Helmholtz solver

Level-dependent shift

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

$$\swarrow \qquad\qquad \searrow$$

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

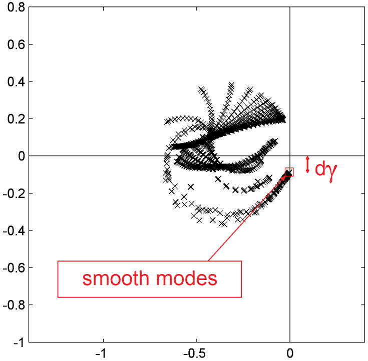
Characterization:

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

Writing $\mathbf{e}^{2h} = \sum_i a_i\,\varphi_i^{2h}$ (φ_i^{2h} eigenmodes), we obtain

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

Level-dependent shift



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

$$\varepsilon^{2h} = \sum_i a_i \left(\frac{\lambda^{2h}-\tilde{\lambda}^{2h}}{\tilde{\lambda}^{2h}}\right)_i \varphi_i^{2h}$$

Only oscillatory eigenmodes contribute to the unwanted error ε^{2h}!

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

The correction step error ε^{2h} is eliminated by post-smoothing.

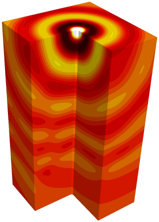
Denote $d\gamma = |\gamma^h - \gamma^{2h}|$.

Level-dependent shift

Seismic 3D model problem

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**)
LVL-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 [Simon 1979]
- GMRES(3) as smoother substitute

Roadmap

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The Helmholtz equation

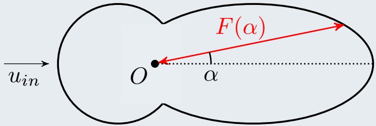
"Representation of the physics behind a wave scattering at an object χ defined on a compact area O located within a domain $\Omega \subset \mathbb{R}^d$."

Scattered wave solution $u(\mathbf{x})$ satisfies inhomogeneous Helmholtz

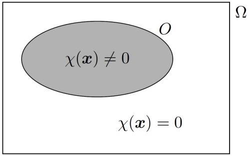
$$\left(-\Delta - k^2(\mathbf{x})\right) u(\mathbf{x}) = f(\mathbf{x}) \quad \text{on} \quad \Omega \subset \mathbb{R}^d, \qquad (2)$$

$f(\mathbf{x}) = k_0^2 \chi(\mathbf{x}) u_{in}(\mathbf{x})$. Numerical solution $u^N(\mathbf{x})$: previous work.

Goal: Far field amplitude map



$\chi(\mathbf{x}) = \frac{k^2(\mathbf{x}) - k_0^2}{k_0^2}$



Far field map

Analytical solution on whole $\mathbb{R}^d$ using Green's function:

$$u(\mathbf{x}') = \int_\Omega G(\mathbf{x},\mathbf{x}')\, k_0^2 \chi(\mathbf{x}) \left(u_{in}(\mathbf{x}) + u^N(\mathbf{x})\right) d\mathbf{x}, \quad \mathbf{x}' \in \mathbb{R}^d.$$

Calculate u in any point $\mathbf{x}' \in \mathbb{R}^d$ outside the numerical box, using only the information inside the numerical box.

Computation: Split the far field integral into a sum $I_1 + I_2$, with

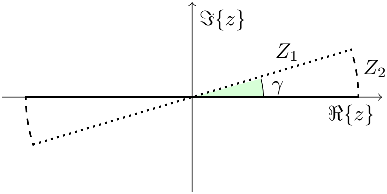
$$I_1 = \underbrace{\int_\Omega G(\mathbf{x},\mathbf{x}')\chi(\mathbf{x})u_{in}(\mathbf{x})d\mathbf{x}}_{\text{all factors known explicitely}} \quad \text{and} \quad I_2 = \underbrace{\int_\Omega G(\mathbf{x},\mathbf{x}')\chi(\mathbf{x})u^N(\mathbf{x})d\mathbf{x}}_{\text{requires } u^N(\mathbf{x}) \text{ for } x \in \Omega}$$

Far field map

Complex contour approach.

For u and χ analytical
the far field integral

$$I_2 = \int_\Omega G(\mathbf{x},\mathbf{x}')\chi(\mathbf{x})u^N(\mathbf{x})d\mathbf{x}$$

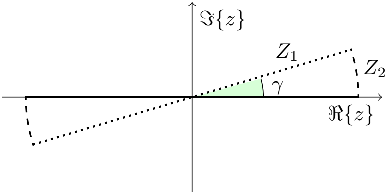


can be calculated over a *complex contour* $Z = Z_1 + Z_2$, rather than over the real domain Ω, i.e.

$$I_2 = \underbrace{\int_{Z_1} G(\mathbf{x},\mathbf{x}')\chi(\mathbf{z})u^N(\mathbf{z})d\mathbf{z}}_{\text{requires } u^N(\mathbf{z}) \text{ for } \mathbf{z}\in Z_1} + \int_{Z_2} G(\mathbf{x},\mathbf{x}')\chi(\mathbf{z})u^N(\mathbf{z})d\mathbf{z}.$$

Far field map

Complex contour approach.



For u and χ analytical the far field integral

$$I_2 = \int_\Omega G(\mathbf{x}, \mathbf{x}')\chi(\mathbf{x}) u^N(\mathbf{x}) d\mathbf{x}$$

can be calculated over a *complex contour* $Z = Z_1 + Z_2$, rather than over the real domain Ω, i.e.

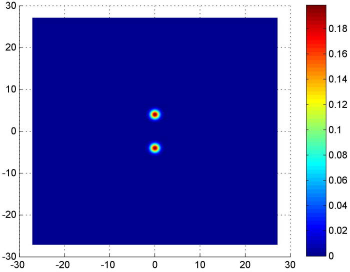
$$I_2 = \underbrace{\int_{Z_1} G(\mathbf{x}, \mathbf{x}')\chi(\mathbf{z}) u^N(\mathbf{z}) d\mathbf{z}}_{\text{requires } u^N(\mathbf{z}) \text{ for } \mathbf{z} \in Z_1} + \int_{Z_2} G(\mathbf{x}, \mathbf{x}')\chi(\mathbf{z}) u^N(\mathbf{z}) d\mathbf{z}.$$

Far field map

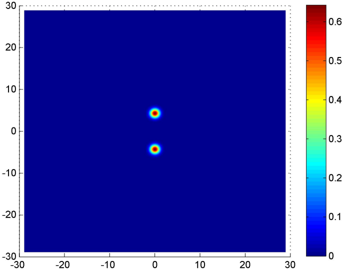
$$\chi(x, y) = -\frac{1}{5}\left(e^{-(x^2+(y-4)^2)} + e^{-(x^2+(y+4)^2)}\right)$$

Object of interest

Real domain with ECS $|\chi(\mathbf{x})|$
$(\theta_{ECS} = 45°)$



Complex contour $|\chi(\mathbf{z})|$
$(\gamma = 14.6°)$

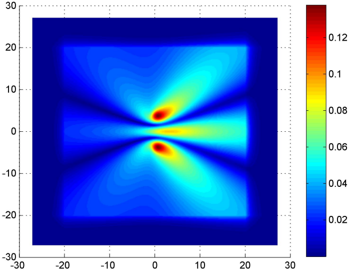


Far field map

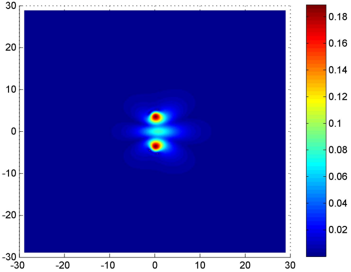
$$\chi(x,y) = -\frac{1}{5}\left(e^{-(x^2+(y-4)^2)} + e^{-(x^2+(y+4)^2)}\right)$$

Scattered wave solution

Real domain with ECS $|u(\mathbf{x})|$
LU factorization



Complex contour $|u(\mathbf{z})|$
V(1,1) cycles ($tol_{res} = 10^{-6}$)

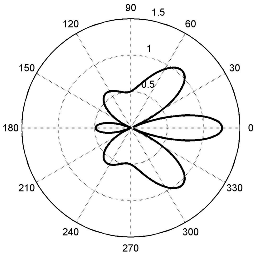


Far field map

$$\chi(x,y) = -\frac{1}{5}\left(e^{-(x^2+(y-4)^2)} + e^{-(x^2+(y+4)^2)}\right)$$

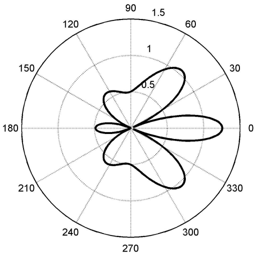
Far field amplitude map

Real domain with ECS $F(\alpha)$



$$\frac{\|F_{re} - F_{ex}\|_2}{\|F_{ex}\|_2} = 9.37\text{e-}5$$

Complex contour $F(\alpha)$



$$\frac{\|F_{co} - F_{ex}\|_2}{\|F_{ex}\|_2} = 1.39\text{e-}4$$

Far field map

3D damped Helmholtz solver ($\gamma = 10^\circ$)

$n_x \times n_y \times n_z$	16^3	32^3	64^3	128^3	256^3
$k_0 = 1/4$	**10** (0.79s.) 0.24	**9** (4.65s.) 0.20	**9** (44.2s.) 0.21	**9** (352s.) 0.20	**9** (2778s.) 0.20
$k_0 = 1/2$	12 (0.92s.) 0.31	**10** (4.96s.) 0.24	**10** (48.3s.) 0.22	**10** (390s.) 0.23	**9** (2797s.) 0.21
$k_0 = 1$	7 (0.62s.) 0.13	13 (6.59s.) 0.32	**11** (54.6s.) 0.27	**10** (387s.) 0.24	**10** (3079s.) 0.24
$k_0 = 2$	2 (0.28s.) 0.00	8 (4.24s.) 0.14	13 (63.9s.) 0.33	**11** (428s.) 0.27	**10** (3006s.) 0.24
$k_0 = 4$	1 (0.20s.) 0.00	2 (1.35s.) 0.00	7 (36.1s.) 0.12	13 (503s.) 0.33	**11** (3306s.) 0.26

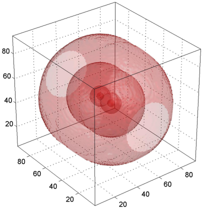
GMRES(3)-smoothed V(1,1) cycles ($tol_{res} = 10^{-6}$) $k_0 h = 0.625$

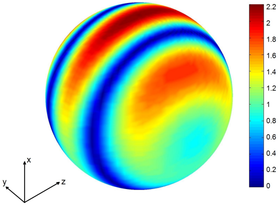
Far field map

3D damped Helmholtz solver ($\gamma = 10^\circ$, $k_0 = 1$)

$n_x \times n_y \times n_z$	16^3	32^3	64^3	128^3	256^3	256^3
CPU time	0.20 s.	0.78 s.	6.24 s.	53.3 s.	462 s.	8×573 s.
$\|r\|_2$	3.3e-5	7.9e-5	2.7e-5	1.1e-5	4.6e-6	1.0e-5

GMRES(3)-smoothed FMG(1,1) cycle [Vasseur 2012]





System specifications: Intel Core i7-2720QM 2.20GHz CPU, 6MB Cache, 8GB RAM. Serial Matlab implementation.

Roadmap

TABLE OF CONTENTS

Conclusions

This thesis contains the following novel and original research contributions:

- ★ Rigourous k-grid LFA analysis to determine complex shift parameter in CSL preconditioner, validating the established rule-of-thumb.
- ★ Theoretical embedding of CSL into $EX(m)$ preconditioner class. Spectral analysis showed more series terms improve preconditioning.
- ★ Level-dependent correction scheme with adaptive complex shift. Used as Helmholtz solver, competitive with CSL-Krylov methods.
- ★ Complex contour method for Far field map of Helmholtz and Schrödinger scattering problems. Significant convergence speed-up and excellent wavenumber scalability.
- ★ Wavelet-based multigrid preconditioner for CT reconstruction, introducing Krylov methods as efficient solvers for tomography.

Conclusions

"During this PhD I have devoted myself to the development and analysis of fast, scalable and robust iterative solution methods for the Helmholtz equation.

Moreover, the use of multigrid methods was succesfully investigated in a wide range of application areas, ranging from Far field map calculation to CT reconstruction.

I believe this thesis shows that multigrid methods - despite being over 50 years old - are still a valuable tool for the solution of Helmholtz and related problems."

Roadmap

TABLE OF CONTENTS

Local Fourier Analysis

Primary aim: find a rigourous method for the choice of the complex shift parameter using LFA to optimize CSL efficiency.

Basic principles in 2D. The l-th level error after m iterations $e_l^{(m)}$ is a formal linear combination of eigenmodes $\varphi_l(\boldsymbol{\theta}, \vec{x})$

$$e_l^{(m)}(\vec{x}) = \Lambda^{(m)}\, \varphi_l(\boldsymbol{\theta}, \vec{x}), \quad \boldsymbol{\theta} \in [-\pi, \pi]^2, \vec{x} \in \Omega, m \geq 0.$$

The evolution of the error amplitude is given by the amplification factor or Fourier symbol $\mathcal{G}_l(\boldsymbol{\theta}, k, \beta)$

$$\Lambda^{(m+1)} = \mathcal{G}_l(\boldsymbol{\theta}, k, \beta)\, \Lambda^{(m)}, \qquad m \geq 0.$$

Local Fourier Analysis

Smoothed two-grid correction scheme - error update step:

$$e_l^{(m+1)} = S^{\nu_2}[I - P_{l+1}^l (A^{l+1})^{-1} R_l^{l+1} A^l] S^{\nu_1}\, e_l^{(m)}, \quad m \geq 0.$$

$$\begin{aligned}
\mathcal{G}_S(\boldsymbol{\theta}, k, \beta) &= 1 - \omega + \frac{2\omega}{4 + (1+\beta i)k^2 h_l^2}(\cos\theta_1 + \cos\theta_2). \\
\mathcal{G}_{A^l}(\boldsymbol{\theta}, k, \beta) &= \frac{4}{h_l^2} - \frac{2}{h_l^2}\cos\theta_1 - \frac{2}{h_l^2}\cos\theta_2 + (1+\beta i)k^2. \\
\mathcal{G}_{R_l^{l+1}}(\boldsymbol{\theta}, k, \beta) &= \frac{1}{4}(\cos\theta_1\cos\theta_2 + \cos\theta_1 + \cos\theta_2 + 1). \\
\mathcal{G}_{P_{l+1}^l}(\boldsymbol{\theta}, k, \beta) &= \frac{1}{4}(\cos\theta_1\cos\theta_2 + \cos\theta_1 + \cos\theta_2 + 1).
\end{aligned}$$

Definition. *Minimal complex shift parameter*

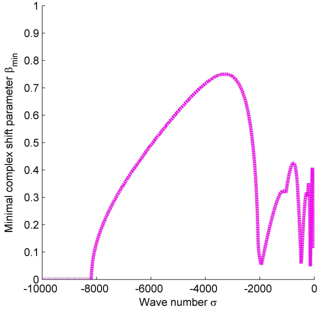
$$\beta_{\min} := \underset{\beta \geq 0}{\operatorname{argmin}} \left\{ \max_{\boldsymbol{\theta} \in [-\pi, \pi]^2} \mathcal{G}(\boldsymbol{\theta}, k, \beta) \leq 1 \right\}. \tag{3}$$

Local Fourier Analysis

Numerical validation: 2D model problem with $N = 32 \times 32$.

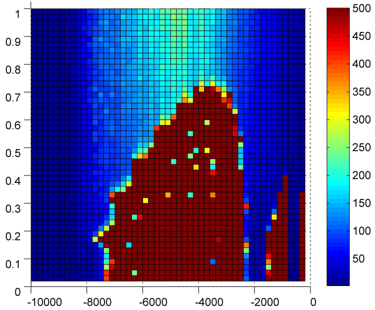
Property 1: Minimality w.r.t. MG convergence.

Theoretical



4-grid LFA minimal complex shift

Experimental



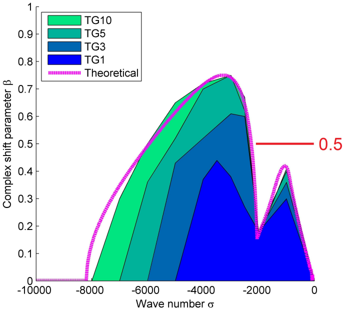
asymptotic V(1,0)-GMRES iteration count

Local Fourier Analysis

Numerical validation: 2D model problem with $N = 32 \times 32$.

Property 2: Near-optimality w.r.t. Krylov convergence.

Theoretical vs. experimental



TG-GMRES iteration-minimum-β

Expansion preconditioners

Definition. General class of shifted preconditioners

$$M(\beta) = -\Delta - k(\vec{x})^2 - P(\beta, \vec{x}). \tag{4}$$

with $P(\beta, \vec{x})$ a linear operator in $\beta \in \mathbb{R}^+$, such that $M(0) = A$.

- Complex Shifted Laplacian (CSL) [Erlangga Vuik Oosterlee 2004]

$$M(\beta) = -\Delta - (1 + i\beta)k^2 \equiv -\Delta - k^2 - P(\beta).$$

- Complex Stretched Grid (CSG) [Reps Vanroose bin Zubair 2010]

$$M(\beta) = -\Delta e^{-i\gamma_\beta} - k^2 \equiv -\Delta - k^2 - P(\beta, \vec{x}).$$

Expansion preconditioners

Definition. Shifted preconditioner $M(\beta)$ inverse

$$f(\beta) := M(\beta)^{-1} = (-\Delta - (1 + \beta i)k^2)^{-1}.$$

Taylor series expansion of $f(\beta)$ around a fixed $\beta_0 \in \mathbb{R}^+$ yields

$$f(\beta) = \sum_{n=0}^{\infty} \frac{f^{(n)}(\beta_0)}{n!}(\beta - \beta_0)^n, \tag{5}$$

with derivatives $f^{(n)}(\beta) = n!\,(k^2 i)^n\,(-\Delta - (1 + \beta i)k^2)^{-(n+1)}$.

Corollary. Original Helmholtz operator A inverse

$$f(0) = M(0)^{-1} = \sum_{n=0}^{\infty} (\beta_0 \sigma i)^n\, M(\beta_0)^{-(n+1)}. \tag{6}$$

Expansion preconditioners

Definition. *Expansion preconditioner of degree m*

$$EX(m) := \sum_{n=0}^{m-1} \alpha_n \left(-\Delta - (1+\beta_0 i)k^2\right)^{-(n+1)}, \qquad (7)$$

where $\alpha_n = (-\beta_0 k^2 i)^n$.

Properties.

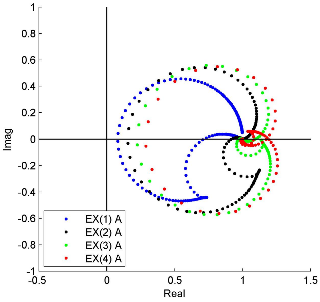
- Asymptotic exactness: $\lim_{m\to\infty} EX(m) = A^{-1}$.
- Accuracy of the expansion: $M(0)^{-1} = EX(m) + \mathcal{O}({\beta_0}^m)$.
- CSL is member of $EX(m)$ class: $EX(1) = (M_{CSL})^{-1}$.

Expansion preconditioners

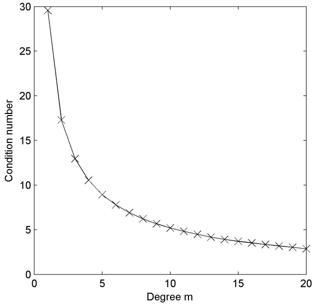
Numerical validation: 1D model problem with $N = 256$ and $k = 140$.

Exact $EX(m)$ preconditioner inversion.

Spectrum



Condition number

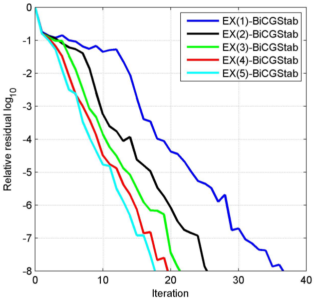


Expansion preconditioners

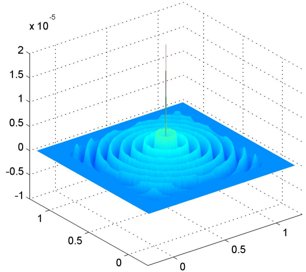
Numerical validation: 2D model problem with $N = 128 \times 128$ and $k = 70$.

Multigrid V(1,1)-cycle(s) EX(m) preconditioner inversion.

Convergence



Solution



Expansion preconditioners

Numerical validation: 2D model problem.

Multigrid V(1,1)-cycle(s) $EX(m)$ preconditioner inversion.

	$N = 128 \times 128$, $k = 70$		$N = 256 \times 256$, $k = 140$	
$EX(m)$	iterations	CPU time	iterations	CPU time
1	37	14.70 s.	140	157.0 s.
2	26	18.97 s.	112	210.8 s.
3	22	23.14 s.	105	277.9 s.
4	20	26.29 s.	104	351.0 s.
5	18	30.51 s.	103	436.2 s.

MG-BiCGStab solver.

Computational cost: m V-cycles required to approximate/compute $EX(m)$.

Schrödinger cross sections

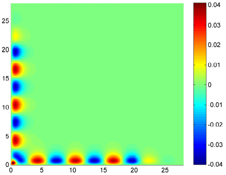
Definition. *The 2D driven Schrödinger equation is*

$$\left(-\frac{1}{2}\Delta + V_1(x) + V_2(y) + V_{12}(x,y) - E\right) u(x,y) = f(x,y),$$

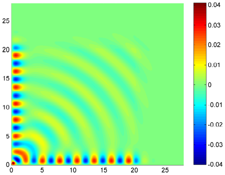
with $x, y \geq 0$, V_i potentials, $E \in \mathbb{R}$ energy of the system.

Solution types.

Single ionization
$-1.0215 < E < 0$



Double ionization
$0 < E$



Schrödinger cross sections

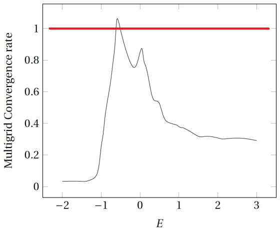
Definition. Single and double ionization cross sections

$$s_n(E) = \int_\Omega \phi_{k_n}(x)\phi_n(y)\left[\phi(x,y) - V_{12}(x,y)u(x,y)\right]\, dx\, dy.$$

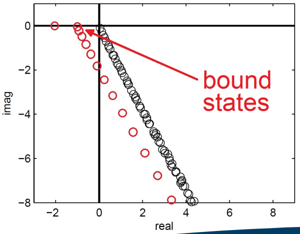
$$f(k_1,k_2) = \int_\Omega \phi_{k_1}(x)\phi_{k_2}(y)\left[\phi(x,y) - V_{12}(x,y)u(x,y)\right]\, dx\, dy.$$

Complex contour approach.

Convergence



Hamiltonian spectrum



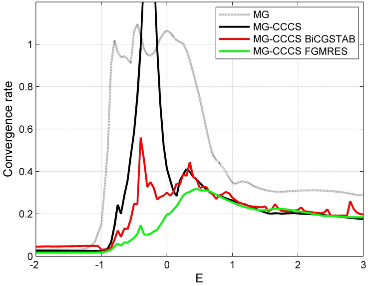
Schrödinger cross sections

Definition. *Coupled channel correction step (CCCS).*

$$u^{(k+1)}(x,y) = u^{(k)}(x,y) + \sum_{m=1}^{M} e_m^A(y)\phi_m(x) + \sum_{l=1}^{L} e_l^B(x)\varphi_l(y),$$

with $M \ll n_x$, $N \ll n_y$.

Numerical results.



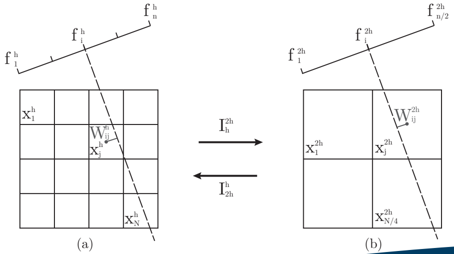
Multigrid-Krylov for ATR

Algebraic Tomographic Reconstruction (ATR) *[Joseph 1982]*

$$Wx = b, \qquad \underbrace{W = (w_{ij}) \in \mathbb{R}^{M\times N}}_{\textit{projection operator}}, \quad \underbrace{b = (b_i) \in \mathbb{R}^{M}}_{\textit{projection data}}.$$

Tikhonov regularization for noisy data

$$\min_x \{\|Wx - \tilde{b}\|_2 + \lambda\|x\|_2\}, \qquad \tilde{b} = b + \varepsilon.$$



Multigrid-Krylov for ATR

Method 1. Simultaneous Iterative Reconstruction Technique

$$x^{(k+1)} = x^{(k)} + CW^T R(b - Wx^{(k)}), \qquad k \geq 1.$$

- ☺ low computational (2 SpMV) and storage cost (2 vectors)
- ☹ slow convergence speed [Gregor Benson 2008]

Method 2. MG-Krylov methods on the normal equations

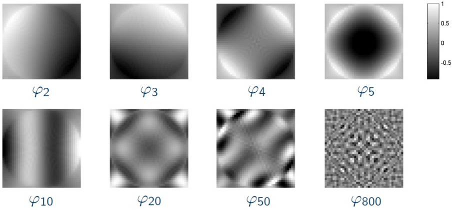
$$W^T Wx = W^T b.$$

- ☺ fast convergence with good preconditioner (non-existing)
- ☹ higher computational and storage cost compared to SIRT
- ☹ standard MG preconditioning fails! [Köstler Rüde 2006]

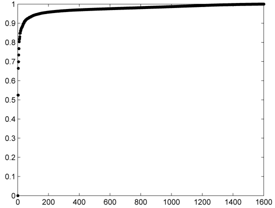
Multigrid-Krylov for ATR

Spectral analysis of SIRT

Eigenmodes



Eigenvalues



Observations:

- majority of eigenvalues $\lambda_i \approx 1$ $\rightarrow$ slow convergence
- *smoothest* modes are damped $\rightarrow$ *no smoothing property!*

Multigrid-Krylov for ATR

Wavelet-based two-grid correction scheme (WTG)

[1D] Two sets of intergrid operators

$$I_{h,1D}^{2h} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 & & & & & & \\ & & 1 & 1 & & & & \\ & & & & \cdot & \cdot & & \\ & & & & & & 1 & 1 \end{bmatrix}, \quad I_{2h,1D}^{h} = (I_{h,1D}^{2h})^T.$$

$$J_{h,1D}^{2h} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 & & & & & & \\ & & 1 & -1 & & & & \\ & & & & \cdot & \cdot & & \\ & & & & & & 1 & -1 \end{bmatrix}, \quad J_{2h,1D}^{h} = (J_{h,1D}^{2h})^T.$$

[2D] Four sets of intergrid operators

$$\begin{aligned} I_{h,LL}^{2h} &= I_{h,1D}^{2h} \otimes I_{h,1D}^{2h}, & I_{2h,LL}^{h} &= (I_{h,LL}^{2h})^T, \\ I_{h,LH}^{2h} &= I_{h,1D}^{2h} \otimes J_{h,1D}^{2h}, & I_{2h,LH}^{h} &= (I_{h,LH}^{2h})^T, \\ I_{h,HL}^{2h} &= J_{h,1D}^{2h} \otimes I_{h,1D}^{2h}, & I_{2h,HL}^{h} &= (I_{h,HL}^{2h})^T, \\ I_{h,HH}^{2h} &= J_{h,1D}^{2h} \otimes J_{h,1D}^{2h}, & I_{2h,HH}^{h} &= (I_{h,HH}^{2h})^T. \end{aligned}$$

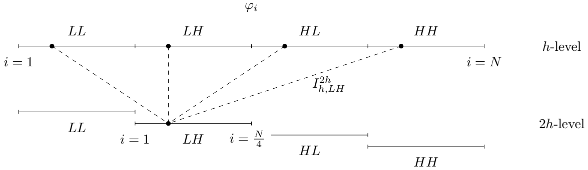
Multigrid-Krylov for ATR

Wavelet-based two-grid correction scheme (WTG)

for $id \in \{LL, LH, HL, HH\}$

1. Calculate the fine grid residual $r^h = b^h - A^h x^h$, and restrict to a coarse grid $r^{2h} = I^{2h}_{h,id} r^h$.
2. Solve the residual equation $A^{2h}_{id} e^{2h} = r^{2h}$ for e^{2h} on the coarse grid.
3. 'Interpolate' the coarse grid error $e^h = I^h_{2h,id} e^{2h}$ to obtain a fine grid error approximation, and correct the initial guess $x^h \leftarrow x^h + e^h$.

Elimination of oscillatory modes in TG correction scheme → no smoother!

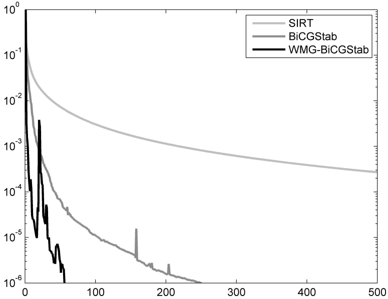


Multigrid-Krylov for ATR

Model with noiseless data

Shepp-Logan phantom

- pixels
  $N = 160 \times 160$
- datapoints
  $M = 400 \times 160$
- $RELERRTOL = 2e{-}2$



Relative residual L_2 norms $\|r_k\|_2/\|r_0\|_2$.

	iterations	CPU time	error L_2	error L_∞
SIRT	1000+	80.6 s.	0.1015	0.2010
BiCGStab	300	25.1 s.	0.0166	0.0317
WMG-BiCGStab	50	17.4 s.	0.0152	0.0669

Multigrid-Krylov for ATR

Model with noisy data

Shepp-Logan phantom

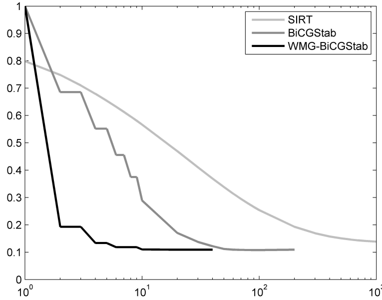
- pixels

  $N = 160 \times 160$

- datapoints

  $M = 400 \times 160$

- with regularization

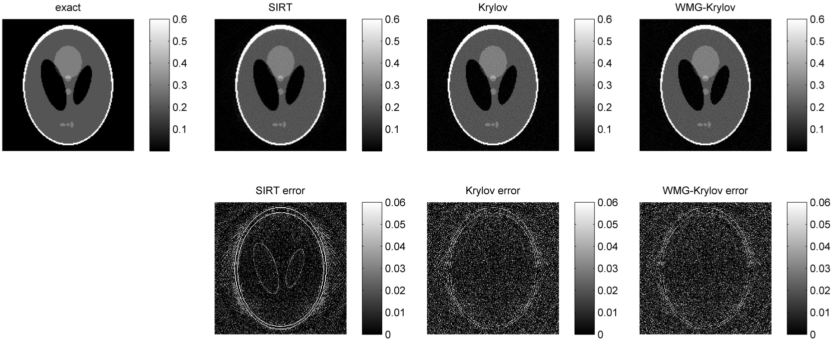


Scaled error L_2 norms $\|x_{ex} - x_k\|_2 / \|x_{ex}\|_2$.

	iterations	CPU time	error L_2	error L_∞
SIRT	1000	81.1 s.	0.1385	0.2697
BiCGStab	100	9.35 s.	0.1074	0.1459
WMG-BiCGStab	14	5.44 s.	0.1083	0.1386

Multigrid-Krylov for ATR

Model with noisy data



Shepp-Logan model with $N = 160 \times 160$ and $M = 400 \times 160$ (noisy, regularized). Numerical solutions after $k_{opt} = 1000$ (SIRT), $k_{opt} = 100$ (BiCGStab) and $k_{opt} = 14$ (WMG-BiCGStab) iterations.