Iterative Helmholtz Solvers

Scalability and Accuracy of Helmholtz solvers

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Outline

Aim and Impact

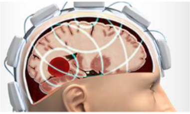
- Joint-work with PhD candidtate Vandana Dwarka
- Contribute to broad research on Helmholtz solvers
- Understand inscalability (convergence) and accuracy (pollution)
- Improve convergence properties
- Alert solver developers to keep accuracy of solution in mind

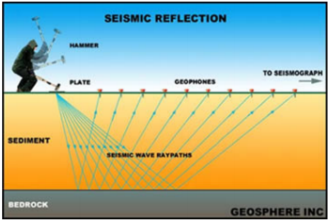
Introduction - The Helmholtz Equation

- Inhomogeneous Helmholtz equation + BC's

$$(-\nabla^2 - k^2)\, u(\mathbf{x}) = f(\mathbf{x}), \mathbf{x} \in \Omega \subseteq \mathbb{R}^n$$

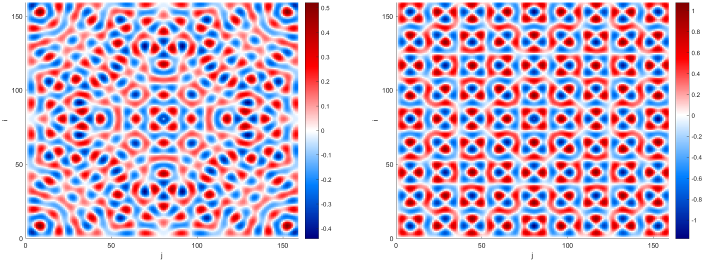
- k is the wave number: $k = \frac{2\pi}{\lambda}$
- Practical applications in seismic and medical imaging





Introduction - Challenges

- Negative & positive eigenvalues ⇒ limits Krylov based solvers
- Fast near-origin moving eigenvalues ⇒ slows convergence
  - CSLP: A with a complex shift
  - Deflation + CSLP
  - Despite improvements problem remains
- Numerical solution is often inaccurate!



- Problems exacerbate in 2D & 3D

Introduction - Numerical Model

- Analytical 1D model problem

$$-\frac{d^2u}{dx^2} - k^2\,u = \delta(x - \frac{1}{2}),$$
$$u(0) = 0, u(1) = 0,$$
$$x \in \Omega = [0,1] \subseteq \mathbb{R},$$

- Discretization using second-order FD with at least 10 gpw
- We obtain a linear system $A\hat{u} = f$

$$A = \frac{1}{h^2}\text{tridiag}[-1 \;\; 2-(kh)^2 \;\; -1],$$

- A is real, symmetric, normal, indefinite and sparse
- Using Radiation BC's A additionally becomes non-Hermitian

Introduction - Spectral Properties

- Near-null eigenvalues near intersection with origin
- The index where this happens for the analytical case is

$$\lambda_{j_{\min}} = 0 \Rightarrow j^2\pi^2 \approx k^2\pi^2,$$
$$\Rightarrow j_{\min} = \lfloor \frac{k}{\pi} \rfloor \text{ or } \lceil \frac{k}{\pi} \rceil.$$

- The index where this happens for the numerical case is

$$\hat{\lambda}_{\hat{j}_{\min}} = 0 \Rightarrow \frac{1}{h^2}\left[2 - 2\cos(j\pi h)\right] \approx k^2$$
$$\Rightarrow \hat{j}_{\min} = \text{round}\left[\frac{\arccos 1 - \kappa^2}{\pi h}\right]$$

- Our research:
  - Near-null eigenvalues ⇒ accuracy issues ⇒ Pollution
  - Near-null eigenvalues ⇒ convergence issues ⇒ Deflation

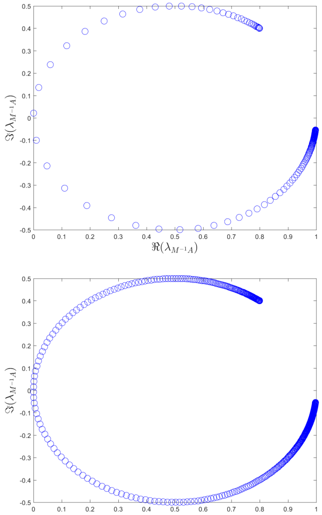
Preconditioning - CSLP

- Preconditioning to speed up convergence of Krylov subspace methods
- Solve $M^{-1}Au = M^{-1}f$, M is CSLP-preconditioner.

$$M = A - (\beta_1 + \beta_2 i)k^2 I,$$
$$(\beta_1, \beta_2) \in [0, 1]$$

- Increasing $k \Rightarrow$ inscalable CSLP-solver
- Project unwanted eigenvalues onto zero = Deflation

Figure: $\sigma(M^{-1}A)$ for $k = 50$ (top) and $k = 150$ bottom.



Preconditioning - Deflation

- Projection principle: solve $PAu = Pf$

$$\tilde{P} = AQ \text{ where } Q = ZE^{-1}Z^T \text{ and } E = Z^TAZ,$$
$$P = I - \tilde{P},\ Z \in \mathbb{R}^{m \times n},\ m < n$$

- Columns of Z span deflation subspace
- Ideally Z contains eigenvectors
- In practice approximations

DEF - I

- Main focus on DEF-preconditioner (Sheikh, A., 2014)

$$P = I - AQ \text{ where } Q = Z{A_{2h}}^{-1}Z^T \text{ and } A_{2h} = Z^TAZ$$

- Inter-grid vectors from multi-grid as deflation vectors
- Inter-grid approximation based on linear interpolation
- Use DEF + CSLP combined $\Rightarrow$ spectral improvement

$$P^TM^{-1}Au = P^TM^{-1}f$$

- Monitor eigenvalues using rigorous Fourier analysis
- Effect aggravates in higher-dimensions
- Near-null eigenvalues unless $\#gpw$ increases along

DEF - II

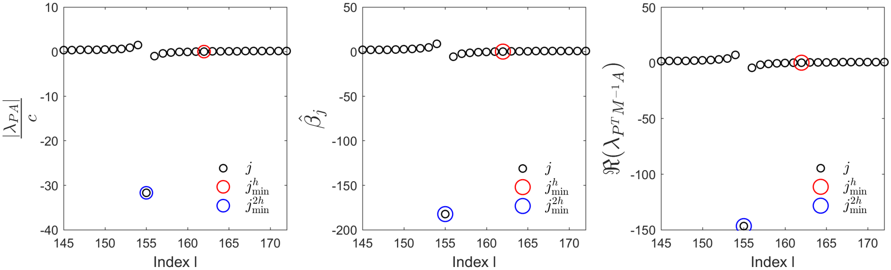
- Near-null eigenvalues arise at projection level
- Block-diagonalize $P \Rightarrow$ eigenvalues

$$\begin{aligned}
\lambda^l(P) &= s^l + c^l, \\
s^l &= \left(1 - \frac{\lambda^l(A)\cos(l\pi\frac{h}{2})^4}{\lambda^l(A_{2h})}\right) = \frac{\lambda^{n+1-l}(A)\sin(l\pi\frac{h}{2})^4}{\lambda^l(A_{2h})}, \\
c^l &= \left(1 - \frac{\lambda^{n+1-l}(A)\sin(l\pi\frac{h}{2})^4}{\lambda^l(A_{2h})}\right) = \frac{\lambda^l(A)\cos(l\pi\frac{h}{2})^4}{\lambda^l(A_{2h})}, \\
\lambda^l(PA) &= \lambda^l(A)s^l + \lambda^{n+1-l}(A)c^l, \\
l &= 1, 2, \ldots, \frac{n}{2}.
\end{aligned}$$

DEF - II

- Investigate near-null eigenvalue of <u>all</u> operators involved

Figure: $\lambda_j(PA), \beta^j, \lambda_j(P^T M^{-1} A)$ for $k = 500$



- Eigenvalues of PA and $P^T M^{-1} A$ behave like $\hat{\beta} = \frac{\lambda^l(A)}{\lambda^l(A_{2h})}$
- If near-kernel of A and A_{2h} misaligned $\Rightarrow$ near-null eigenvalues reappear!
- Equivalent to $j^h_{\min} \neq j^{2h}_{\min}$

DEF - III

- Recall: deflation space spanned by linear approximation basis vectors
- Transfer coarse-fine grid ⇒ interpolation error ⇒ near-kernel A_{2h} shifts
- Measure effect by projection error E

$$E(kh) = \|(I - P)\phi_{j_{\min},h}\|^2,$$

$$P = Z(Z^TZ)^{-1}Z^T$$

Figure: Restricted & interpolated eigenvectors (left $kh = 0.625$, right $k^3h^2 = 0.625$

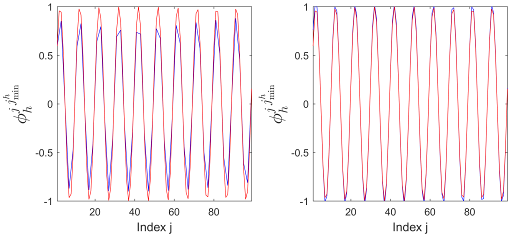


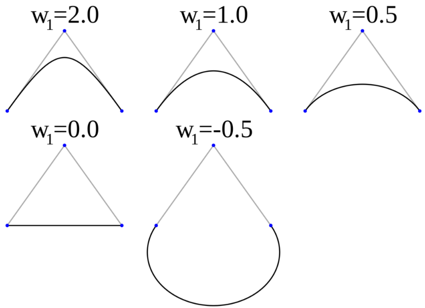
Table: Projection error DEF-scheme

k	$E(0.625)$	$E(0.3125)$
10^2	0.8818	0.1006
10^3	9.2941	1.0062
10^4	92.5772	10.0113
10^5	926.135	100.1382
10^6	9261.7129	1001.3818

Our Approach - Introduction

- Higher-order deflation vectors
- Rational quadratic Bezier curve $\Rightarrow$ one control-point
- Weight-parameter w to adjust control-point

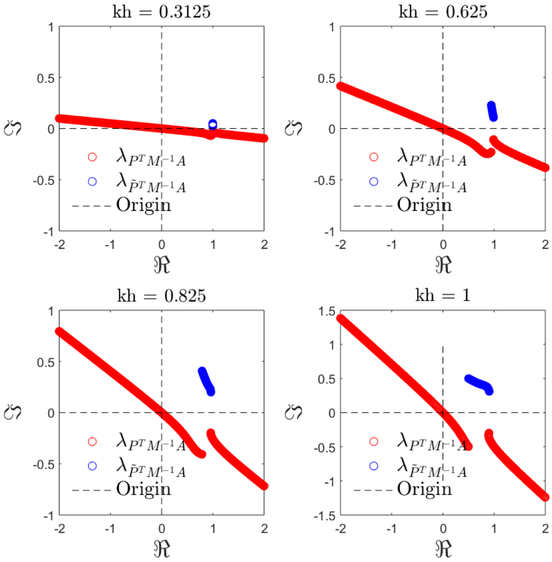
Figure: Effect of changing weight



- w determined such that projection error minimized
- Rigorous Fourier analysis confirms favourable spectrum

Our Approach - Spectral Analysis (1D)

Figure: Spectrum of old (red) and new (blue) method for $k = 10^6$



Numerical Experiments - 1D

Table: GMRES-iterations with tol $= 10^{-7}$ using the new scheme $APD(w)$ and CSLP(1,0.5).

k	APD(0.1250)	APD(0.0575)	APD(0.01875)	APD(0.00125)
	$kh = 1$	$kh = 0.825$	$kh = 0.625$	$kh = 0.3125$
10^2	6	5	4	3
10^3	6	5	4	3
10^4	6	5	4	3
10^5	6	5	4	3
10^6	6	5	4	3

- DEF + CSLP takes 367 its. and 16.1104 sec. for $k = 10^4$
- We obtain wave number independence for all kh
- Weight-parameter w less important as kh decreases

Projection Error - 1D

Table: Projection error $E(kh)$ for $APD(w)$ and CSLP(1,0.5)

k	APD(0.1250)	APD(0.0575)	APD(0.01875)	APD(0.00125)
	$kh = 1$	$kh = 0.825$	$kh = 0.625$	$kh = 0.3125$
10^2	0.0127	0.0075	0.0031	0.0006
10^3	0.0233	0.0095	0.0036	0.0007
10^4	0.0246	0.0095	0.0038	0.0007
10^5	0.0246	0.0095	0.0038	0.0007
10^6	0.0246	0.0095	0.0038	0.0007

- Weight-parameter w chosen to minimize projection error
- In all cases projection error *strictly* < 1

Numerical Experiments - 2D

Table: GMRES-iterations with tol $= 10^{-7}$ using the new scheme $APD(w)$ and CSLP(1,0.5). AD contains no CSLP.

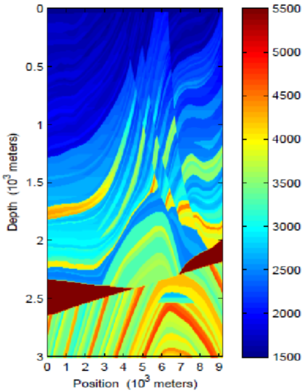
k	APD(0.1250)	APD(0.0575)	AD(0)
	$kh = 0.625$	$kh = 0.3125$	$kh = 0.3125$
100	4	4	3
250	5	4	4
500	5	5	5
750	7	5	5
1000	8	8	7

- DEF + CSLP takes 471 iterations and 1195.9730 sec. for $k = 250$
- Close to wave number independence
- Weight-parameter w and CSLP less important as kh decreases

Marmousi - 2D

Table: Solve time (s) and GMRES-iterations for 2D Marmousi

	DEF-TL	APD-TL	DEF-TL	APD-TL
	10 gpw			
f	Solve time (s)		Iterations	
1	1.72	4.08	3	4
10	7.20	3.94	16	6
20	77.34	19.85	31	6
40	1175.99	111.78	77	6
	20 gpw			
1	9.56	3.83	3	5
10	19.64	15.45	7	5
20	155.70	122.85	10	5
40	1500.09	1201.45	15	5



Numerical Experiments - 3D

Table: GMRES-iterations with tol $= 10^{-7}$ using the new scheme $APD(w)$ and CSLP(1,0.5). $kh = 0.625$.

k	APD(0.125)	APD(0)
	Iterations	Iterations
10	4	4
25	4	5
50	4	5
75	4	5

- DEF + CSLP takes 66 iterations for $k = 40$
- Two-level method memory constrained $\Rightarrow$ multilevel

Conclusion

- Deflation projects unwanted eigenvalues to zero
- Large $k \Rightarrow$ near-null eigenvalues reappear
- Near-kernel alignment of A and A_{2h}
- Misalignment affects both accuracy and convergence
- New deflation scheme: higher-order approximation
- Obtain faster convergence

References - I

- Upcoming articles
  http://ta.twi.tudelft.nl/nw/users/vuik/pub_it_helmholtz.html
- Further reading

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- Further reading

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