Iterative Helmholtz Solvers

Scalability of deflation-based Helmholtz solvers

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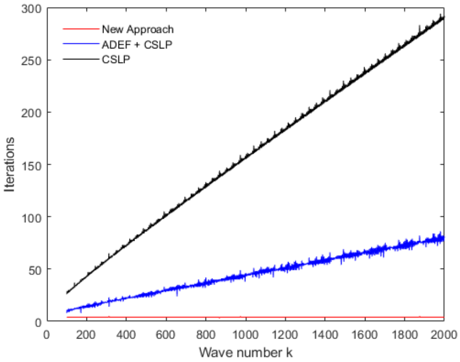
Outline

Aim and Impact

- Contribute to broad research on Helmholtz solvers
- Obtain understanding of inscalability
- Improve convergence properties
- Link results to accuracy issues (pollution)

Evolution of iterative Helmholtz Solvers

- Direct Solvers
- Preconditioned iterative solvers
  1. Factorization (ILU)
  2. Real shift
  3. Complex shift - CSLP
- Deflation-based preconditioning



Problem Definition

- Analytical 1D model problem

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

- Numerical 1D model problem using second order FD

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

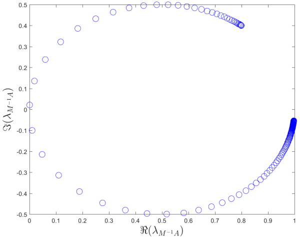
- Discretization on $\Omega = [0,1]$ with $h = \frac{1}{n}$
- $k \approx \lfloor 2\pi/\#\text{gpw} \rfloor \Rightarrow kh$ is the grid resolution
- Rule of thumb $kh = 0.625 = 10$ gpw
- Coefficient matrix A is indefinite

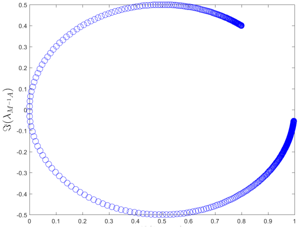
CSLP

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

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

- Optimal shift letting $(\beta_1, \beta_2) = (1, 0.5)$
- Increasing $k \Rightarrow$ increasing near-null eigenvalues $\Rightarrow$ inscalable CSLP-solver
- Project unwanted eigenvalues onto zero $=$ Deflation





Deflation

- Projection principle: solve $PAu = Pf$

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

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

ADEF - I

- Main focus on ADEF-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
- Approximation based on linear interpolation
- Use ADEF + CSLP combined $\Rightarrow$ spectral improvement
- Monitor eigenvalues using rigorous Fourier analysis
- Near-null eigenvalues unless $\#gpw$ increases along
- Effect aggravates in higher-dimensions

ADEF - II

- Near-null eigenvalues arise at projection level
- Block-diagonalize $P \Rightarrow$ eigenvalues (Ramos Garcia, L., 2017)

$$\lambda^l(P) = \alpha^l + \beta^l,$$

$$\alpha^l = \left(1 - \frac{\lambda^l(A)\cos(l\pi\frac{h}{2})^4}{\lambda^l(A_{2h})}\right) = \frac{\lambda^{n+1-l}(A)\sin(l\pi\frac{h}{2})^4}{\lambda^l(A_{2h})},$$

$$\beta^l = \left(1 - \frac{\lambda^{n+1-l}(A)\sin(l\pi\frac{h}{2})^4}{\lambda^l(A_{2h})}\right) = \frac{\lambda^l(A)\cos(l\pi\frac{h}{2})^4}{\lambda^l(A_{2h})},$$

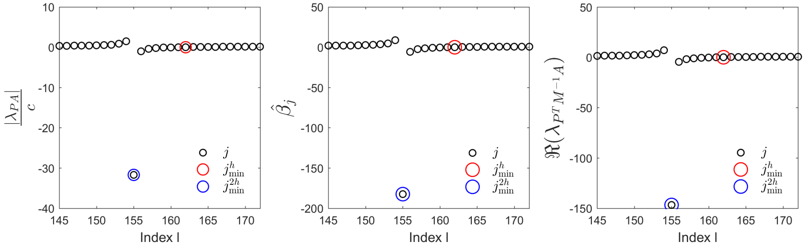
$$\lambda^l(PA) = \lambda^l(A)\alpha^l + \lambda^{n+1-l}(A)\beta^l,$$

$$l = 1, 2, \ldots, \frac{n}{2}.$$

ADEF - III

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

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



- Eigenvalues of PA and $P^TM^{-1}A$ 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!
- Reminiscent of pollution!

ADEF - VI

- 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

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

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

Figure: Restricted & interpolated eigenvectors

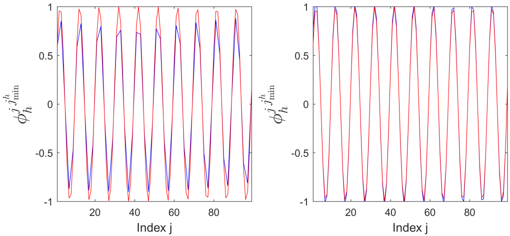


Table: Projection error ADEF-scheme

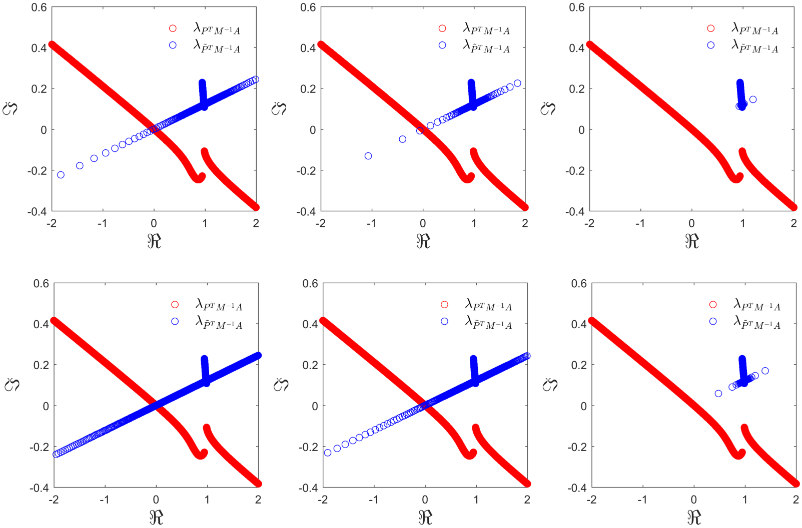
k	$E(0.625)$	$E(0.3125)$
10^2	0.8818	0.1006
10^3	9.2941	1.0062
10^4	92.5772	10.0113
10^5	926.135	100.1382
10^6	9261.7129	1001.3818

Newly Proposed Scheme

- Higher-order deflation vectors based
- Weight-parameter ε to adjust control-points
- ε determined such that $E(kh)$ minimized
- Deflation vectors now quadratic
- Rigorous Fourier analysis confirms favourable spectrum

Spectral Analysis (1D)

Figure: $k = 10^5$ (Upper), $k = 10^6$ (Lower)



Numerical Experiments - 1D

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

k	APD(0.1250)	APD(0.0575)	APD(0.01875)	**APD(0)**	APD(0.00125)
	$kh = 1$	$kh = 0.825$	$kh = 0.625$	$kh = 0.625$	$kh = 0.3125$
10^2	6	5	4	**4**	3
10^3	6	5	4	**6**	3
10^4	6	5	4	**12**	3
10^5	6	5	4	**59**	3
10^6	6	5	5	**509**	3

- ADEF + CSLP takes 367 its. and 16.1104 sec. for $k = 10^4$
- We solved $k = 10^6$ with the new scheme in 3.4697 sec.
- Weight-parameter ε less important as kh decreases

Projection Error - 1D

Table: Projection error $E(kh)$ for $APD(\varepsilon)$ + 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	0.0219	0.0096	0.0036	0.0007
10^3	0.0243	0.0097	0.0039	0.0007
10^4	0.0246	0.0102	0.0041	0.0007
10^5	0.0246	0.0154	0.0070	0.0009
10^6	0.0246	0.0167	0.0361	0.0022

- Weight-parameter ε 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 and CSLP(1,0.5). AD contains no CSLP.

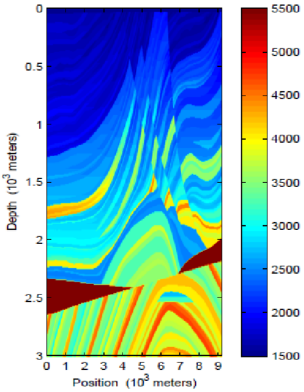
k	APD(0.1250)	APD(0.0575)	AD(0)
	$kh = 0.625$	$kh = 0.3125$	$kh = 0.3125$
100	4	4	3
250	5	4	4
500	5	5	5
750	7	5	5
1000	8	8	7

- ADEF + CSLP takes 471 iterations and 1195.9730 sec. for $k = 250$
- We solved $k = 10^3$ with problem size $(11 \times 10^6) \times (11 \times 10^6)$ in 616.2462 sec.
- Weight-parameter ε and CSLP less important as kh decreases

Marmousi - 2D

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

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



Conclusion

- Deflation projects unwanted eigenvalues to zero
- Large $k \Rightarrow$ near-null eigenvalues reappear
- Near-kernel alignment of A and A_{2h}
- Interpolation error $\Rightarrow$ misalignment
- New deflation scheme: higher-order approximation
- Even better results with weight-parameter
- Outperforms in terms of spectral and convergence properties

References

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

C. Vuik et. al.
Modern Solvers for Helmholtz Problems.
Birkhuser, 2017.

A. Sheikh
Development of the Helmholtz Solver based on a Shifted Laplace Preconditioner and a Multigrid Deflation technique.
PhD Thesis, Delft University of Technology, 2014

L. Garcia Ramos, R. Nabben
On the Spectrum of Deflated Matrices with Applications to the Deflated Shifted Laplace Preconditioner for the Helmholtz Equation
SIAM Journal on Matrix Analysis and Applications, 39(1):262286, 2018