A Scalable version of the ADEF-Solver

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Outline

Intro - Helmholtz Equation

- Time-dependent wave equation + separation of variables

$$(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2})u(\mathbf{x}, t) = \mathbf{0}$$

- Homogeneous Helmholtz equation

$$(-\nabla^2 - k^2)\, u(\mathbf{x}) = \mathbf{0}, \mathbf{x} \in \Omega \subseteq \mathbb{R}^n$$

- Practical applications non-homogeneous Helmholtz equation
- k is the wave number

$$k = \frac{2\pi}{\lambda}$$

- Boundary conditions at $\partial\Omega$
- In this interim thesis:
  1. Non-homogeneous 1D
  2. Dirichlet

Analytical Model

- Analytical 1D model problem

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

- Sturm-Liouville + Green's function $\Rightarrow$ exact solution

$$
\begin{aligned}
G(x, L/2) &= \frac{2}{L}\sum_{j=1}^{\infty} \frac{\sin(j\pi x/L)\sin((j\pi L/2/L))}{j^2\pi^2 - k^2/L}\\
k^2 &\neq \frac{j^2\pi^2}{L}\\
j &= 1, 2, 3, \ldots
\end{aligned}
$$

Numerical Model

- Discretization on $\Omega = [0, 1]$
- Second-order finite difference scheme using step-size $h = \frac{1}{n}$
- $k \approx \lfloor 2\pi/\#\text{gpw} \rfloor \Rightarrow \kappa = kh$ is the grid resolution
- Rule of thumb $\kappa = 0.625$
- We obtain a linear system

$$
\begin{aligned}
Au &= f, \\
A = \Delta - k^2 I &= \frac{1}{h^2}\text{tridiag}[-1 \;\; 2 - k^2 \;\; -1], \\
A, I &\in \mathbb{R}^{(n-1)\times(n-1)}, \\
u, f &\in \mathbb{R}^{(n-1)}.
\end{aligned}
$$

- A is real, symmetric, normal, indefinite, tridiagonal and sparse

Continuous vs. Discrete Spectrum - I

- Continuous eigenvalues for the analytical model

$$\lambda_j = j^2\pi^2 - k^2,\ j = 1, 2, 3, \ldots$$

- Discrete eigenvalues for the numerical model

$$\lambda_l = \frac{1}{h^2}\left[2 - 2\cos(l\pi h) - k^2h^2\right],$$
$$l = 1, 2, 3, \ldots, n-1$$

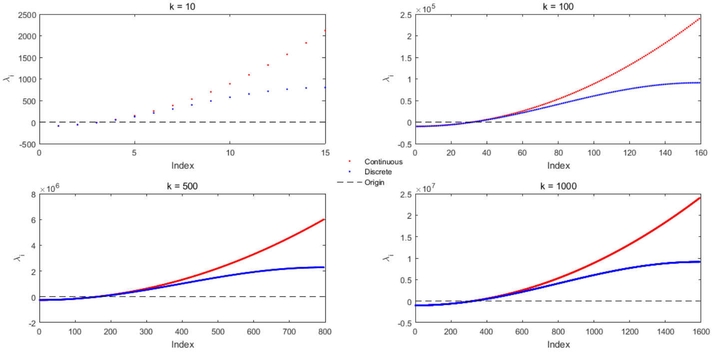
- Orthonormal eigenvectors for continuous and discrete

$$\theta_l = \sin\left(l\pi x\right),\ 1 \le l \le n-1$$

- Negative eigenvalues with increasing $k \Rightarrow$ indefinite A

Continuous vs. Discrete Spectrum - II

Figure: *Eigenvalues of the continuous and discrete Helmholtz operator*



Near-null Eigenvalues - I

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

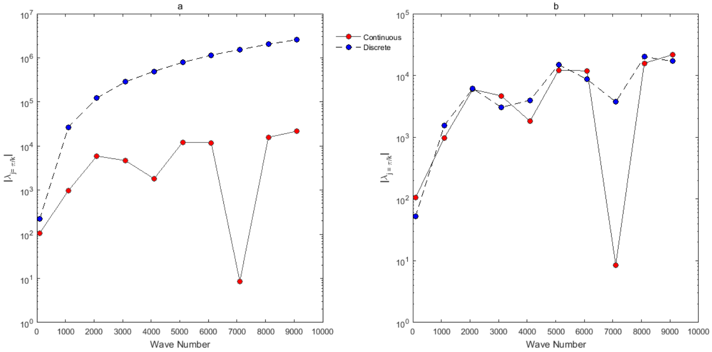
$$\lambda_{\hat{j}} = 0 \Rightarrow j^2\pi^2 \approx k^2\pi^2,$$
$$\Rightarrow \hat{j} \approx \frac{k}{\pi} = \lfloor \frac{k}{\pi} \rfloor \text{ or } \lceil \frac{k}{\pi} \rceil.$$

- The index where this happens for the discrete case is

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

Near-null Eigenvalues - II

Figure: *Order of magnitude smallest absolute eigenvalue. (a)* $\kappa = 0.625$, *(b)* $\kappa = 0.0625$



Intro - Numerical Solution Methods

- Solve linear system $Au = f$ using iterative numerical method
- Krylov subspace methods for Helmholtz problems
- General matrix GMRES or Bi-CGSTAB compatible
- In this interim thesis: GMRES-method

Multigrid - I

- BIM error propagation operator $\Rightarrow e_{k+1} = Se_k = S^k e_0$

$$S = I - M^{-1}A$$

- Low frequency vs. High frequency error
- Coarse-grid defect correction (CGC) for $H > h$
- CGC Error propagation operator

$$C = I - I_H^h A_H^{-1} I_h^H A,$$
$$A_H = I_h^H A I_H^h$$

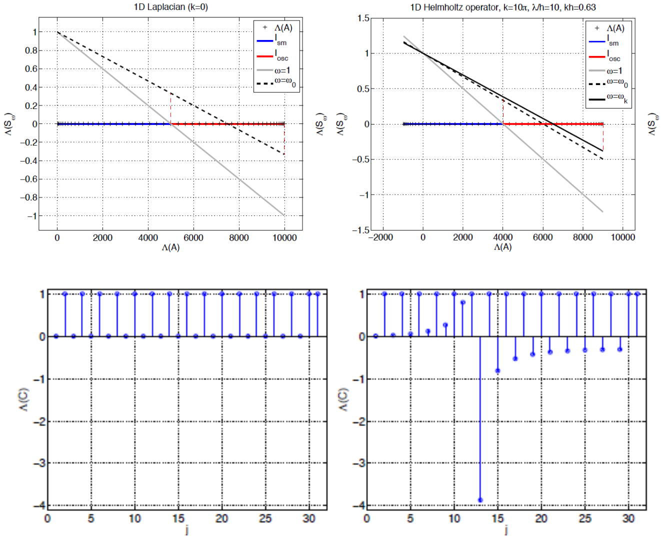
- Multigrid = BIMs + coarse-grid correction

$$e_{k+1} = \tilde{C} e_k = S^{\nu_1} C S^{\nu_1} e_k$$

- Standard multigrid unsuitable for Helmholtz problems

Multigrid - II

Figure: *Eigenvalues of smoothing (upper) and coarse-grid operator (lower)*



Pollution - I

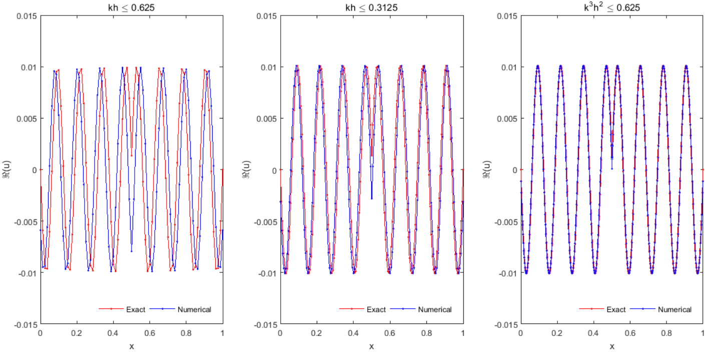
- Large $k \Rightarrow$ oscillating solution
- Pollution of the numerical solution
- Numerical dispersion
- Total error for the model problem

$$\text{error}_{total} = \frac{\|u-\hat{u}\|}{\|u\|} \leq C_1 kh + C_2 k^3 h^2,\ kh < 1$$

- $\kappa = 0.625$ not sufficient
- Set $k^3 h^2 \leq 0.625$ or use higher-order discretization.

Pollution - II

Figure: *Exact and numerical solution for $k = 50$. The point-source has been placed at $x = 0.5$.*



Intro - Preconditioning

- Preconditioning to speed up convergence
- Solve $M^{-1}Au = \widehat{A}u = M^{-1}f$
- Various M for the Helmholtz problem:
  1. $M := A = LU$
  2. $M := -\Delta$
  3. $M := -\Delta - \beta_1 k^2 I,\ \beta_1 \in \mathbb{R}^+$
  4. $M := -\Delta - (\beta_1 + i\beta_2)k^2 I,\ \beta_1, \beta_2 \in [0,1]$
- In this interim thesis: CSLP preconditioner

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

CSLP - I

- A and M^{-1} commute $\Rightarrow$ eigenvalues are given by

$$\lambda_j(\widehat{A}) = \lambda_j(M^{-1}A) = \frac{\lambda_j(A)}{\lambda_j(M)}$$

- $\widehat{A}$ is complex, symmetric, normal yet non-Hermitian
- Continuous eigenvalues

$$\lambda_j(\widehat{A}) = \frac{j^2\pi^2 - k^2}{j^2\pi^2 - (\beta_1 + i\beta_2)k^2}, \ \beta_1, \beta_2 \in [0, 1]$$

- Discrete eigenvalues

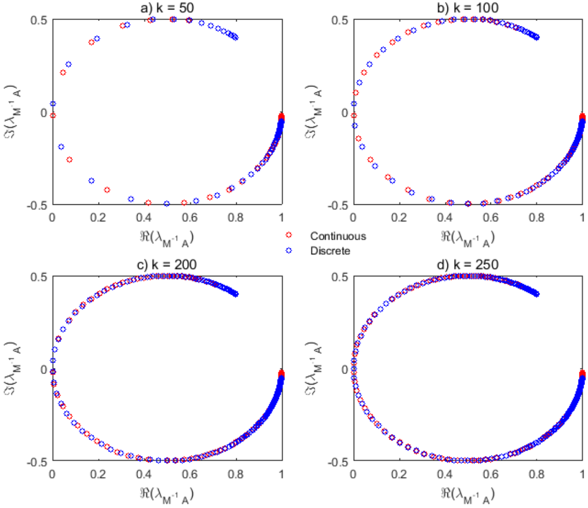
$$\lambda_l(\widehat{A}) = \frac{\omega - k^2}{\omega - (\beta_1 + i\beta_2)k^2}, \ \ \beta_1, \beta_2 \in [0, 1]$$

$$\omega = \frac{1}{h^2}(2 - 2\cos(l\pi h))$$

- Optimal shift letting $(\beta_1, \beta_2) = (1, 0.5)$

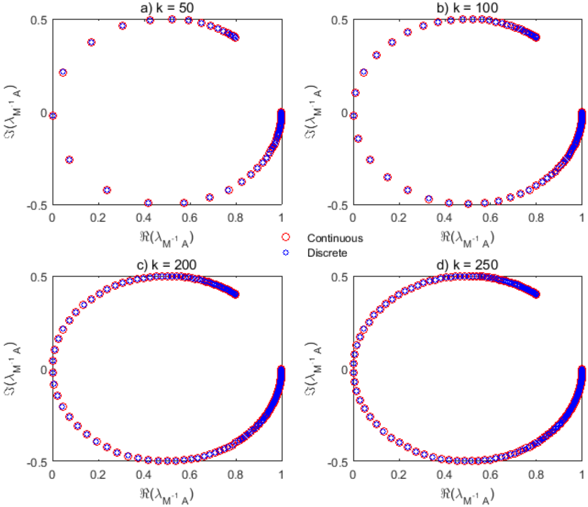
Near-null Eigenvalues - I

Figure: *Eigenvalues of the preconditioned system* $\widehat{A}$



Near-null Eigenvalues - II

Figure: *Eigenvalues of the preconditioned system $\widehat{A}$ using $\kappa = 0.0625$*



Near-null Eigenvalues - III

Table: *Smallest absolute eigenvalue of h^2A and $\widehat{A}$*

k	$\lfloor \frac{k}{\pi} \rfloor$	$\widehat{l}$	$\widehat{l} - \lfloor \frac{k}{\pi} \rfloor$	$\min \lvert \lambda(h^2A) \rvert$	$\min \lvert \lambda(M^{-1}A) \rvert$
100	31	32	1	8.658989e-03	1.961650e-03
500	159	162	3	6.237295e-04	1.019831e-05
1000	318	324	6	6.237295e-04	1.019831e-05
5000	1591	1619	28	1.572319e-04	6.480688e-07
10000	3183	3237	54	7.592379e-05	1.511108e-07
20000	6366	6475	109	4.064631e-05	4.330941e-08

Convergence - I

- Increasing $k \Rightarrow$ increasing near-null eigenvalues $\Rightarrow$ inscalable CSLP-solver
- CSLP convergence is step-size independent
- CSLP outperforms other preconditioners
- Number of iterations increases linearly with k
- Large k CSLP diverges

Convergence - II

Table: *Number of full GMRES iterations and relative residual for the CSLP-solver.*

k	Iterations	Rel. Res.
100	28	3.230682e-08
500	89	6.074832e-08
1000	159	4.987300e-08
5500	752	8.011798e-08
5700	1493	3.428289e-03

Intro - Deflation

- Project unwanted eigenvalues onto zero
- Solve $PAu = Pf \Rightarrow$ implement as preconditioner

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

- Columns of Z span deflation subspace
- Various P for the Helmholtz problem:
  1. $A = M^{-1}A$
  2. $A = \tilde{M}^{-1}A$, where $\tilde{M}$ is an approximation of M
  3. $A = A$
  4. $A = M$

ADEF - I

- Main focus on ADEF-preconditioner

$$P = I - AQ + \gamma Q \text{ where } Q = ZE^{-1}Z^T \text{ and } E = Z^T AZ$$

- Recall CGC Error propagation operator

$$C = I - I_H^h A_H^{-1} I_h^H A \text{ where } A_H = I_h^H A I_H^h$$

- Inter-grid vectors from multigrid as deflation vectors

$$Z = I_{2h}^h = \frac{1}{2}\begin{pmatrix} \frac{1}{2} & 1 & \frac{1}{2} \end{pmatrix}$$

- Use ADEF + CSLP combined $\Rightarrow$ spectral improvement

$$M^{-1}Au = M^{-1}f$$

$$M^{-1}PAu = M^{-1}Pf$$

$$P^T M^{-1}Au = \widehat{P}u = P^T M^{-1}f$$

- Systems have equivalent spectrum

$$\sigma(M^{-1}PA) = \sigma(P^T M^{-1}A) = \sigma(\widehat{P})$$

ADEF - II

- Discrete eigenvalues using rigorous Fourier analysis.
- A + CSLP-matrix M share orthonormal eigenvectors.
- Block-diagonalize $\widehat{P}$

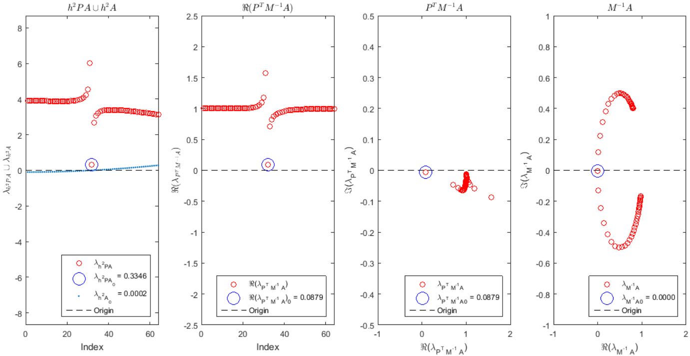
$$V = \left[\theta^1, \theta^{n-1}, \theta^2, \theta^{n-2}, ..., \theta^{n/2-1}, \theta^{n/2}\right],$$
$$\theta^l = \sin(l\pi x) \text{ for } 1 \leq l \leq n-1$$

- Zero eigenvalue of multiplicity $n/2 - 1$
- Remaining $n/2 - 1$ eigenvalues

$$\lambda^l(\widehat{P}) = \frac{a_l + ib_l}{c_l + id_l} \text{ for } 1 \leq l \leq n/2 - 1.$$

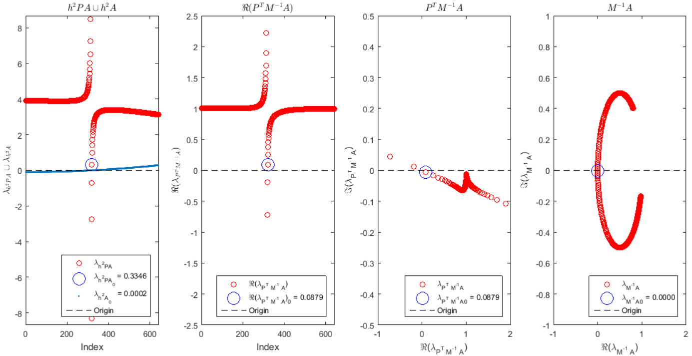
Near-null Eigenvalues - I

Figure: *Discrete eigenvalues of* $h^2 PA$, $\Re(\widehat{P})$, $\widehat{P}$ *and* $\widehat{M}$ *resp. for* $k = 100$. *The marker corresponds to index* $\widehat{l}$.



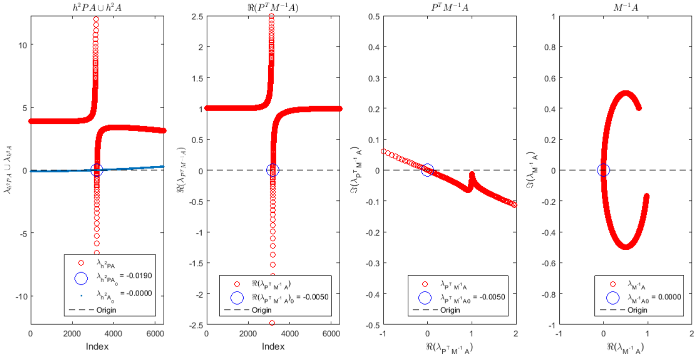
Near-null Eigenvalues - II

Figure: *Eigenvalues of h^2PA, $\Re(\widehat{P})$, $\widehat{P}$ and $\widehat{M}$ resp. for $k = 1000$. The marker corresponds to index $\widehat{l}$.*



Near-null Eigenvalues - IV

Figure: *Eigenvalues of h^2PA, $\Re(\widehat{P})$, $\widehat{P}$ and $\widehat{M}$ resp. for $k = 10000$. The marker corresponds to index $\widehat{l}$.*



Convergence - I

Table: *Number of full GMRES iterations using the ADEF- and CSLP-solver.*

	$\kappa = 0.625$				$\kappa = 0.3125$			
k	ADEF		CSLP		ADEF		CSLP	
	Iter.	Rel. Res.	Iter.	Rel. Res.	Iter.	Rel. Res.	Iter.	Rel. Res.
100	16	1.6650e-08	44	7.6988e-08	10	2.2809e-08	44	7.4631e-08
500	41	4.1160e-08	160	9.6237e-08	19	6.2831e-08	155	6.1181e-08
1000	67	5.1416e-08	296	4.7705e-08	27	7.0026e-08	283	8.5375e-08
5000	251	8.6474e-08	1200	3.3587e-02	81	5.9620e-08	1200	6.9000e-03

Convergence - II

Table: *Number of full GMRES iterations using the ADEF- and CSLP-solver with shifts* $(\beta_1, \beta_2) = (1, 0.25)$ *and* $(1, 1)$.

	$\kappa = 0.625$		$\kappa = 0.3125$	
k	ADEF(1,0.25)	ADEF(1,1)	ADEF(1,0.25)	ADEF(1,1)
	Iter.	Iter.	Iter.	Iter.
100	14	17	10	10
200	22	25	11	12
300	27	29	15	16
400	32	35	17	17
500	38	42	19	19
600	43	46	20	21
700	48	51	21	21
800	53	57	24	24

Research Questions

To what extent is the ADEF-solver scalable?

1. What causes to current solver to remain inscalable?
2. What parameters can be identified to influence solver scalability?
   - Parameters on operator level
   - Parameters on geometric level
3. Is there a relation between the pollution error and the cause for inscalability? If affirmative, will reducing the pollution error lead to better scalability?
   - Perturbed wave number and spectral changes
4. If time permits: how do different discretization schemes affect the accumulation of numerical pollution?

Test-Problems

- 1D Helmholtz Test-Problems
  1. constant wave-number problem + Dirichlet boundary conditions
  2. constant wave-number problem + Dirichlet and Sommerfeld boundary conditions
- 2D Helmholtz Test-Problems
  1. constant wave-number problem + Dirichlet and Sommerfeld boundary conditions
  2. non-constant wave number wedge-problem + Dirichlet and Sommerfeld boundary conditions
  3. non-constant wave number Marmousi-problem + Dirichlet and Sommerfeld boundary conditions

Thank you! Questions? :)