Multigrid for Helmholtz Equations

Using Classical Components

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Research Motivation

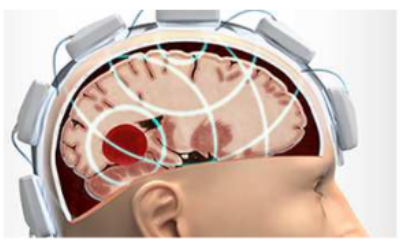
- Blueprint for numerically solving high frequency wave problems.
- Requires robust and scalable solvers.
- Incremental results starting with scalable solvers for the Helmholtz equation (time-harmonic Maxwell).
- Open problem for 45 years

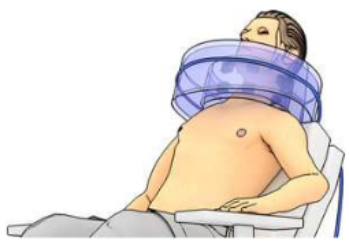
Introduction - The Helmholtz Equation

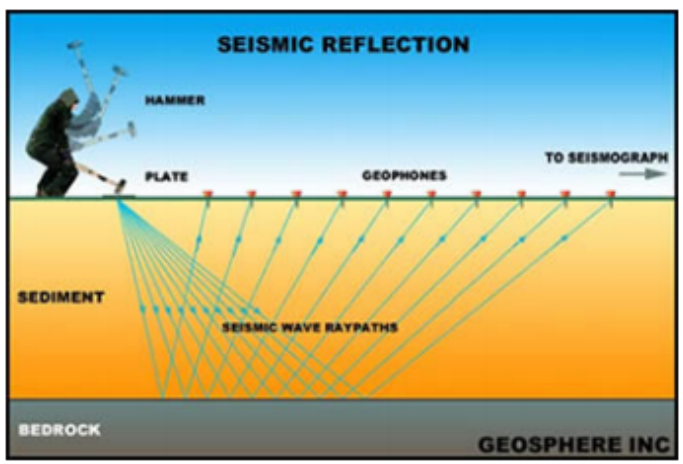
- Inhomogeneous Helmholtz equation + BC's

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

- k is the dimensionless wave number: $k = \frac{2\pi}{\lambda}$
- Practical applications in quantum mechanics, imaging problems and plasma fusion







Introduction - Numerical Model

- Start with 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 Sommerfeld BC's A becomes non-Hermitian $\Rightarrow$ non-selfadjoint

Introduction - Challenges

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  - Additional accuracy requirements: pollution criteria
  - No general theory for these indefinite systems

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  - Additional accuracy requirements: pollution criteria
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- Computational challenges
  - Very large linear systems due to pollution criteria
  - Iterations to converge grow with k (inscalable)
  - Problems exacerbate in 2D & 3D
  - Multigrid solvers diverge for indefinite Helmholtz (also still an open problem!)

Preconditioning - CSL

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

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

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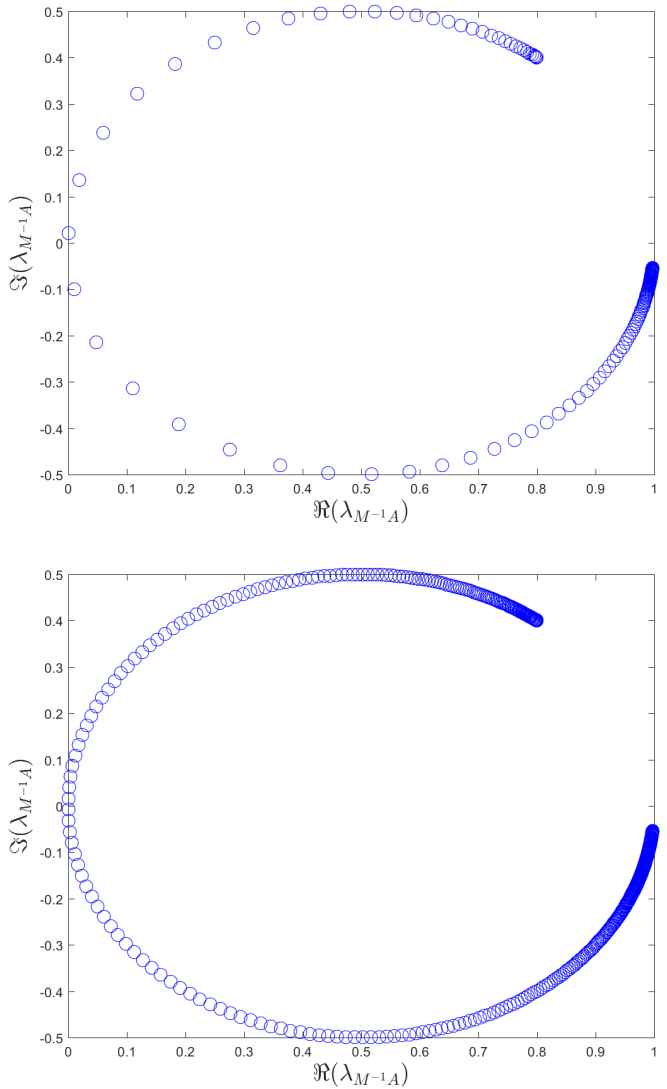
- L is the discretized Laplace operator
- Increasing $k \Rightarrow$ eigenvalues move fast towards origin $\Rightarrow$ inscalable CSL-solver

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



Preconditioning - CSL

Table: GMRES iterations using tol $= 10^{-6}$ with (β_1, β_2) for 1D problem. CSL inversion using multigrid.

k	$(1, 1)$	$(1, 0.5)$
50	25	20
100	41	30
500	138	87
1 000	254	156
5 000	1 153	693

- Already convergence issues for simple toy problem!
- Direct solve of CSL expensive
- Approximate solve of CSL needs more iterations
- Wavenumber k increases $\Rightarrow$ more near-zero eigenvalues $\Rightarrow$ more iterations
- Project unwanted eigenvalues onto zero = Deflation

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: inter-grid vectors from multigrid (linear interpolation polynomial)
- Use DEF + CSL combined $\Rightarrow$ spectral improvement

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

- Monitor eigenvalues using RFA (Dirichlet)

Preconditioning - Deflation

- Deflation space spanned by linear approximation basis vectors
- Transfer coarse-fine grid $\Rightarrow$ interpolation error
- Measure effect by projection error E

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

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

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

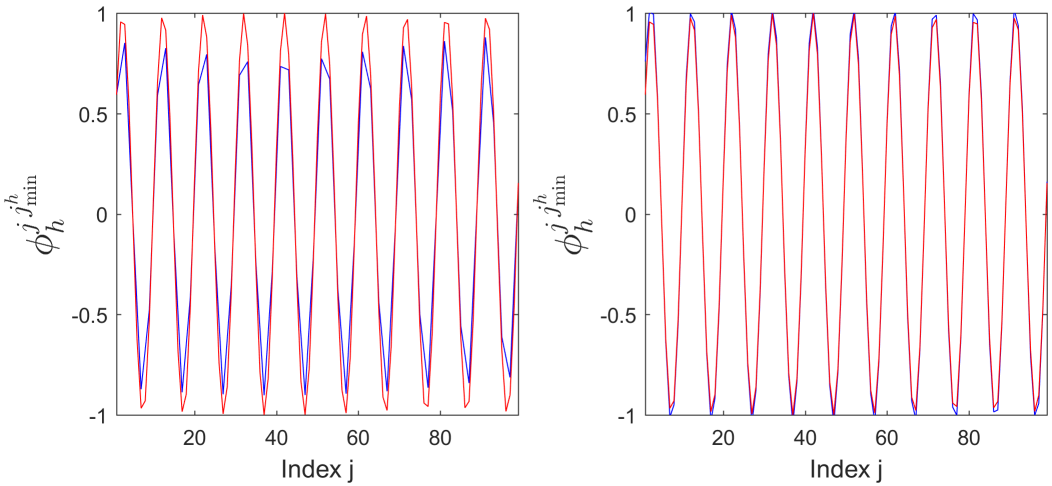


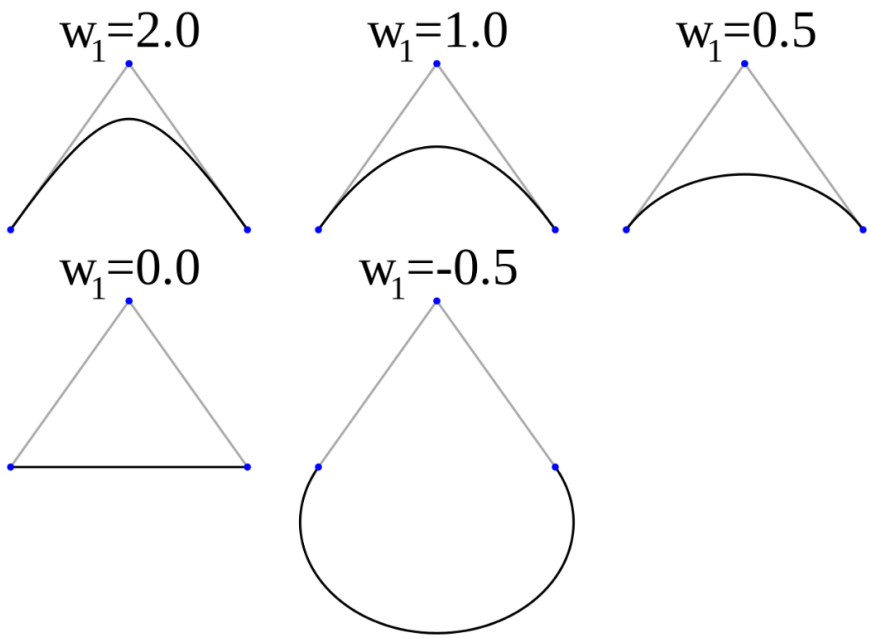
Table: Projection error DEF-scheme

k	$E(0.625)$	$E(0.3125)$
10^2	0.88	0.10
10^3	9.29	1.00
10^4	92.57	10.01
10^5	926.13	100.13
10^6	9 261.71	1 001.38

Higher-order Deflation

- 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

Projection Error

Table: Projection error $E(kh)$ for various w for 1D

k	$w = 0.1250$	$w = 0.0575$	$w = 0.01875$	$w = 0.00125$
	$kh = 1$	$kh = 0.825$	$kh = 0.625$	$kh = 0.3125$
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
- RFA confirms favourable spectrum

Two-Level Deflation - 2D

Table: GMRES-iterations with tol $= 10^{-6}$ using Sommerfeld BC's and MG-approximation of CSL(1,1). AD contains no CSL.

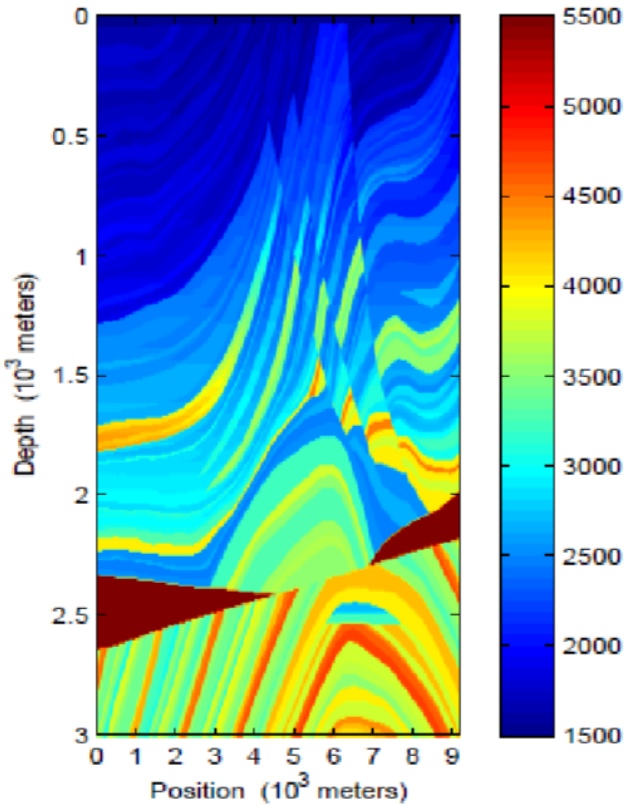
k	APD(0.1250)	APD(0.0575)	AD(0)
	$kh = 0.625$	$kh = 0.3125$	$kh = 0.3125$
100	4	4	3
250	5	4	4
500	5	5	5
750	7	5	5
1000	8	8	7

- DEF (linear) + CSL needs 471 iterations for $k = 250$
- Close to k-independence
- Weight-parameter w and CSL less important as kh decreases

Two-Level Deflation - 2D Marmousi

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	1 175.99	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	1 500.09	1 201.45	15	5



Two-Level Deflation - 3D

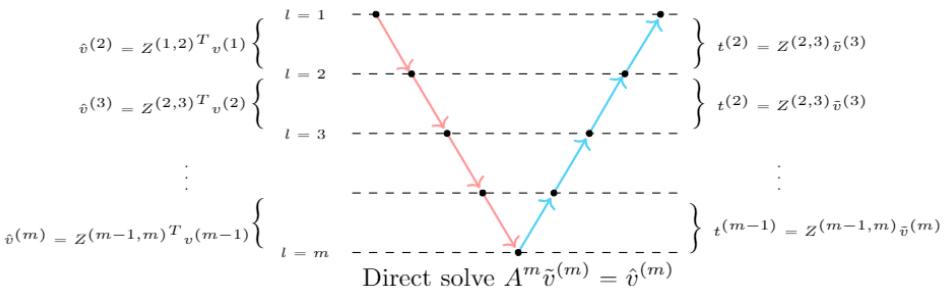
Table: GMRES-iterations with tol $= 10^{-6}$ using Sommerfeld BC's and MG-approximation of CSL(1,1). AD contains no CSL.

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

- DEF (linear) + CSL takes 66 iterations for $k = 40$
- k-independent convergence
- Two-level method memory $\Rightarrow$ multilevel methods

Multilevel Deflation

- Apply two-level method recursively
- Only 1 FGMRES it. per level



- Krylov 'smoother' vs Multigrid
- 10 iterations on indefinite levels
- 1 Jacobi iteration on all others
- Reduce time and memory

Algorithm 3.1 Two-level Deflation FGMRES

Initialization:
Choose u_0 and dimension k of the Krylov subspaces.
Define $(k+1) \times k$ $\bar{H}_k$ and initialize to zero.
Arnoldi process: $r_0 = f - Au_0$, $\beta = \|r_0\|_2, v_1 = r_0/\beta$.
for $j = 1, 2, ...k$ **do**
  $\hat{v} = Z^T v_j$
  $\tilde{v} = E^{-1}\hat{v}$
  $t = Z\tilde{v}$
  $s = At$
  $\tilde{r} = v_j - s$
  $r = M^{-1}\tilde{r}$
  $x_j = r + t$
  $w = Ax_j$
  for $i = 1, 2, ...j$ **do**
    $h_{i,j} = (w, v_j)$ $w = w - h_{i,j}v_i$
  end
  Compute $h_{j+1,j} = \|w\|_2$ and $v_{j+1} = w/h_{j+1,j}$.
  Define $X_k = [x_1, x_2, \ldots, x_k]$
  $\bar{H}_k = \{h_{i,j}\}_{1 \leqslant i \leqslant j+1, 1 \leqslant j \leqslant k}$
end
Form approximate solution:
Compute $u_k = u_0 + X_k y_k$ where $y_k = \arg\min_y \|\beta e_1 - \bar{H}_k y\|_2$.
Restart:
If satisfied stop, else set $u_0 \leftarrow u_k$ and repeat Arnoldi process.

Multilevel Deflation - Spectral Analysis

Spectrum of the coarse linear systems for $k = 100$ for 1D. $m \leq 3$ denotes the levels with $m = 0$ the original fine grid matrix $E_0 = A$.

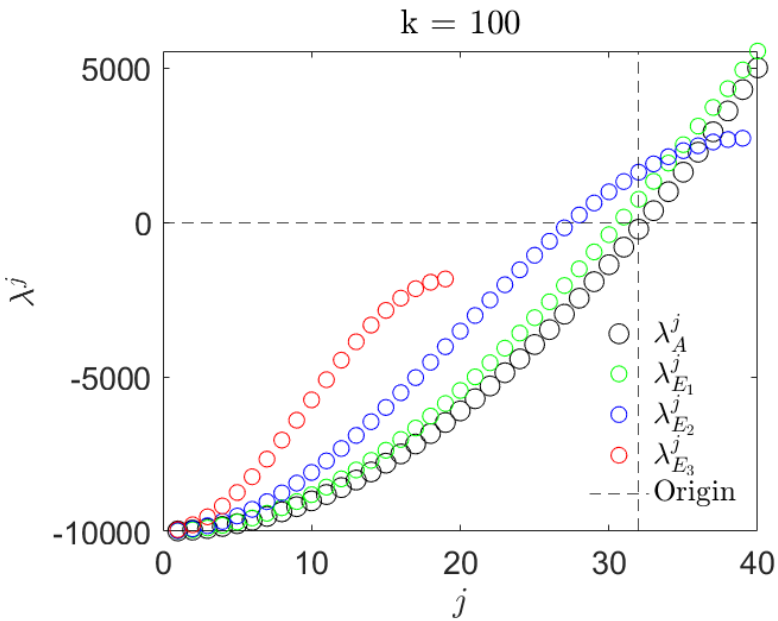


Figure: Linear Interpolation

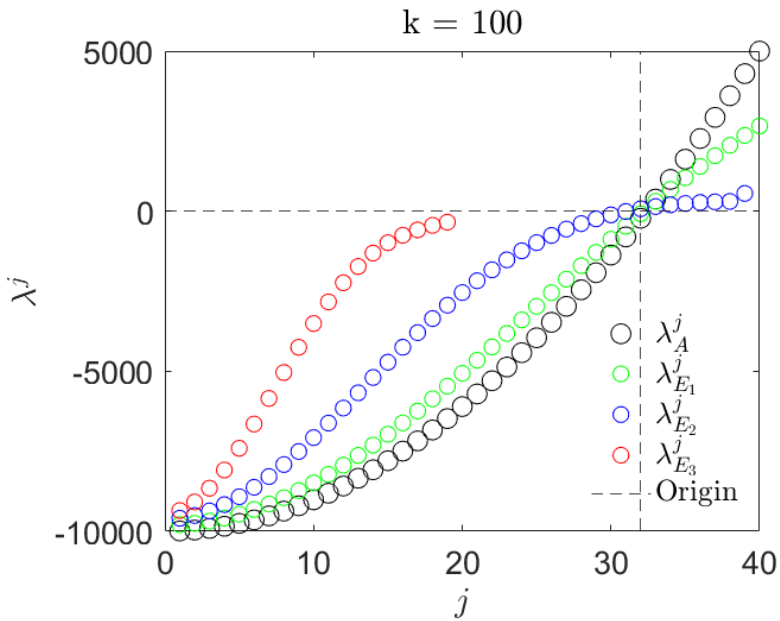


Figure: Quadratic Rational Bezier

Multilevel Deflation - Spectral Analysis

Spectrum of the deflation + CSL preconditioned system (20 gpw) for 1D.

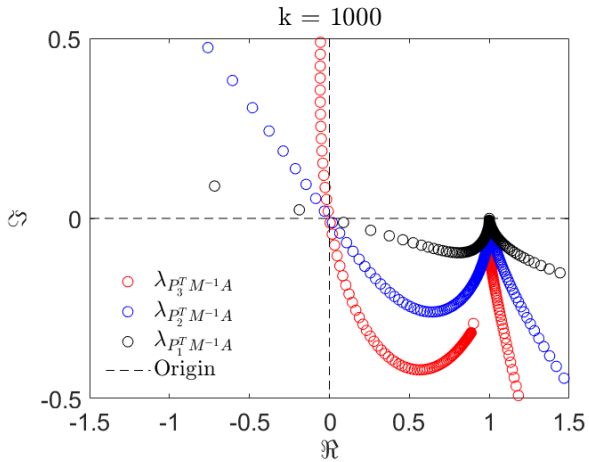


Figure: Linear interp. (Dirich.)

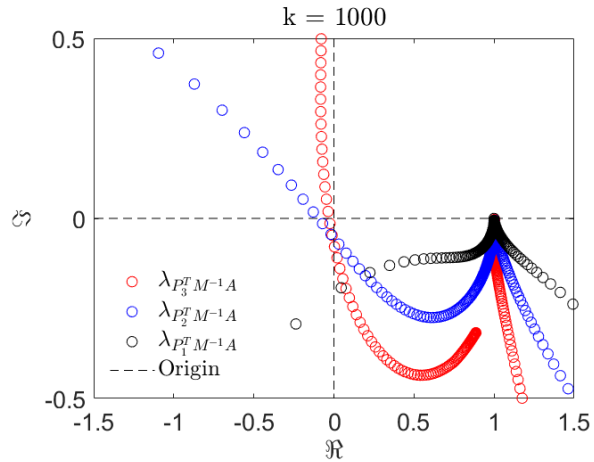


Figure: Linear interp. (Somm)

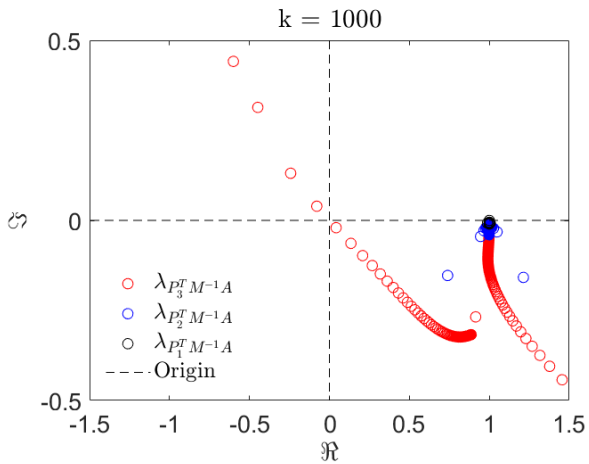
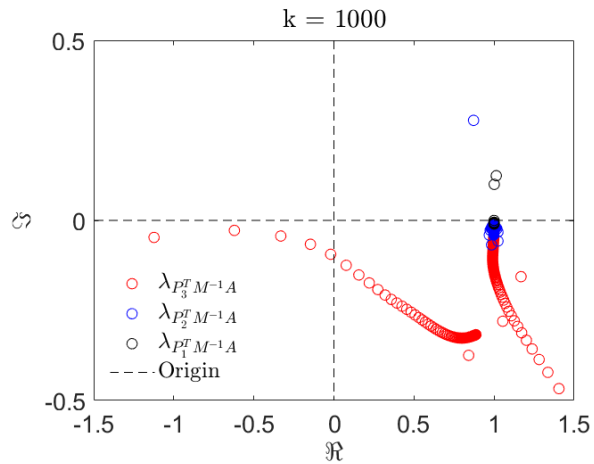


Figure: Quadr. (Dirich.)



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Multilevel Deflation - 3D

Table: Number of outer FGMRES-iterations for $kh = 0.625$. Column 1 quadratic, column 2 linear deflation vectors.

k	APD	DEF
	Iterations	Iterations
10	9	11
20	9	12
40	11	17
80	14	45

- Both methods benefit from multilevel implementation
- Reduced time and memory
- But iterations slightly depend on k again

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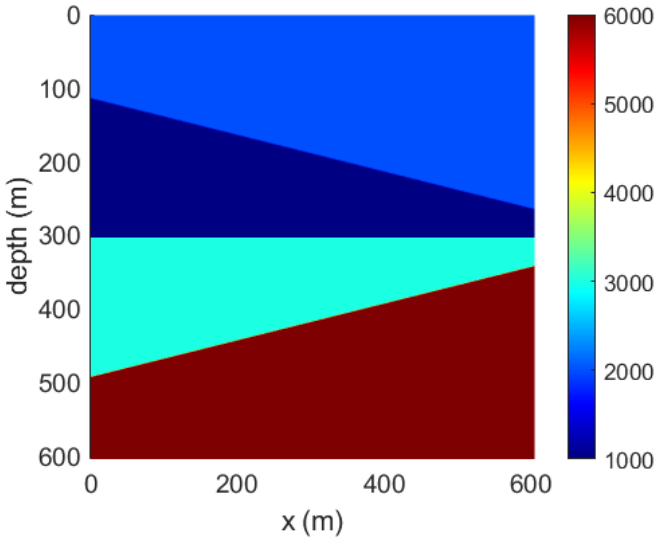
What about heterogeneous problems?

Multilevel Deflation - 2D Wedge



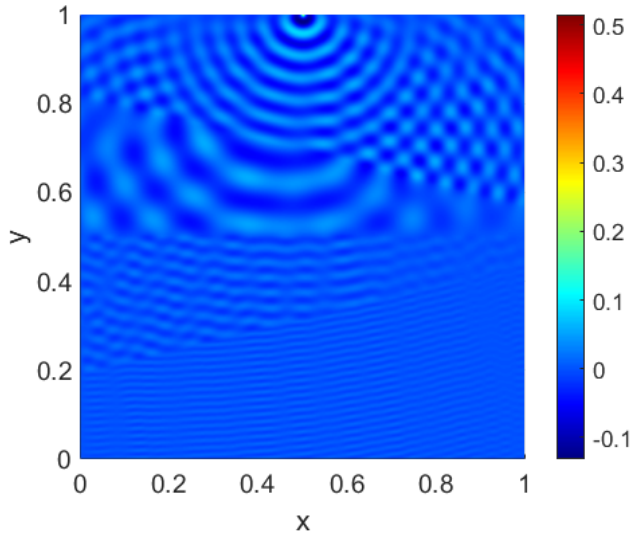


Table: Outer FGMRES-iterations and CPU time for $kh = 0.625$.

	$c(x,y) \in [500, 3\,000]$ m/s			$c(x,y) \in [1\,000, 6\,000]$ m/s		
f (Hz)	Iterations	CPU(s)	n	Iterations	CPU(s)	n
10	12	4.10	41 209	9	0.58	10 201
20	18	37.14	162 409	12	3.97	41 209
30	22	118.22	366 025	16	18.99	91 809
40	29	370.91	648 025	19	34.29	162 409
60	35	1 097.31	1 456 849	22	174.03	366 025

$f = 60$ corresponds to a dimensionless wavenumber $k = 753$.

Status-quo

- Iterative solvers with preconditioners:
  - Two-level deflation
  - Multilevel deflation
- Trade-off: either $k-$independent convergence or better memory/time complexity yet slight $k-$ dependence.

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What about multigrid as a stand-alone solver?

Multigrid - Challenges for Helmholtz

- Still open-problem
- Near-zero eigenvalues coarser level(s) (reminiscent of problem with deflation!)
- Smoother amplifies error
- Literature mostly for constant k
- Most works use restricted hierarchy (no full coarsening)

Multigrid - Our Contributions

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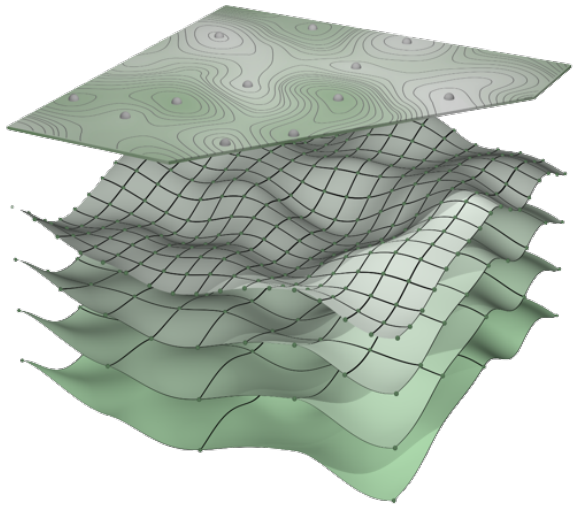
- Some remarks:
  - Main focus on convergent solver, not fast solver
  - We focus on 2D problems. So far no 3D cases in literature.

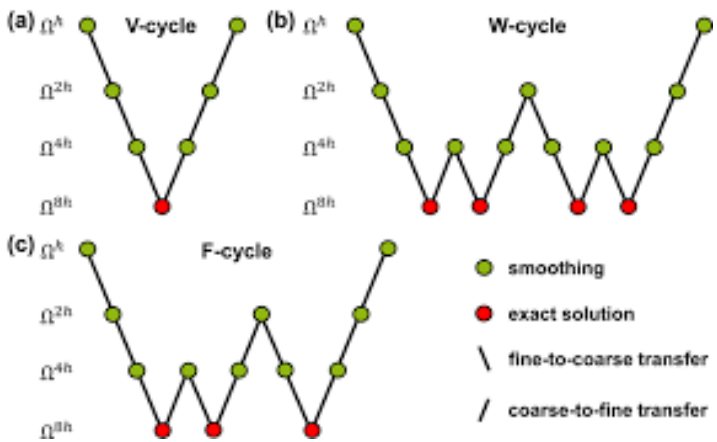
Multigrid - Overview

- Standard multigrid diverges
- But, convergence if:

  Higher-order prolongation/restriction

  Coarsening on CSL instead of original Helmholtz operator
- Small number of smoothing steps using $\omega-$Jacobi
- No restriction on coarsest grid
- Works for both $V/W-$cycles





Multigrid - Two-Grid V(1,1)

Table: Two-grid spectral radius using h.o. scheme and $w-$Jacobi smoothing. Coarsening on Helmholtz.

k	Bezier		Linear	
	$kh = 0.625$	$kh = 0.3125$	$kh = 0.625$	$kh = 0.3125$
50	0.2436	0.2852	1.290	0.9217
100	0.2441	0.2076	3.325	1.0225
250	0.2443	0.1538	5.4108	21.5327
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- H.o. scheme gives spectral radius *strictly* < 1
- Analogous to projection error *strictly* < 1 for deflation!

Multigrid - Two-Grid V(1,1)

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- Still exact solve on second-level $\Rightarrow$ memory constraints

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Can we create deeper V-cycles with more levels?

Multigrid - Divergence

Table: Number of $V(\nu,\nu)$-cycles using the Beziér scheme and coarsening on the **original Helmholtz operator**. $\times$ shows no convergence within 500 iterations.

	$k=10$			$k=20$			$k=40$		
	$N=256$ $N_D=4$			$N=1024$ $N_D=16$			$N=4096$ $N_D=64$		
Level	2	3	4	2	3	4	2	3	4
$\nu=1$	46	46	78	50	48	$\times$	52	49	$\times$
$\nu=2$	24	24	47	26	25	$\times$	27	25	$\times$
$\nu=4$	14	14	14	14	14	$\times$	15	15	$\times$
$\nu=8$	8	9	8	9	9	$\times$	9	17	$\times$

Multigrid - GMRES(3) Smoothing

Table: Number of V- ($\gamma = 1$) and W-cycles ($\gamma = 2$). ν is the number of GMRES(3) relaxations. Coarsening on CSL with shift k^{-1}.

	$k = 50$		$k = 100$		$k = 150$		$k = 200$		$k = 250$	
	$N = 6\,724$ $N_D = 8$		$N = 26\,244$ $N_D = 8$		$N = 57\,600$ $N_D = 4$		$N = 102\,400$ $N_D = 8$		$N = 160\,000$ $N_D = 4$	
γ	1	2	1	2	1	2	1	2	1	2
$\nu = 1$	14	7	24	10	39	19	51	24	64	29
$\nu = 2$	8	5	13	7	22	10	28	13	34	16
$\nu = 3$	6	5	10	6	16	9	20	10	24	12
$\nu = 4$	6	5	8	5	12	7	15	9	18	10
$\nu = 5$	5	5	7	5	11	7	13	8	15	9

- Iteration count with $\gamma = 2$ close to k-independent
- If GMRES(3) and Bezier are used, coarsening on original Helmholtz is possible as well! Here, linear would diverge!

Multigrid - GMRES(3) Smoothing

Table: Number of V- ($\gamma = 1$) and W-cycles ($\gamma = 2$). ν is the number of GMRES(3) relaxations. Coarsening on CSL with shift k^{-1}.

	$k = 50$		$k = 100$		$k = 150$		$k = 200$		$k = 250$	
	$N = 6\,724$ $N_D = 8$		$N = 26\,244$ $N_D = 8$		$N = 57\,600$ $N_D = 4$		$N = 102\,400$ $N_D = 8$		$N = 160\,000$ $N_D = 4$	
γ	1	2	1	2	1	2	1	2	1	2
$\nu = 1$	14	7	24	10	39	19	51	24	64	29
$\nu = 2$	8	5	13	7	22	10	28	13	34	16
$\nu = 3$	6	5	10	6	16	9	20	10	24	12
$\nu = 4$	6	5	8	5	12	7	15	9	18	10
$\nu = 5$	5	5	7	5	11	7	13	8	15	9

- Iteration count with $\gamma = 2$ close to k-independent
- If GMRES(3) and Bezier are used, coarsening on original Helmholtz is possible as well! Here, linear would diverge!

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γ	1	2	1	2	1	2	1	2	1	2
$\nu = 1$	14	7	24	10	39	19	51	24	64	29
$\nu = 2$	8	5	13	7	22	10	28	13	34	16
$\nu = 3$	6	5	10	6	16	9	20	10	24	12
$\nu = 4$	6	5	8	5	12	7	15	9	18	10
$\nu = 5$	5	5	7	5	11	7	13	8	15	9

- Iteration count with $\gamma = 2$ close to k-independent
- If GMRES(3) and Bezier are used, coarsening on original Helmholtz is possible as well! Here, linear would diverge!

What about heterogeneous problems?

Multigrid -(Smooth Changes)

Figure: $k(x, y)$

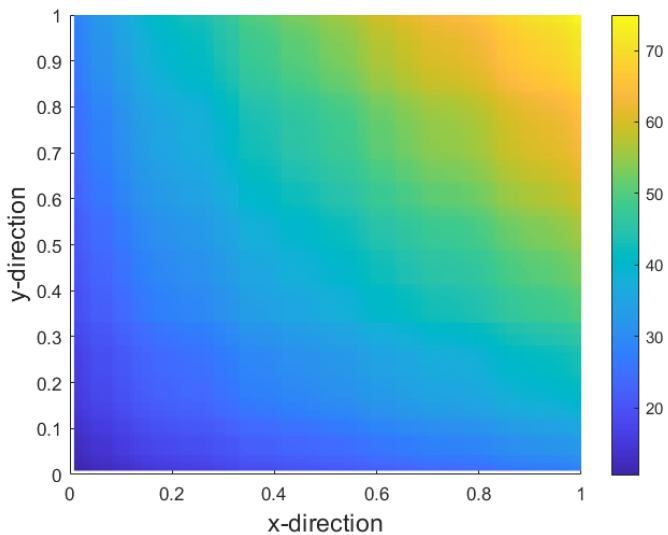

Figure: $u(x, y)$

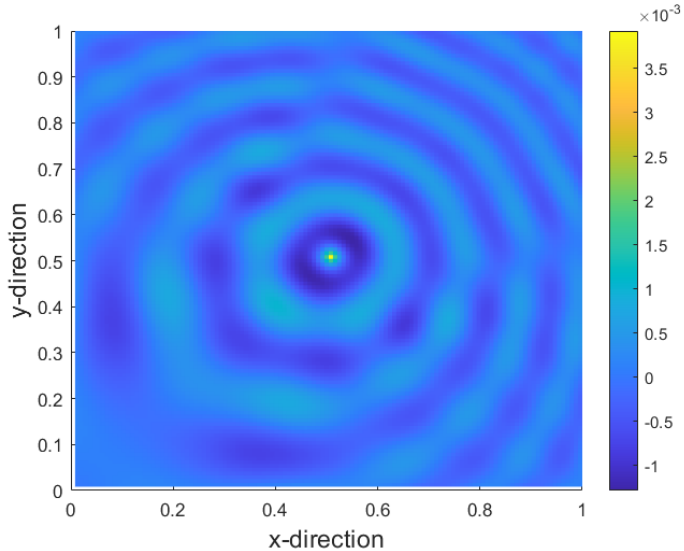

Table: Number of V- ($\gamma = 1$) and W-cycles ($\gamma = 2$). ν denotes the number of ω-Jacobi relaxations.

	$(k_1, k_2) = (10, 50)$		$(k_1, k_2) = (10, 75)$	
γ	1	2	1	2
$\nu = 4$	65	60	90	88
$\nu = 5$	62	59	86	86
$\nu = 6$	61	58	85	85
$\nu = 7$	60	57	84	84
$\nu = 8$	59	57	83	83

Multigrid - (Sharp Changes)

Figure: $k(x, y)$

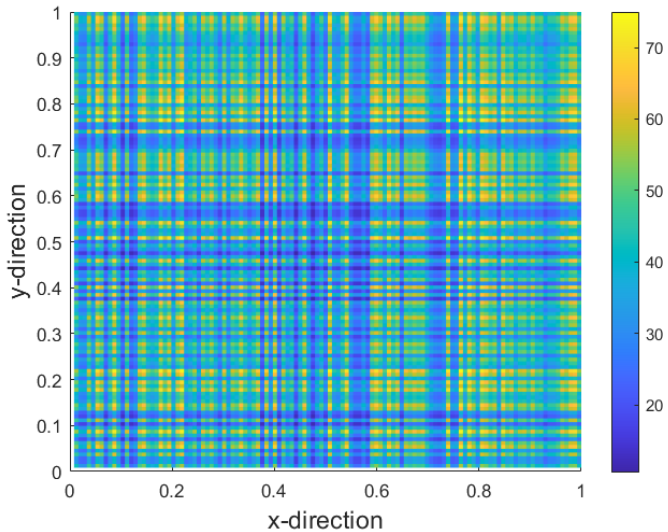

Figure: $u(x, y)$

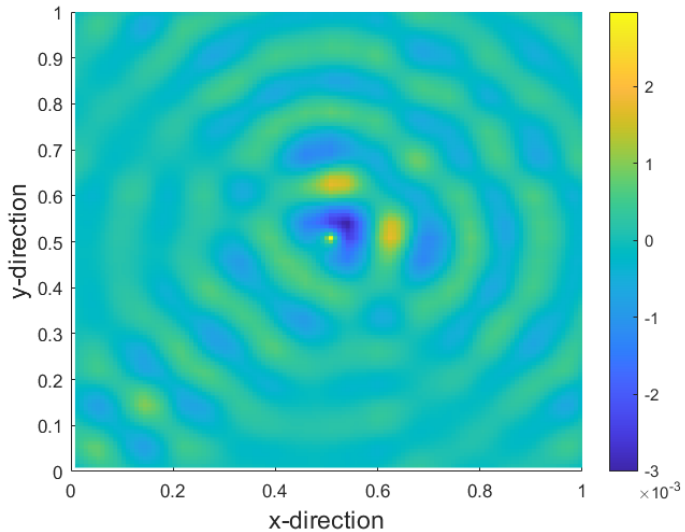

Table: Number of V- ($\gamma = 1$) and W-cycles ($\gamma = 2$) with tol 10^{-5}. ν denotes the number of ω-Jacobi smoothing steps.

	$(k_1, k_2) = (10, 50)$		$(k_1, k_2) = (10, 75)$	
γ	1	2	1	2
$\nu = 4$	102	96	111	107
$\nu = 5$	97	95	103	105
$\nu = 6$	95	95	101	104
$\nu = 7$	94	94	102	104
$\nu = 8$	94	94	102	104

Multigrid - (Sharp Changes)

Figure: $k(x, y)$

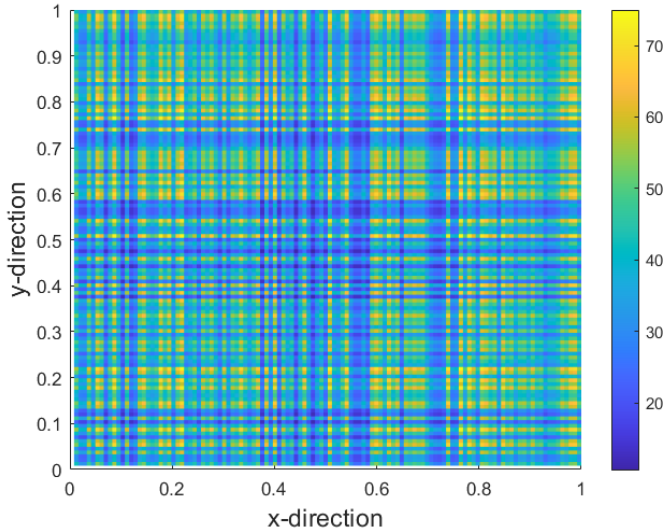

Figure: $u(x, y)$

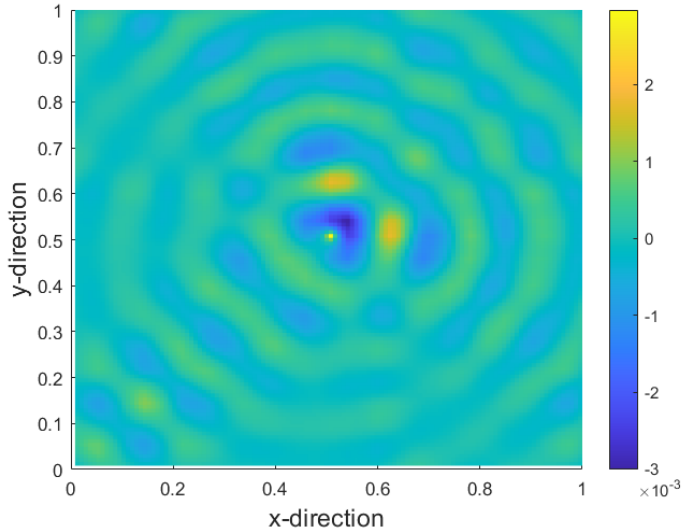

Table: Number of V- ($\gamma = 1$) and W-cycles ($\gamma = 2$) with tol 10^{-5}. ν denotes the number of GMRES(3) smoothing steps.

	$(k_1, k_2) = (10, 50)$		$(k_1, k_2) = (10, 75)$	
γ	1	2	1	2
$\nu = 1$	28	12	31	12
$\nu = 2$	16	8	17	7
$\nu = 3$	12	7	12	6
$\nu = 4$	10	6	10	6
$\nu = 5$	9	6	9	6

Conclusion

- Wave problems lead to indefinite systems
- Near-zero eigenvalues of fine/coarse systems
- New deflation scheme: higher-order approximation
- Two-level method k-independent convergence but memory constrained
- Use higher-order scheme in multilevel methods
  1. Multilevel deflation (preconditioner)
  2. Multigrid (stand-alone solver)

     First convergent classical solver for the 2D indefinite Helmholtz

     First converging scheme for non-constant wavenumbers in 2D.
- Properties of our Multigrid method

  Higher-order prolongation/restriction

  Coarsening on CSL instead of original Helmholtz operator

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