Multigrid for Helmholtz revisited

Methods for Indefinite Systems

Delft University of Technology

Vandana Dwarka

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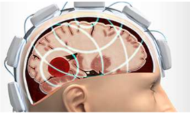
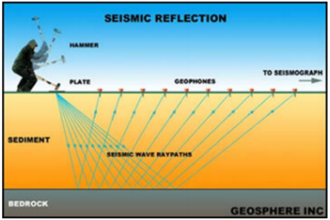
Introduction

- 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

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

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

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

- Using Sommerfeld BC's A becomes non-Hermitian indefinite

Preconditioning - CSLP

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

$$
\begin{aligned}
M &= L - (\beta_1 - \beta_2 i)k^2 I, \\
&= A + \beta_2 i k^2 I, \\
&(\beta_1, \beta_2) \in (0, 1]
\end{aligned}
$$

- L is the discretized Laplace operator

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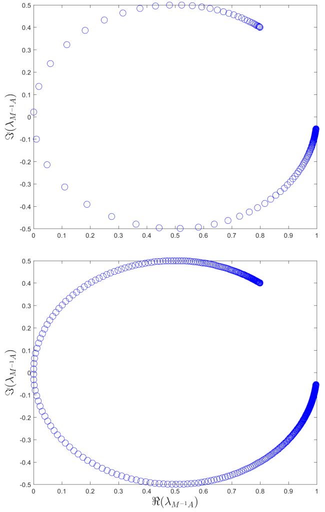
$$M = L - (\beta_1 - \beta_2 i)k^2 I,$$
$$= A + \beta_2 i k^2 I,$$
$$(\beta_1, \beta_2) \in (0, 1]$$

- L is the discretized Laplace operator
- Increasing $k \Rightarrow$ eigenvalues move fast towards origin $\Rightarrow$ inscalable CSLP-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 1D-problem!
- k increases $\Rightarrow$ more near-zero eigenvalues $\Rightarrow$ more iterations
- Project unwanted eigenvalues onto zero = Deflation

Preconditioning - Deflation

- Projection principle: solve $PAu = Pf$

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

- Columns of Z span deflation subspace
- Ideally Z contains eigenvectors
- In practice approximations: inter-grid vectors from multigrid (linear interpolation polynomial)
- Use DEF + CSLP 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

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

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

Preconditioning - Deflation

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

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

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

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

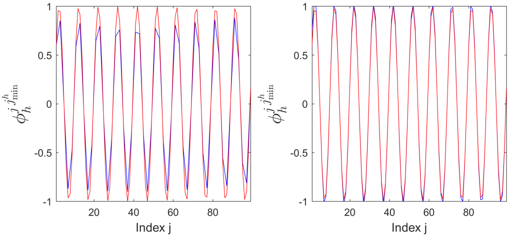


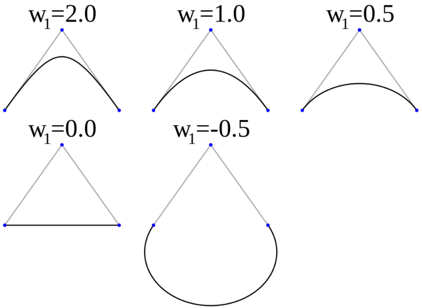
Table: Projection error DEF-scheme

k	$E(0.625)$	$E(0.3125)$
10^2	0.88	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 ⇒ 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
- Confirmed with RFA and spectral analysis for Dirichlet BC

Two-Level Deflation - 3D

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

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

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

Multilevel methods

Multilevel Deflation

- Pros

  Close to linear complexity

  Memory efficient

  Recursive structure

  Use as preconditioner with FGMRES
- Cons

  Needs more inner cycles

  Convergence depends weakly on k

Multigrid

- Pros

  Linear complexity

  Memory efficient

  Recursive structure

  Use as stand-alone or preconditioner
- Cons

  Diverges for Helmholtz

  Slow convergence small k

Multigrid - Challenges for Helmholtz

- Still open-problem
- Near-zero eigenvalues coarser level(s)
- Smoother amplifies error
- Literature mostly for constant k and restricted hierarchy (no full coarsening)

Multigrid - Two-Grid V(1,1)

- Constant k using Sommerfeld BC
- Damped Jacobi smoothing
- Coarsening on Helmholtz operator

Table: Two-grid spectral radius using h.o. scheme

k	Quadratic 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
500	0.2443	0.1354	15.5047	21.5327
1000	0.2443	0.1350	27.7478	21.5327

- H.o. scheme gives spectral radius *strictly* < 1
- Analogous to projection error *strictly* < 1 for deflation!

Multigrid - 2D

- Constant k using Sommerfeld BC
- Construct two-grid V(1,1)-cycle
- Coarsening on Helmholtz operator

k	$\omega-$Jacobi		Gaus-Seidel	
	$kh = 0.625$	$kh = 0.3125$	$kh = 0.625$	$kh = 0.3125$
50	14	14	6	5
100	14	14	6	5
250	14	14	6	5
500	14	14	6	5

- Both cases k-independence
- Still exact solve on second-level $\Rightarrow$ memory constraints
- Can we create a deeper V-cycle?

Multigrid - 2D

- Constant k using Sommerfeld BC
- Three-grid cycle with $kh_{coarsest} = 2.5 \approx \frac{2\pi}{2.5}$

Figure: V-cycle

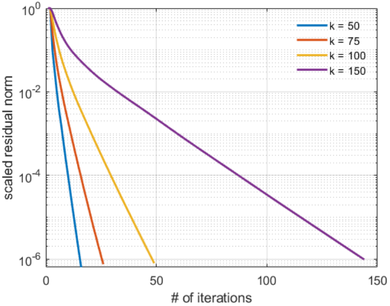
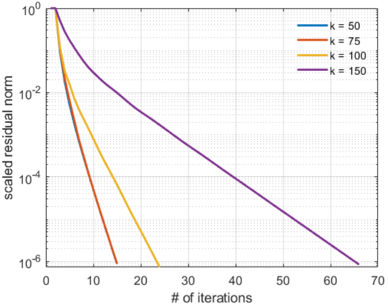


Figure: F-cycle



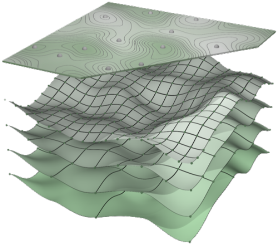
- Deeper cycle diverges despite h.o. scheme $\Rightarrow$ coarsen on CSLP using level-dependent scheme + GMRES(3) smoothing (Cools)

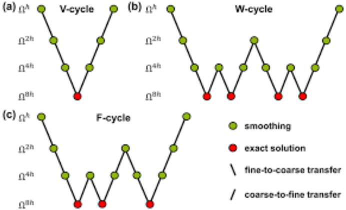
Multigrid

- With CSL coarsening, level-dependent parameter (Cools)
- But, level-indep. convergence if:

    Higher-order prolongation/restriction (deflation!)
    Coarsening on CSL

- Small number of smoothing steps using $\omega-$Jacobi
- No restriction on coarsest grid
- Works for both $V/W-$cycles





Multigrid - Idea of Proof

We assume post-smoothing, then the iteration matrix T_0 is:

$$T_0 = \left(I - P{A_c}^{-1}P'A\right)\left(I - X^{-1}A\right).$$

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We write T_0 as $T_0 = I - DA$, such that

$$T_0^H T_0 = I - \Gamma$$

Next, if Γ is HPD, then the two-grid iteration converges.

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We show that:

1. Coarsening on CSL instead of A and
2. Using h.o. interpolation & restriction,

leads to Γ HPD.

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Next, if Γ is HPD, then the two-grid iteration converges.
We show that:

1. Coarsening on CSL instead of A and
2. Using h.o. interpolation & restriction,

leads to Γ HPD.
Remark:

1. Γ can be HPD, while DA is **not**

Multigrid - Idea of Proof

Consequently, our two-grid iteration matrix becomes:

$$T_0 = \left(I - P{C_c}^{-1}P'A\right)\left(I - X^{-1}A\right).$$

with $C_c = P'CP$, X damped-Jacobi.

Multigrid - Idea of Proof

Consequently, our two-grid iteration matrix becomes:

$$T_0 = \left(I - P C_c^{-1} P' A\right)\left(I - X^{-1} A\right).$$

with $C_c = P'CP$, X damped-Jacobi.

	Linear				Bezier			
k	A, A_c		A, C_c		A, A_c		A, C_c	
5	$\times$	0.960	$\times$	0.960	$\checkmark$	0.865	$\checkmark$	0.865
10	$\times$	1.004	$\times$	0.999	$\times$	0.887	$\checkmark$	0.887
20	$\times$	1.081	$\times$	1.015	$\times$	0.896	$\checkmark$	0.896
30	$\times$	1.122	$\times$	1.021	$\times$	0.898	$\checkmark$	0.898

Table: Spectral radius of T_0 with 1 post-smoothing step using damped-Jacobi.

Multigrid - 2D

- Constant k using Sommerfeld BC

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

	$k = 50$		$k = 100$		$k = 150$		$k = 200$		$k = 250$	
	$N = 6\ 724$ $N_D = 8$		$N = 26\ 244$ $N_D = 8$		$N = 57\ 600$ $N_D = 4$		$N = 102400$ $N_D = 8$		$N = 160\ 000$ $N_D = 4$	
γ	1	2	1	2	1	2	1	2	1	2
$\nu = 4$	58	58	104	108	155	159	209	213	267	271
$\nu = 5$	58	58	104	104	150	166	194	229	238	287
$\nu = 6$	55	58	99	102	139	167	183	222	226	283
$\nu = 7$	53	60	97	101	136	163	179	219	221	280
$\nu = 8$	53	60	95	104	131	161	178	212	218	277

- Coarsening on CSLP (shift $= 0.7$)
- Linear interpolation still diverges ($k = 50, \gamma = 1$)
- What about GMRES(3) smoothing? (Elman)

Multigrid - 2D

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	$k = 50$		$k = 100$		$k = 150$		$k = 200$		$k = 250$	
	$N = 6\ 724$ $N_D = 8$		$N = 26\ 244$ $N_D = 8$		$N = 57\ 600$ $N_D = 4$		$N = 102\ 400$ $N_D = 8$		$N = 160\ 000$ $N_D = 4$	
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

- Coarsening + on CSLP (shift $= k^{-1}$)
- Iteration count with $\gamma = 2$ close to k-independent
- Linear interpolation 199 iterations ($k = 50, \gamma = 1$)
- What about heterogeneous problems?

Multigrid - 2D random k (high-contrast)

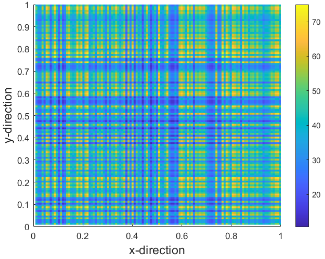


Figure: $k(x, y)$

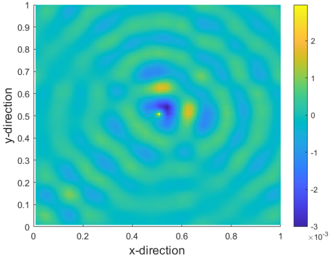


Figure: $u(x, y)$

Table: Number of V- ($\gamma = 1$) and W-cycles ($\gamma = 2$). 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

Multigrid - 2D Wedge Model

Figure: $k(x,y)$

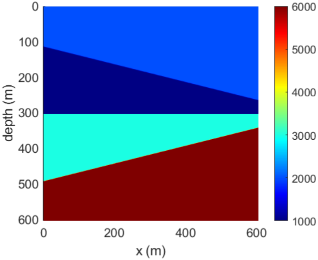
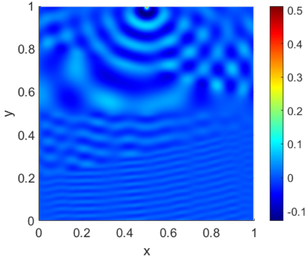


Figure: $u(x,y)$



f (Hz)	$k(x,y) = \dfrac{2L\pi f}{c(x,y)}$	Iterations
4	[4.18 , 25.13]	78
8	[8.37 , 50.26]	179
12	[12.56 , 75.39]	381
14	[14.66 , 87.96]	610
16	[16.75 , 100.53]	794

Table: Number of V-cycles ($\gamma = 1$) with coarsening until size of the system is less than 10×10. We use tolerance 10^{-8} with fixed 8 pre- and post-smoothing with damped Jacobi.

Conclusion

- Non-Hermitian indefinite systems cause many convergence issues
- Deflation gives k-independent convergence, but memory constrained (two-level)
- Use higher-order approximation from deflation for multigrid
- H.o. scheme + CSL coarsening $\Rightarrow$ convergence
- We lose k-independent convergence

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