A decade of fast and robust Helmholtz solvers

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Contents

The Helmholtz equation

The Helmholtz equation without damping

$$-\Delta \mathbf{u}(x,y) - k^2(x,y)\mathbf{u}(x,y) = \mathbf{g}(x,y) \ \text{ in } \Omega$$

$\mathbf{u}(x,y)$ is the pressure field,
$\mathbf{k}(x,y)$ is the wave number,
$\mathbf{g}(x,y)$ is the point source function and
Ω is the domain. Absorbing boundary conditions are used on Γ.

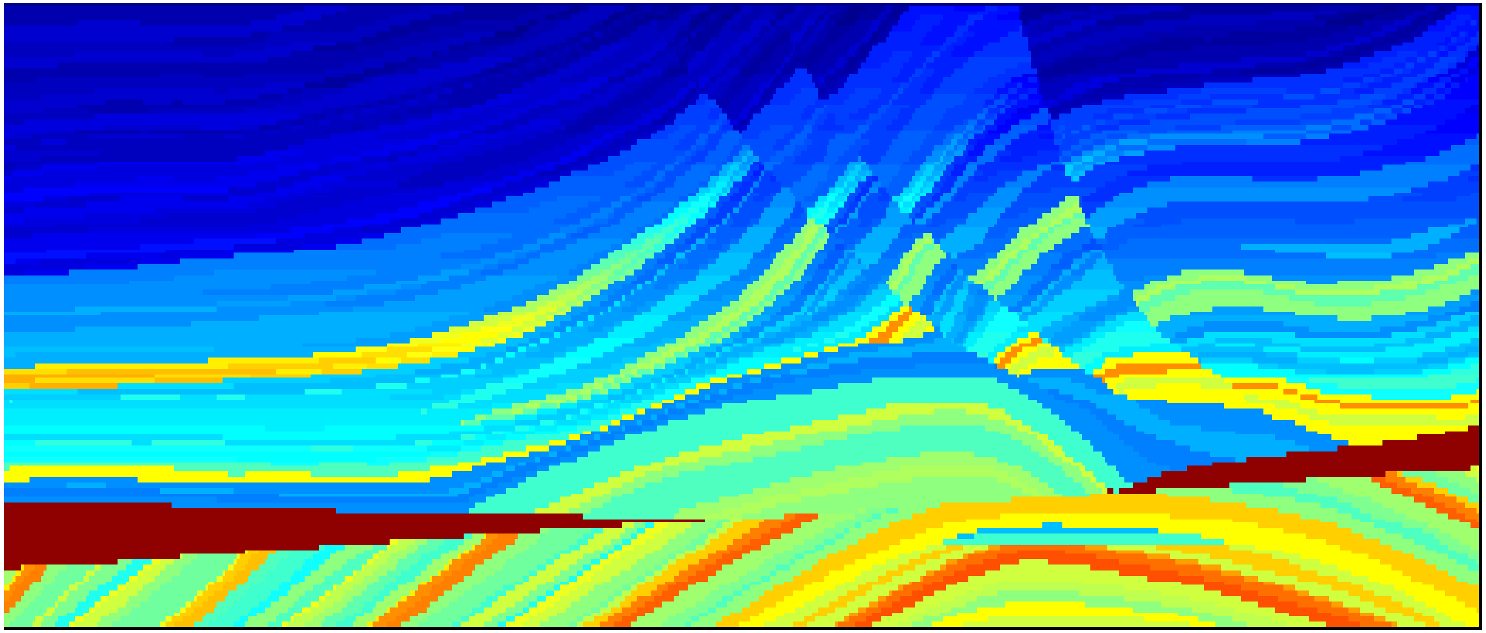
$$\frac{\partial \mathbf{u}}{\partial n} - \iota \mathbf{u} = 0$$

n is the unit normal vector pointing outwards on the boundary.

Perfectly Matched Layer (PML) and Absorbing Boundary Layer (ABL)

Application: geophysical survey

hard Marmousi Model



Problem description

- Second order Finite Difference stencil:

$$\begin{bmatrix} & -1 & \\ -1 & 4-k^2h^2 & -1 \\ & -1 & \end{bmatrix}$$

- Linear system $Au = g$: properties
  Sparse & complex valued
  Symmetric & Indefinite for large k
- For high resolution a very fine grid is required: $30-60$ gridpoints per wavelength (or $\approx 5-10 \times k$) $\rightarrow A$ is extremely large!
- Is traditionally solved by a Krylov subspace method, which exploits the sparsity.

Survey of solution methods

Special Krylov methods

- COCG van der Vorst and Melissen, 1990
- QMR Freund and Nachtigal, 1991

General purpose Krylov methods

- CGNR Paige and Saunders, 1975
- Short recurrences
  Bi-CGSTAB van der Vorst, 1992
  IDR(s) Van Gijzen and Sonneveld, 2008
- Minimal residual
  GMRES Saad and Schultz, 1986
  GCR Eisenstat, Elman and Schultz, 1983
  GMRESR van der Vorst and Vuik, 1994

Preconditioning

Equivalent linear system $M_1^{-1}AM_2^{-1}\tilde{x} = \tilde{b}$, where $M = M_1 \cdot M_2$ is the preconditioning matrix and

$$\tilde{x} = M_2 x, \quad \tilde{b} = M_1 b.$$

Requirements for a preconditioner

- better spectral properties of $M^{-1}A$
- cheap to perform $M^{-1}r$.

Spectrum of A is $\{\mu_i - k^2\}$, with k is constant and μ_i are the eigenvalues of the Laplace operator. Note $\mu_1 - k^2$ may be negative.

Preconditioning

ILU	Meijerink and van der Vorst, 1977
ILU(tol)	Saad, 2003
SPAI	Grote and Huckle, 1997
Multigrid	Lahaye, 2001
	Elman, Ernst and O' Leary, 2001
AILU	Gander and Nataf, 2001
	analytic parabolic factorization
ILU-SV	Plessix and Mulder, 2003
	separation of variables

Preconditioning

Laplace operator	Bayliss and Turkel, 1983
Definite Helmholtz	Laird, 2000
Shifted Laplace	Y.A. Erlangga, C. Vuik and C.W.Oosterlee, 2003

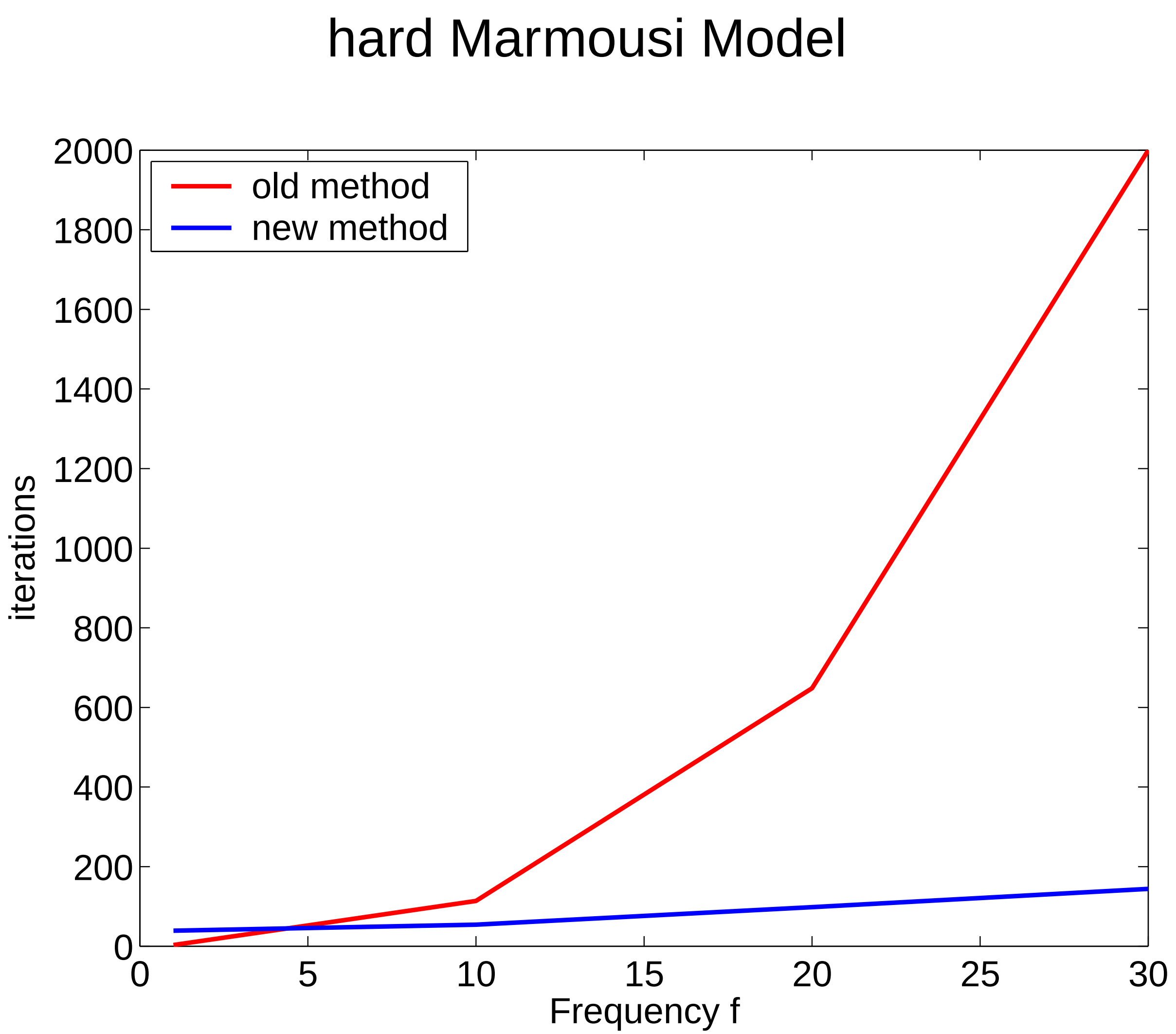
Shifted Laplace preconditioner

$$M \equiv -\Delta - (\beta_1 - \mathrm{i}\beta_2)k^2, \;\; \beta_1, \beta_2 \in \mathbb{R}, \;\; \text{and} \;\; \beta_1 \leq 0.$$

Condition $\beta_1 \leq 0$ is used to ensure that M is a (semi) definite operator.

$\rightarrow \beta_1, \beta_2 = 0$	:	Bayliss and Turkel
$\rightarrow \beta_1 = 1, \beta_2 = 0$	:	Laird
$\rightarrow \beta_1 = -1, \beta_2 = 0.5$	:	Y.A. Erlangga, C. Vuik and C.W.Oosterlee

Application: geophysical survey



Numerical experiments

Example with constant k in Ω

Iterative solver: Bi-CGSTAB

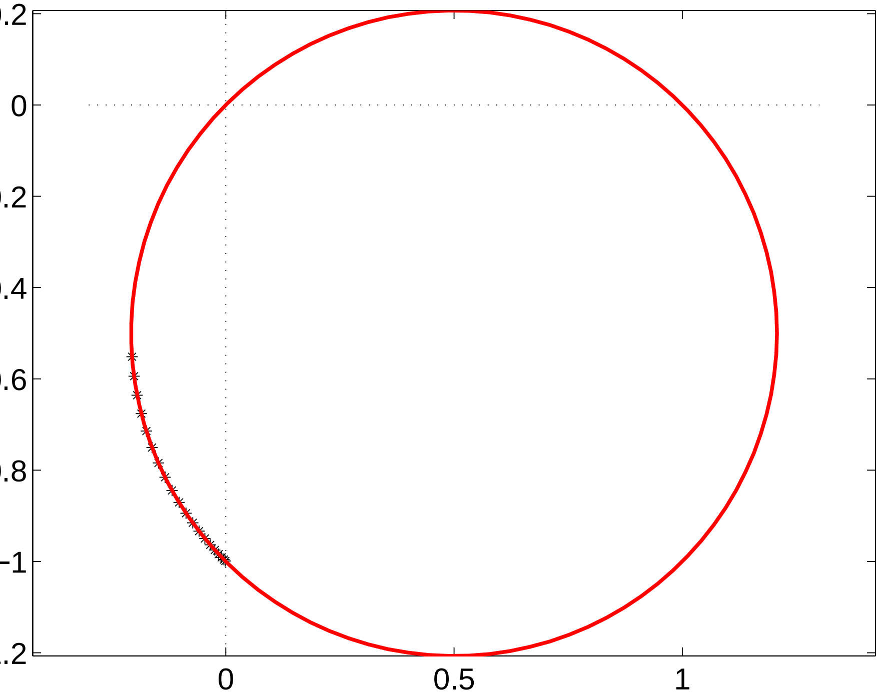
Preconditioner: Shifted-Laplace operator, discretized using the same method as the Helmholtz operator.

k	ILU(0.01)	M_0	M_1	M_i
5	9	13	13	13
10	25	29	28	22
15	47	114	45	26
20	82	354	85	34
30	139	> 1000	150	52

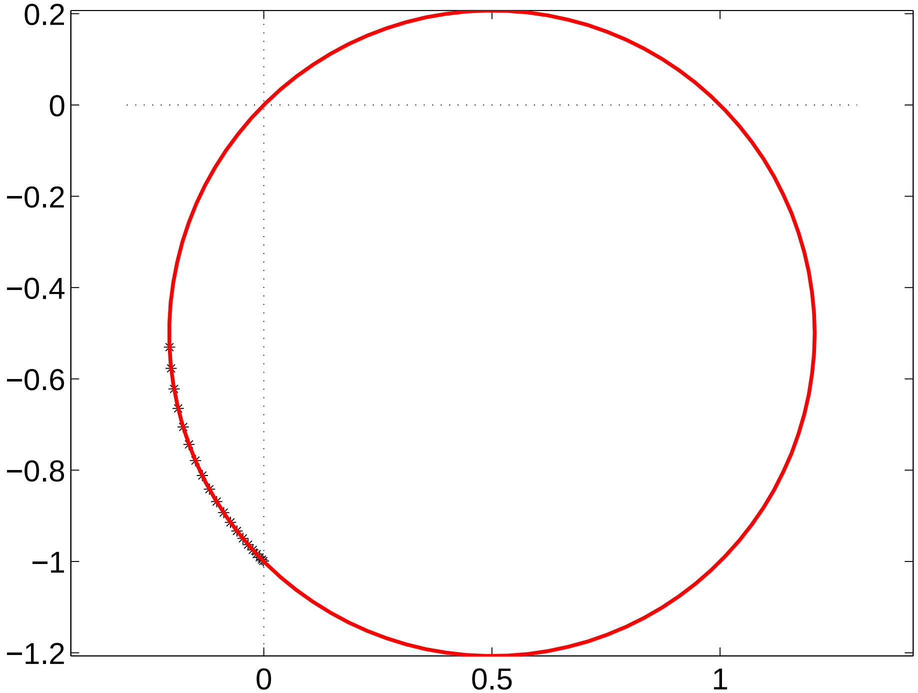
Eigenvalues for Complex preco $k = 100$

20 smallest eigenvalues

75 grid points



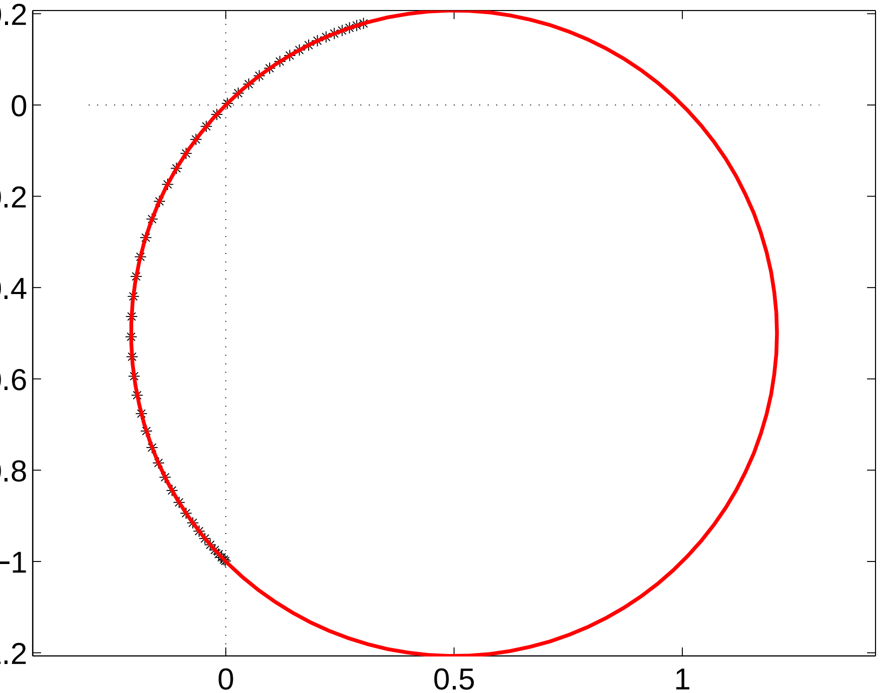
150 grid points



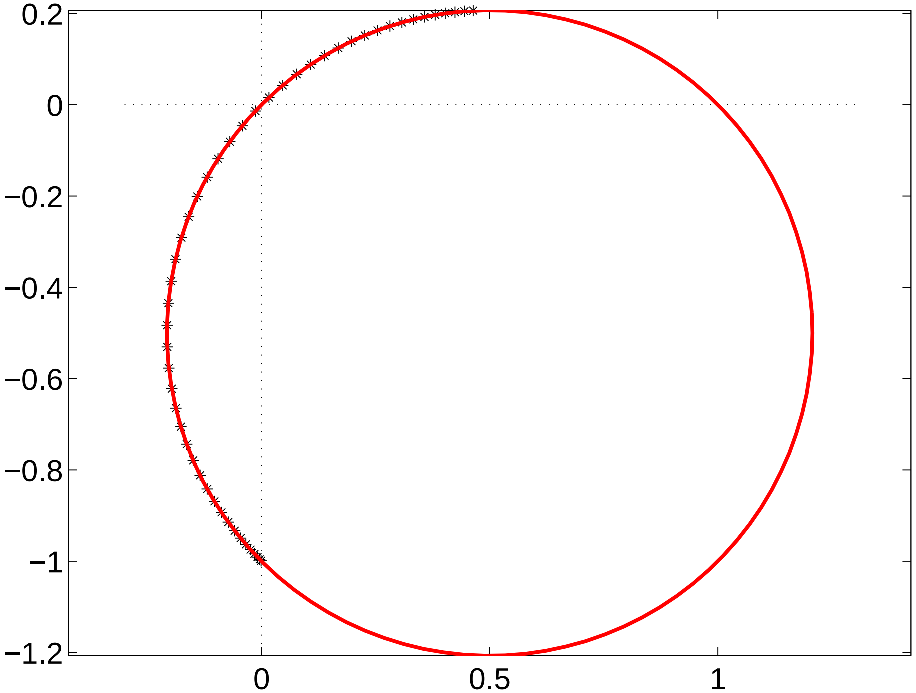
Eigenvalues for Complex preco $k = 100$

50 smallest eigenvalues

75 grid points



150 grid points

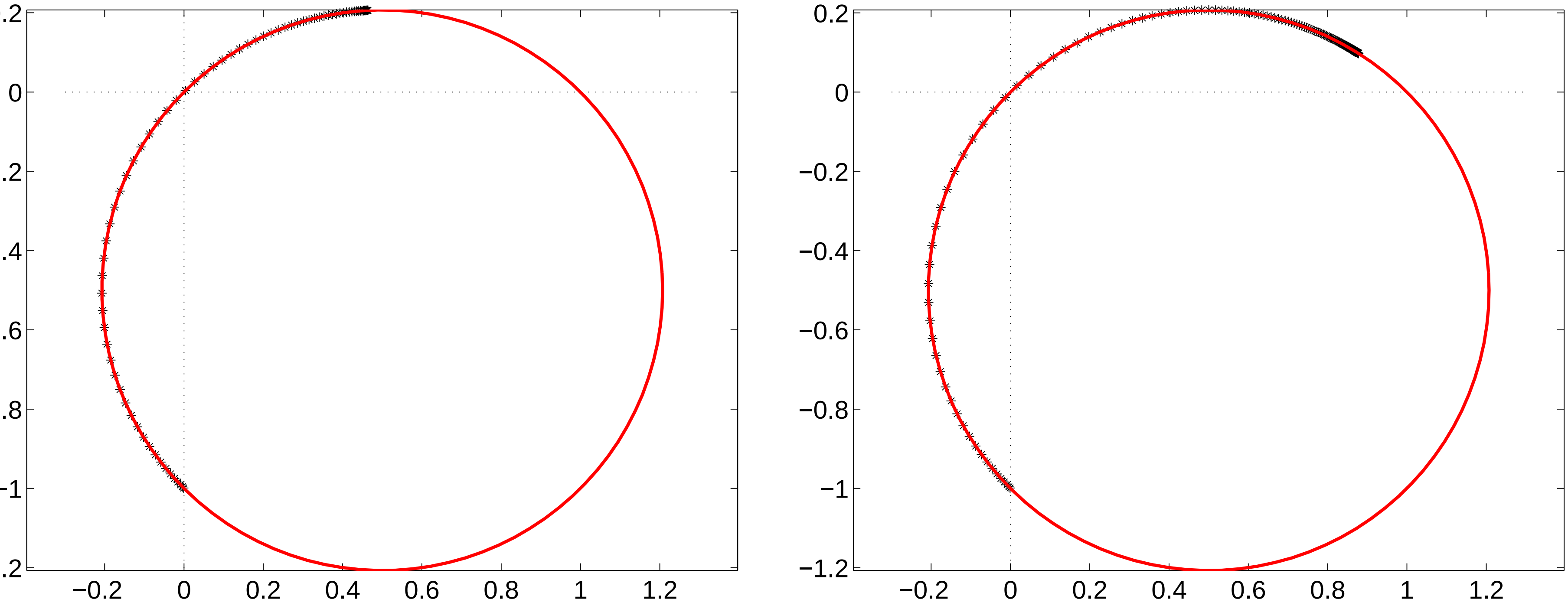


Eigenvalues for Complex preco $k = 100$

spectrum is independent of the grid size

75 grid points

150 grid points



Inner iteration

Possible solvers for solution of $Mz = r$:

- ILU approximation of M
- inner iteration with ILU as preconditioner
- Multigrid

Multigrid components
- geometric multigrid
- Gauss-Seidel with red-black ordering
- matrix dependent interpolation, full weighting restriction

- Galerkin coarse grid approximation

Inner iteration

- geometric multigrid
- ω-JAC smoother
- bilinear interpolation, restriction operator full weighting
- Galerkin coarse grid approximation
- F(1,1)-cycle
- M^{-1} is approximated by *one* multigrid iteration

Numerical results for a wedge problem

k_2	10	20	40	50	100
grid	32^2	64^2	128^2	192^2	384^2
No-Prec	201(0.56)	1028(12)	5170(316)	–	–
ILU(A,0)	55(0.36)	348(9)	1484(131)	2344(498)	–
ILU(A,1)	26(0.14)	126(4)	577(62)	894(207)	–
ILU(M,0)	57(0.29)	213(8)	1289(122)	2072(451)	–
ILU(M,1)	28(0.28)	116(4)	443(48)	763(191)	2021(1875)
MG(V(1,1))	13(0.21)	38(3)	94(28)	115(82)	252(850)

Spectrum of shifted Laplacian preco

References: Manteuffel, Parter, 1990; Yserentant, 1988

Since L and M are SPD we have the following eigenpairs

$$Lv_j = \lambda_j M v_j, \text{ where, } \lambda_j \in \mathbb{R}^+$$

The eigenvalues σ_j of the preconditioned matrix satisfy

$$(L - z_1 M)v_j = \sigma_j (L - z_2 M)v_j.$$

Theorem 1

Provided that $z_2 \neq \lambda_j$, the relation

$$\sigma_j = \frac{\lambda_j - z_1}{\lambda_j - z_2} \text{ holds.}$$

Spectrum of shifted Laplacian preco

Theorem 2

If $\beta_2 = 0$, the eigenvalues $\sigma_r + \mathrm{i}\sigma_i$ are located on the straight line in the complex plane given by

$$\beta_1 \sigma_r - (\alpha_1 - \alpha_2)\sigma_i = \beta_1.$$

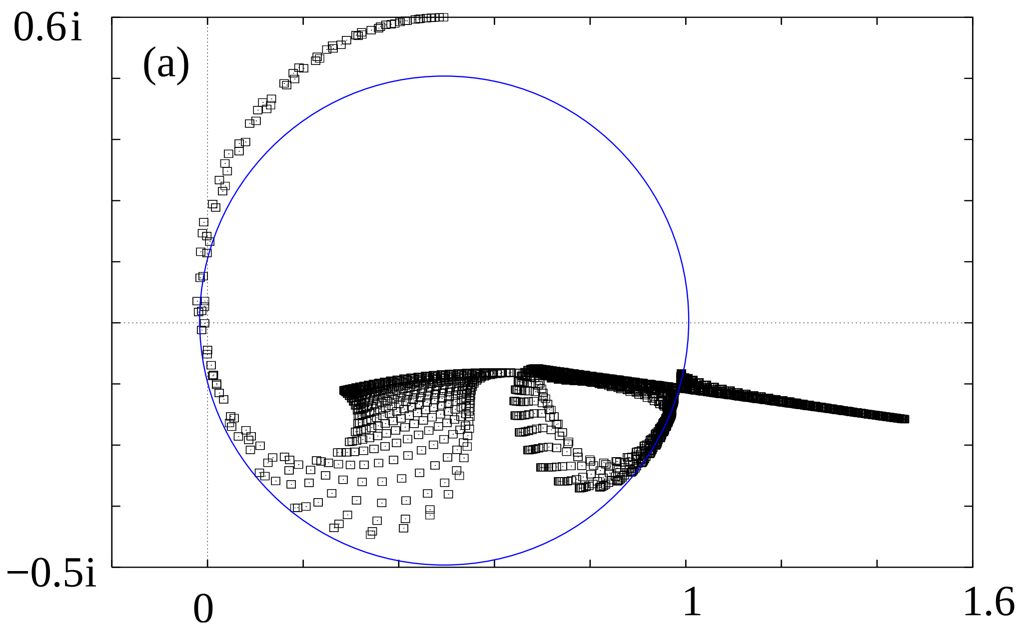
Theorem 3

If $\beta_2 \neq 0$, the eigenvalues $\sigma_r + \mathrm{i}\sigma_i$ are on the circle in the complex plane with center c and radius R:

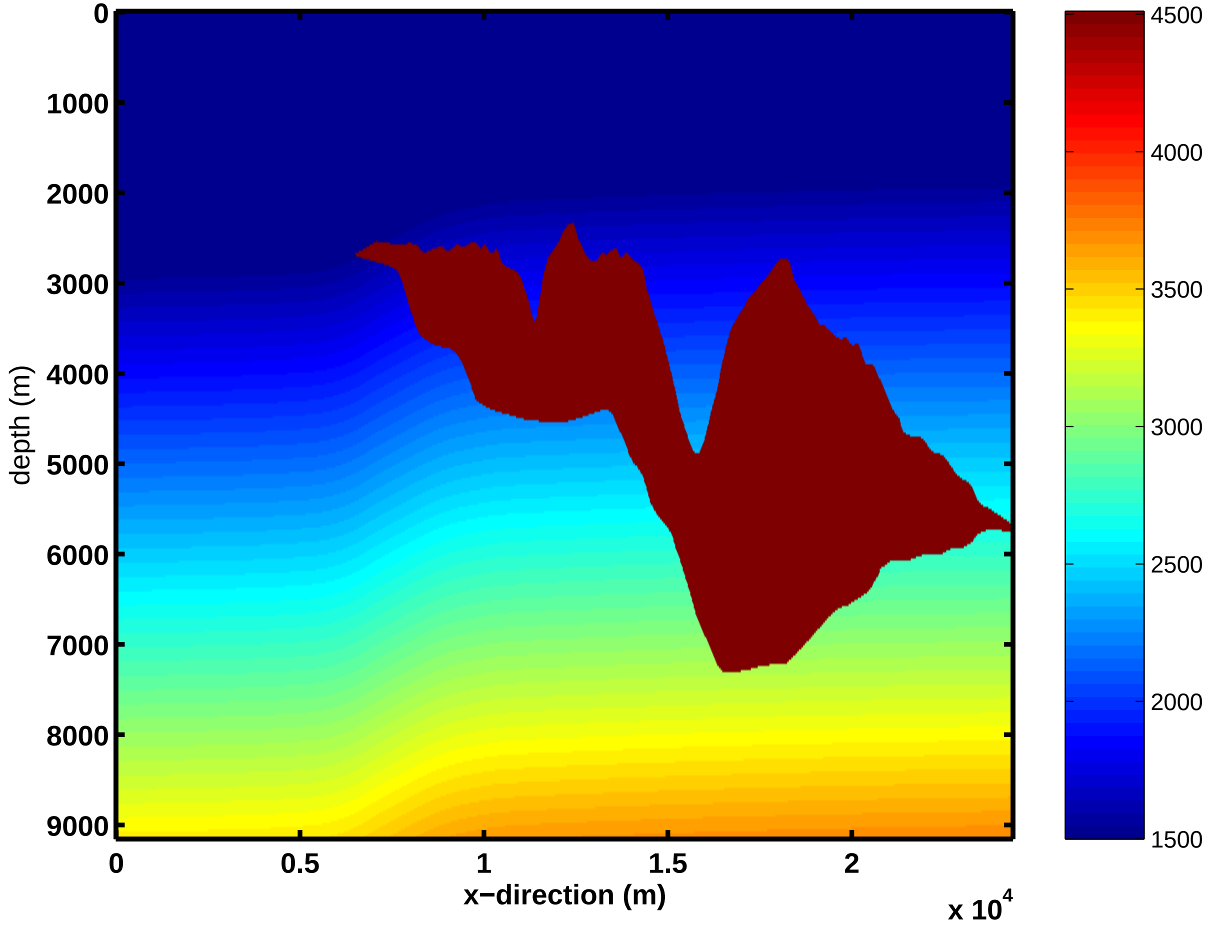
$$c = \frac{z_1 - \bar{z}_2}{z_2 - \bar{z}_2}, \quad R = \left| \frac{z_2 - z_1}{z_2 - \bar{z}_2} \right|.$$

Note that if $\beta_1\beta_2 > 0$ the origin is not enclosed in the circle.

Spectrum with inner iteration



Sigsbee model



Sigsbee model

$dx = dz = 22.86$ m; $D = 24369 \times 9144$ m^2; grid points 1067×401.

Bi-CGSTAB	5 Hz		10 Hz	
	CPU (sec)	Iter	CPU (sec)	Iter
NO preco	3128	16549	1816	9673
With preco	86	48	92	58

Second Level Preconditioning

- ILU and variants
- From Laplace to complex Shifted Laplace Preconditioner (2005)
- Shifted Laplace Preconditioner (SLP)

$$M := -\Delta \mathbf{u} - (\beta_1 - \iota\beta_2)k^2\mathbf{u}$$

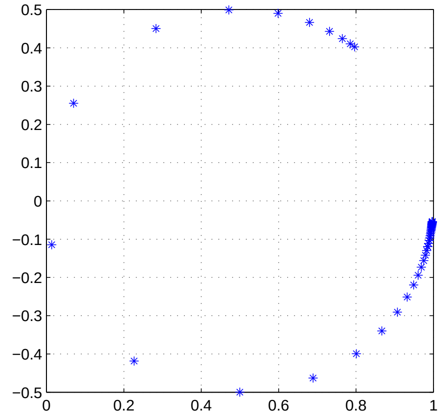
- Results shows: $(\beta_1, \beta_2) = (1, 0.5)$ is the shift of choice
- What is the effect of SLP?

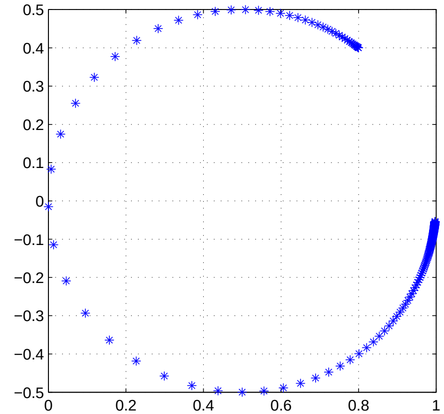
Shifted Laplace Preconditioner

- Introduces damping, Multi-grid approximation is possible
- The modulus of all eigenvalues of the preconditioned operator is bounded by 1
- Small eigenvalues move to zero, as k increases.

Spectrum of $M^{-1}(1, 0.5)A$ for

$k = 30$ and $k = 120$





Some Results at a Glance

Number of GMRES iterations. Shifts in the preconditioner are $(1, 0.5)$

Grid	$k = 10$	$k = 20$	$k = 30$	$k = 40$	$k = 50$	$k = 100$
$n = 32$	**10**	17	28	44	70	14
$n = 64$	10	**17**	28	36	45	163
$n = 96$	10	17	**27**	35	43	97
$n = 128$	10	17	27	**35**	43	85
$n = 160$	10	17	27	35	**43**	82
$n = 320$	10	17	27	35	42	**80**

Number of iterations depends linearly on k.

Deflation improves the convergence

Number of GMRES iterations. Shifts in the preconditioner are $(1, 0.5)$

Grid	$k = 10$	$k = 20$	$k = 30$	$k = 40$	$k = 50$	$k = 100$
$n = 32$	**5/10**	8/17	14/28	26/44	42/70	13/14
$n = 64$	4/10	**6/17**	8/28	12/36	18/45	173/163
$n = 96$	3/10	5/17	**7/27**	9/35	12/43	36/97
$n = 128$	3/10	4/17	6/27	**7/35**	9/43	36/85
$n = 160$	3/10	4/17	5/27	6/35	**8/43**	25/82
$n = 320$	3/10	4/17	4/27	5/35	5/42	**10/80**

Erlangga and Nabben, 2008, seems to be independent of k.

with / without deflation.

Erlangga and Nabben algorithm

Setting up:

For $k = 1$, set $A^{(1)} = A$, $M^{(1)} = M$, construct $Z^{(1,2)}$, $\lambda_{max}^{(k)} = 1, \ \forall \ k$.

From above, $\hat{A}^{(1)} = A^{(1)} {M^{(1)}}^{-1}$ and $P_{\lambda_{max}}^{(1)} = I - \hat{Q}^{(1)}\hat{A}^{(1)} + \hat{Q}^{(1)}$ with $\hat{Q}^{(1)} = Z^{(1,2)} {\hat{A}^{(2)}}^{-1} {Z^{(1,2)}}^T$

For $k = 2, \ldots, m$, construct $Z^{(k-1,k)}$ and compute

$$A^{(k)} = {Z^{(k-1,k)}}^T A^{(k-1)} Z^{(k-1,k)}, \ M^{(k)} = {Z^{(k-1,k)}}^T M^{(k-1)} Z^{(k-1,k)}$$

and

$$P_{\lambda_{max}}^{(k)} = I - Z^{(k,k+1)} {\hat{A}^{(k+1)}}^{-1} {Z^{(k,k+1)}}^T \left(\hat{A}^{(k)} - I \right) \text{ with } \hat{A}^{(k)} = A^{(k)} {M^{(k)}}^{-1}$$

Inside Iterations

Solve: $A^{(2)}{M^{(2)}}^{-1}v_R^{(2)} = (v_R)^{(2)}$ with Krylov

$v_A^{(2)} = A^{(2)}v^{(2)}$;

$s^{(2)} = {M^{(2)}}^{-1}v_A^{(2)}$;

$t^{(2)} = s^{(2)} - \lambda_{max}^{(2)}v^{(2)}$;

Restriction: $(v_R)^{(3)} = {Z^{(2,3)}}^T t^{(2)}$

If $k = m$

$v_R^{(m)} = {A^{(m)}}^{-1}(v'_R)^{(m)}$

else

Solve: $A^{(3)}{M^{(3)}}^{-1}v_R^{(3)} = (v_R)^{(3)}$ with Krylov

$\ldots$

Interpolation: $v_I^{(2)} = Z^{(2,3)}v_R^{(3)}$

$q^{(2)} = v^{(2)} - v_I^{(2)}$

$w^{(2)} = {M^{(2)}}^{-1}q^{(2)}$

$p^{(2)} = A^{(2)}w^{(2)}$

Deflation: or two-grid method

For any deflation subspace matrix

$$Z \in R^{n\times r}, \quad \text{with deflation vectors} \quad Z = [z_1, ..., z_r], \quad rank Z = r$$

$$P = I - AQ, \quad \text{with} \quad Q = ZE^{-1}Z^T \quad \text{and} \quad E = Z^TAZ$$

Solve $PAu = Pg$ preconditioned by M^{-1} or $M^{-1}PA = M^{-1}Pg$
For e.g. say,

$$\textbf{spec}(A) = \{\lambda_1, \lambda_2, \lambda_3, ..., \lambda_n\}$$

and if Z is the matrix with columns the r eigenvectors then

$$\textbf{spec}(PA) = \{0, ..., 0, \lambda_{r+1}, ...\lambda_n\}$$

Deflation

We use multi-grid inter-grid transfer operator (Prolongation) as deflation matrix.

Setting $Z = I_h^{2h}$ and $Z^T = I_{2h}^h$ then

$$P = I - AQ, \quad \text{with} \quad Q = I_h^{2h} E^{-1} I_{2h}^h \text{ and } E = I_{2h}^h A I_h^{2h}$$

where

P can be interpreted as a coarse grid correction and

Q as the coarse grid operator

Fourier Analysis

Dirichlet boundary conditions for analysis.

With above deflation,

$$\textbf{spec}(PM^{-1}A) = f(\beta_1, \beta_2, k, h)$$

is a complex valued function.

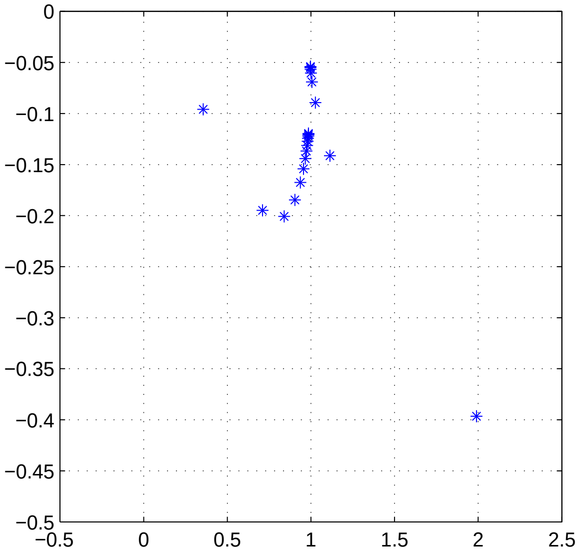
Setting $kh = 0.625$,

- Spectrum of $PM^{-1}A$ with shifts $(1, 0.5)$ is clustered around 1 with a few outliers.
- Spectrum remains almost the same, when the imaginary shift is varied from 0.5 to 1.

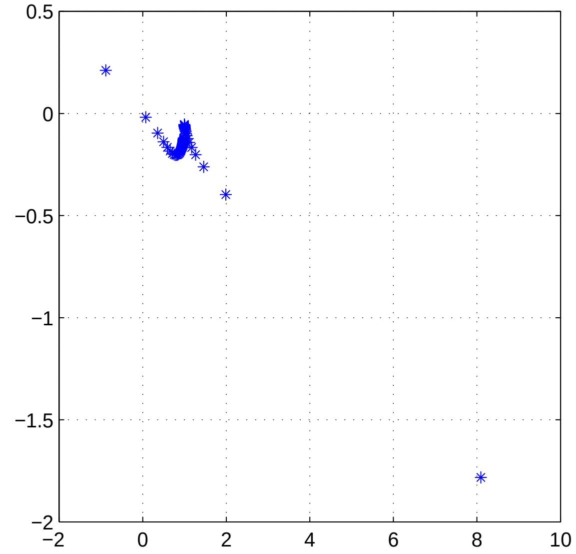
Fourier Analysis

Analysis shows spectrum clustered around 1 with few outliers.

$k = 30$



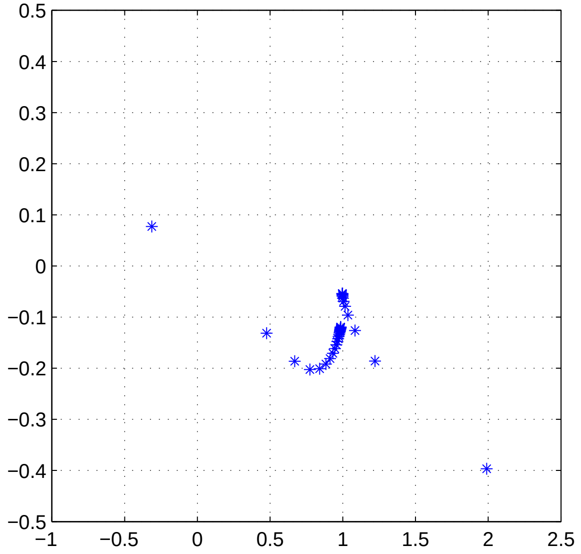
$k = 120$



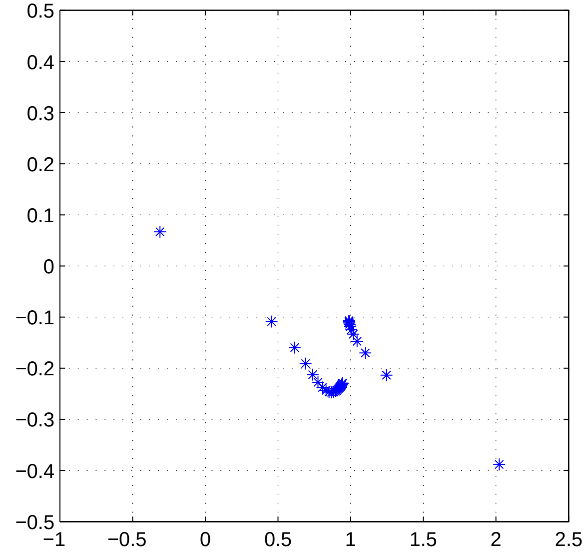
Fourier Analysis

Analysis shows that an increase in the imaginary shift does not change the spectrum.

$(\beta_1, \beta_2) = (1, 0.5)$



$(\beta_1, \beta_2) = (1, 1)$



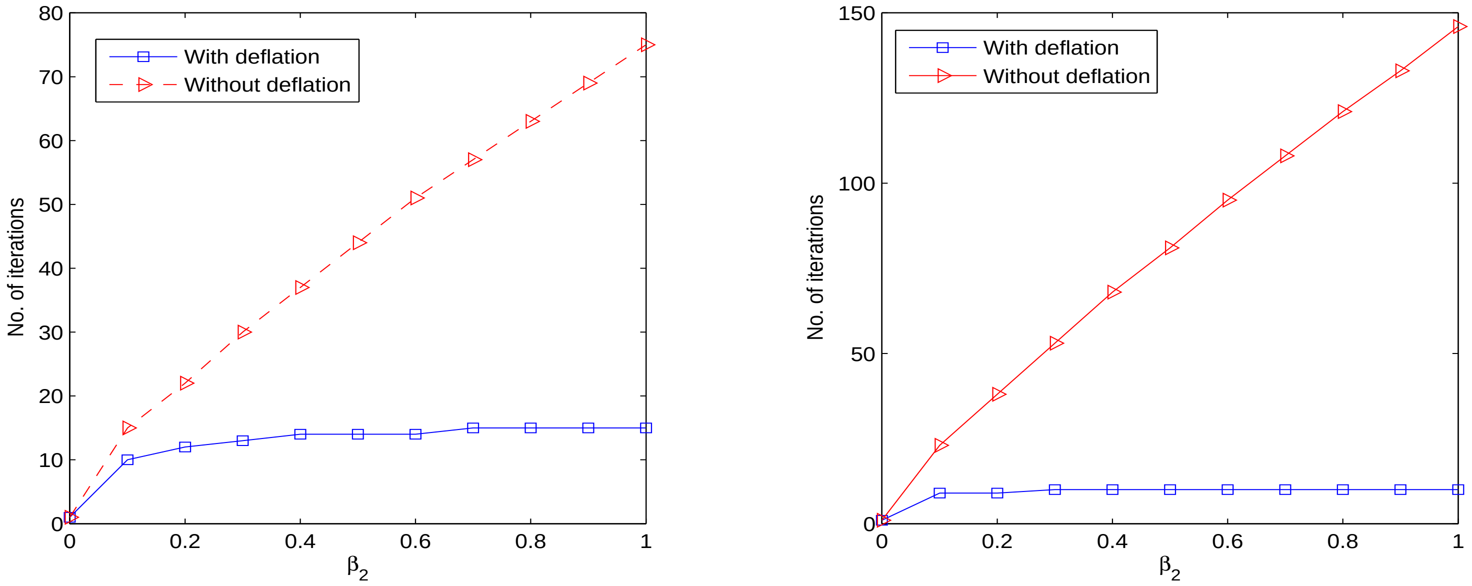
Numerical results

Sommerfeld boundary conditions are used for test problem.

What is the effect of an increase in the imaginary shift in SLP?

Constant wavenumber problem

Wedge problem



Numerical results

Number of GMRES iterations with/without deflation. Shifts in the preconditioner are $(1, 0.5)$

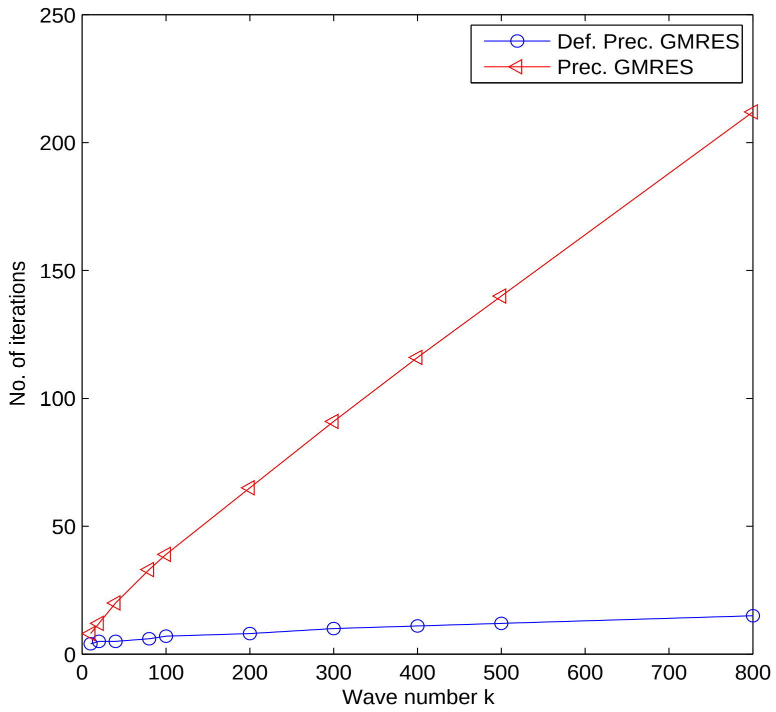
Grid	$k = 10$	$k = 20$	$k = 30$	$k = 40$	$k = 50$	$k = 100$
$n = 32$	**5/10**	8/17	14/28	26/44	42/70	13/14
$n = 64$	4/10	**6/17**	8/28	12/36	18/45	173/163
$n = 96$	3/10	5/17	**7/27**	9/35	12/43	36/97
$n = 128$	3/10	4/17	6/27	**7/35**	9/43	36/85
$n = 160$	3/10	4/17	5/27	6/35	**8/43**	25/82
$n = 320$	3/10	4/17	4/27	5/35	5/42	**10/80**

Numerical results

Number of GMRES iterations with/without deflation to solve a Wedge problem. Shifts in the preconditioner are $(1, 0.5)$

Grid	$freq = 10$	$freq = 20$	$freq = 30$	$freq = 40$	$freq = 50$
74×124	**7/33**	20/60	79/95	267/156	490/292
148×248	5/33	**9/57**	17/83	42/112	105/144
232×386	5/33	7/57	**10/81**	25/108	18/129
300×500	4/33	6/57	8/81	**12/105**	18/129
374×624	4/33	5/57	7/80	9/104	**13/128**

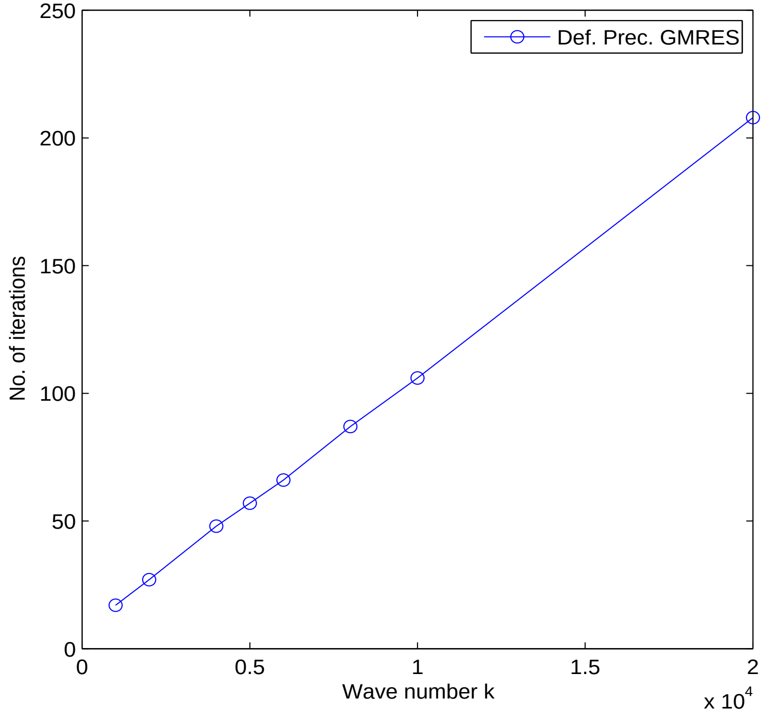
Numerical results



- Number of GMRES iterations for the 1D Helmholtz equation

$$10 \leq k \leq 800$$

Numerical results



Number of GMRES iterations for the 1D Helmholtz equation

$$1000 \leq k \leq 20000$$

Numerical results

Number of GMRES outer-iterations in multilevel algorithm.
$(\beta_1, \beta_2) = (1, 0.5)$ $kh = .3125$ or 20 gp/wl
and MG Vcycle(1,1) for SLP

Grid	$k = 10$	$k = 20$	$k = 40$	$k = 80$	$k = 160$
MLMGV(4,2,1)	9	11	16	27	100+
MLMGV(6,2,1)	9	10	14	21	47
MLMGV(8,2,1)	9	10	13	20	38
MLMGV(8,3,2)	9	10	13	19	37

Results

Petsc solve-time in Seconds; a Two-level solver.

Solver	20	40	80	120	160	200
SLP	0.01(23)	0.24(54)	2.62(113)	11.60(168)	33.59(222)	83.67(274)
Def/SLP	0.03(10)	0.14(14)	0.82(23)	2.92(37)	8.98(61)	23.13(87)

SLP : GCR preconditioned with SLP $M(1,1)$.
Def/SLP: Deflated and preconditioned GCR.

Grid resolution is such that there are 10 grid points per wavelength.

Results

Petsc time and Krylov outer-iterations in multilevel algorithm.

$(\beta_1, \beta_2) = (1, 1)$

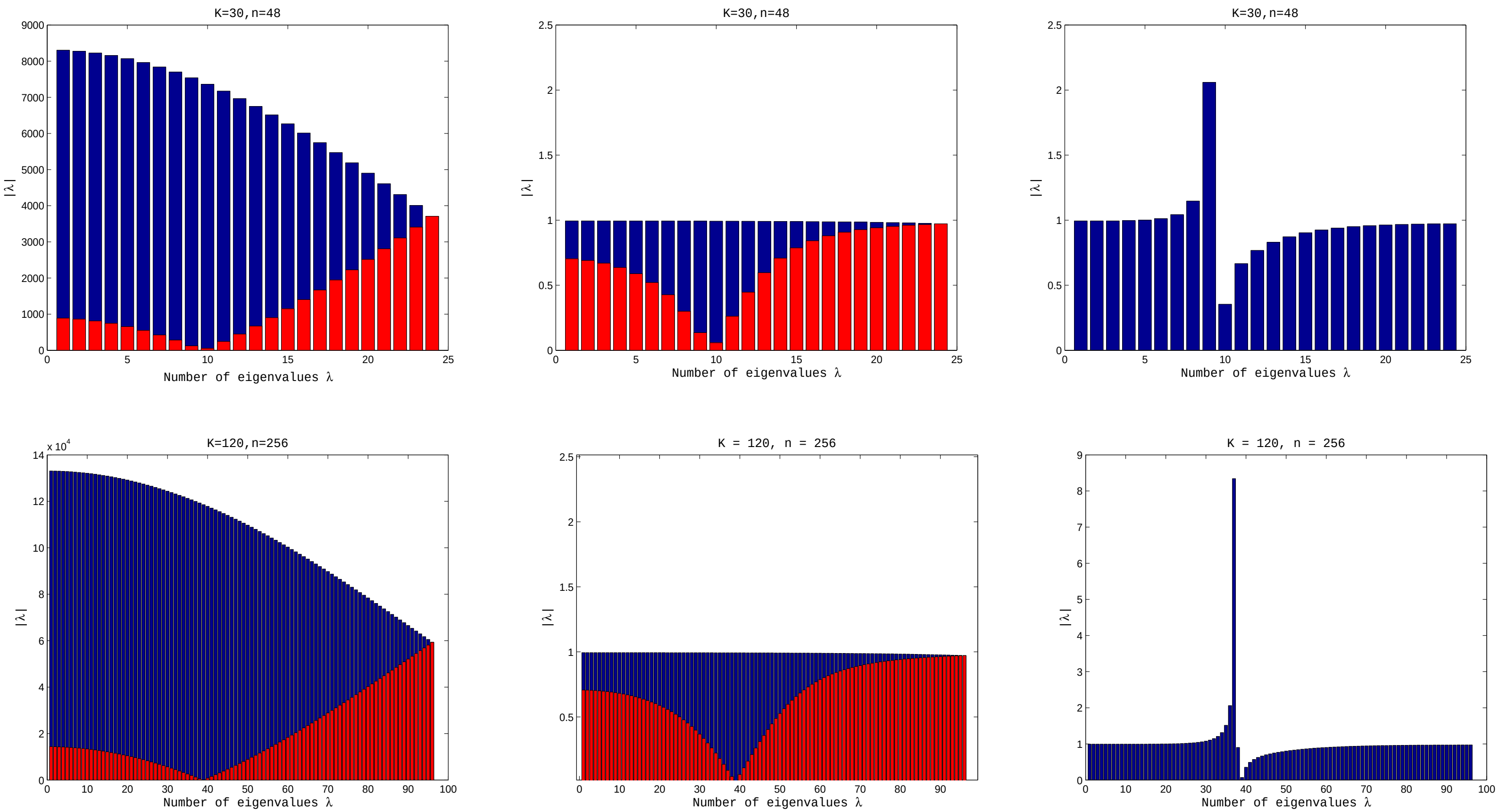
$kh = .625$ or 10 gp/wl

MLMGV is Multilevel with VCycle(1,1), MLMGF is Multilevel with FCycle(1,1)

-	$k = 10$	$k = 20$	$k = 40$	$k = 80$	$k = 120$
MLMGV(8,2,1)	16(1.3)	27(2.8)	58(7.3)	116(38.7)	177(76.8)
MLMGF(8,2,1)	10(0.9)	11(4.3)	16(12.9)	28(39.2)	41(60.5)

Fourier Analysis

Spectrum of A, $M^{-1}A$ and $PM^{-1}A$ (from left to right) in bar-graph.



TUDelft

Conclusions

- The proposed preconditioner (shifted Laplacian + multi-grid) is independent of the grid size and linearly dependent of k.
- With physical damping the proposed preconditioner is also independent of k.
- Without deflation, when imaginary shift is increased in SLP, spectrum remains bounded above 1, but lower part moves to zero.
- Flexibility to increase imaginary shift, when deflation is combined with SLP.
- Further research Multilevel scheme, applying similarly for coarse problem in deflation. Questions: gain in CPU time? why not scalable? ...

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