

An Efficient Two-level Preconditioner for Multi-Frequency Wave Propagation Problems

M. Baumann^{*,†} and M.B. Van Gijzen[†]

*Email: M.M.Baumann@tudelft.nl

[†]Delft Institute of Applied Mathematics
Delft University of Technology
Delft, The Netherlands

January 31, 2017

Motivation (1/3)

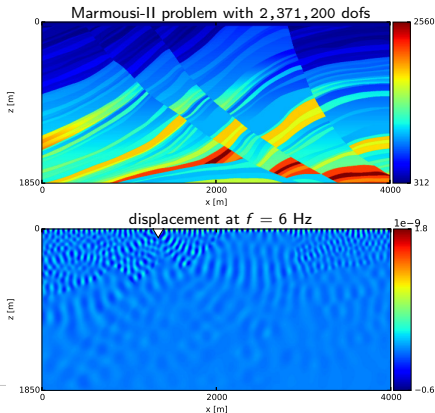
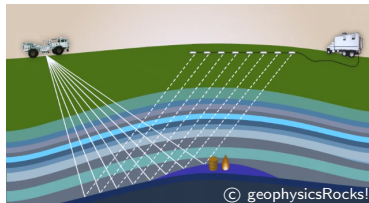
Seismic exploration:

- elastic wave equation
- in frequency-domain
- 'only' forward problem

Solve

$$(K + i\omega_k C - \omega_k^2 M)\mathbf{x}_k = \mathbf{b}$$

for multiple frequencies ω_k .



Motivation (1/3)

Seismic exploration:

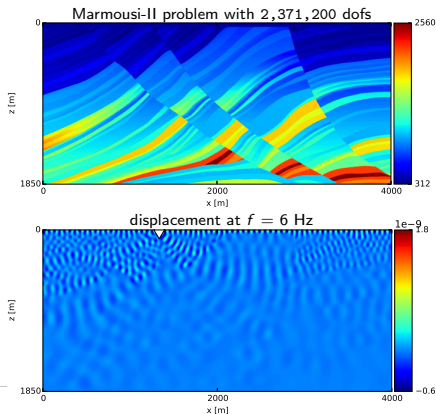
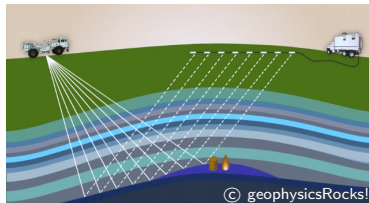
- elastic wave equation
- in frequency-domain
- 'only' forward problem

Solve

$$(K + i\omega_k C - \omega_k^2 M)\mathbf{x}_k = \mathbf{b}$$

for multiple frequencies ω_k .

$$K \succeq 0, \quad C \succeq 0, \quad M \succ 0$$



Motivation (2/3)

$$\dots (K + i\omega_k C - \omega_k^2 M)\mathbf{x}_k = \mathbf{b}$$

Linearization:

$$\left(\begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} - \omega_k \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} \right) \begin{bmatrix} \omega_k \mathbf{x}_k \\ \mathbf{x}_k \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}, \quad k = 1, \dots, N_\omega$$

Single preconditioner:

$$\begin{aligned} \mathcal{P}(\tau)^{-1} &= \left(\begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} - \tau \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} \right)^{-1} \\ &= \begin{bmatrix} I & \tau I \\ 0 & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & (K + i\tau C - \tau^2 M)^{-1} \end{bmatrix} \begin{bmatrix} 0 & I \\ I & -iC + \tau M \end{bmatrix} \end{aligned}$$

Motivation (2/3)

$$\dots (K + i\omega_k C - \omega_k^2 M)\mathbf{x}_k = \mathbf{b}$$

Linearization:

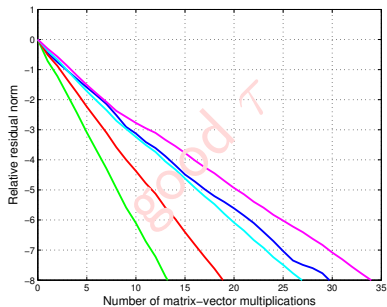
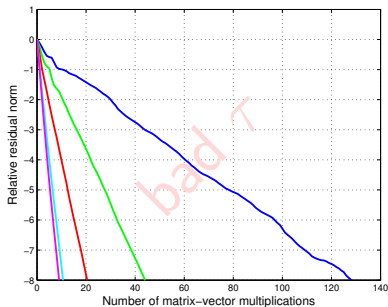
$$\left(\begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} - \omega_k \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} \right) \begin{bmatrix} \omega_k \mathbf{x}_k \\ \mathbf{x}_k \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}, \quad k = 1, \dots, N_\omega$$

Single preconditioner:

$$\begin{aligned} \mathcal{P}(\tau)^{-1} &= \left(\begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} - \tau \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} \right)^{-1} \\ &= \begin{bmatrix} I & \tau I \\ 0 & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & (K + i\tau C - \tau^2 M)^{-1} \end{bmatrix} \begin{bmatrix} 0 & I \\ I & -iC + \tau M \end{bmatrix} \end{aligned}$$

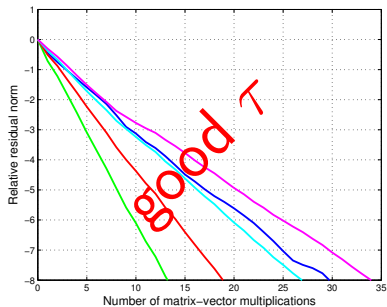
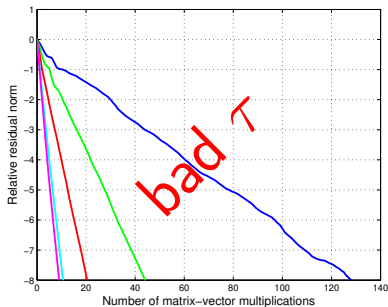
Motivation (3/3)

Convergence behavior for two different τ .



Motivation (3/3)

Convergence behavior for two different τ .



Outlook

- 1 The shift-and-invert preconditioner for GMRES
- 2 Optimization of seed frequency
- 3 Shifted Neumann preconditioners
- 4 Numerical experiments

Shift-and-invert preconditioner for GMRES

$$\mathcal{A} := \begin{bmatrix} iC & K \\ I & 0 \end{bmatrix}, \quad \mathcal{B} := \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix}$$

Want to solve

$$(\mathcal{A} - \omega_k \mathcal{B})\mathbf{x}_k = \mathbf{b}, \quad k = 1, \dots, N_\omega,$$

with a single preconditioner $\mathcal{P}(\tau) = (\mathcal{A} - \tau \mathcal{B})$:

$$(\mathcal{A} - \omega_k \mathcal{B})\mathcal{P}_k^{-1}\mathbf{y}_k = \mathbf{b} \quad \Leftrightarrow \quad (\mathcal{A}(\mathcal{A} - \tau \mathcal{B})^{-1} - \eta_k I)\mathbf{y}_k = \mathbf{b}$$

Shift-and-invert preconditioner for GMRES

$$\mathcal{A} := \begin{bmatrix} iC & K \\ I & 0 \end{bmatrix}, \quad \mathcal{B} := \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix}$$

Want to solve

$$(\mathcal{A} - \omega_k \mathcal{B})\mathbf{x}_k = \mathbf{b}, \quad k = 1, \dots, N_\omega,$$

with a single preconditioner $\mathcal{P}(\tau) = (\mathcal{A} - \tau \mathcal{B})$:

$$(\mathcal{A} - \omega_k \mathcal{B})\mathcal{P}_k^{-1}\mathbf{y}_k = \mathbf{b} \quad \Leftrightarrow \quad (\mathcal{A}(\mathcal{A} - \tau \mathcal{B})^{-1} - \eta_k I)\mathbf{y}_k = \mathbf{b}$$

Shift-and-invert preconditioner for GMRES

$$\mathcal{A} := \begin{bmatrix} iC & K \\ I & 0 \end{bmatrix}, \quad \mathcal{B} := \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix}$$

Want to solve

$$(\mathcal{A} - \omega_k \mathcal{B}) \mathbf{x}_k = \mathbf{b}, \quad k = 1, \dots, N_\omega,$$

with a single preconditioner $\mathcal{P}(\tau) = (\mathcal{A} - \tau \mathcal{B})$:

$$(\mathcal{A} - \omega_k \mathcal{B}) \mathcal{P}_k^{-1} \mathbf{y}_k = \mathbf{b} \quad \Leftrightarrow \quad \left(\begin{array}{cc} C & -\eta_k I \end{array} \right) \mathbf{y}_k = \mathbf{b}$$

- $C := \mathcal{A}(\mathcal{A} - \tau \mathcal{B})^{-1}$
- $\eta_k := \omega_k / (\omega_k - \tau)$

Multi-shift GMRES... Did you know?

For shifted problems,

$$(\mathcal{C} - \eta_k I) \mathbf{y}_k = \mathbf{b}, \quad k = 1, \dots, N_\omega,$$

Krylov spaces are shift-invariant

► GMRES

$$\mathcal{K}_m(\mathcal{C}, \mathbf{b}) \equiv \mathcal{K}_m(\mathcal{C} - \eta I, \mathbf{b}) \quad \forall \eta \in \mathbb{C}.$$

Multi-shift GMRES:

$$(\mathcal{C} - \eta_k I) \mathbf{V}_m = \mathbf{V}_{m+1} (\mathbf{H}_m - \eta_k I)$$

Reference

A. Frommer and U. Glässner. *Restarted GMRES for Shifted Linear Systems*. SIAM J. Sci. Comput., **19**(1), 15–26 (1998)

Multi-shift GMRES... Did you know?

For shifted problems,

$$(\mathcal{C} - \eta_k I) \mathbf{y}_k = \mathbf{b}, \quad k = 1, \dots, N_\omega,$$

Krylov spaces are shift-invariant

► GMRES

$$\mathcal{K}_m(\mathcal{C}, \mathbf{b}) \equiv \mathcal{K}_m(\mathcal{C} - \eta I, \mathbf{b}) \quad \forall \eta \in \mathbb{C}.$$

Multi-shift GMRES:

$$(\mathcal{C} - \eta_k I) \mathbf{V}_m = \mathbf{V}_{m+1} (\mathbf{H}_m - \eta_k \mathbf{I})$$

Reference

A. Frommer and U. Glässner. *Restarted GMRES for Shifted Linear Systems*. SIAM J. Sci. Comput., **19**(1), 15–26 (1998)

Optimization of seed frequency

$$\left(\mathcal{A}(\mathcal{A} - \tau \mathcal{B})^{-1} - \frac{\omega_k}{\omega_k - \tau} I \right) \mathbf{y}_k = \mathbf{b}$$

Theorem: GMRES convergence bound

[Saad, Iter. Methods]

Let the eigenvalues of a matrix be enclosed by a circle with radius R and center c . Then the GMRES-residual norm after i iterations $\|\mathbf{r}^{(i)}\|$ satisfies,

$$\frac{\|\mathbf{r}^{(i)}\|}{\|\mathbf{r}^{(0)}\|} \leq c_2(X) \left(\frac{R(\tau)}{|c(\tau)|} \right)^i,$$

where X is the matrix of eigenvectors, and $c_2(X)$ its condition number in the 2-norm.

Optimization of seed frequency

$$\left(\mathcal{A}(\mathcal{A} - \tau \mathcal{B})^{-1} - \frac{\omega_k}{\omega_k - \tau} I \right) \mathbf{y}_k = \mathbf{b}$$

Theorem: msGMRES convergence bound

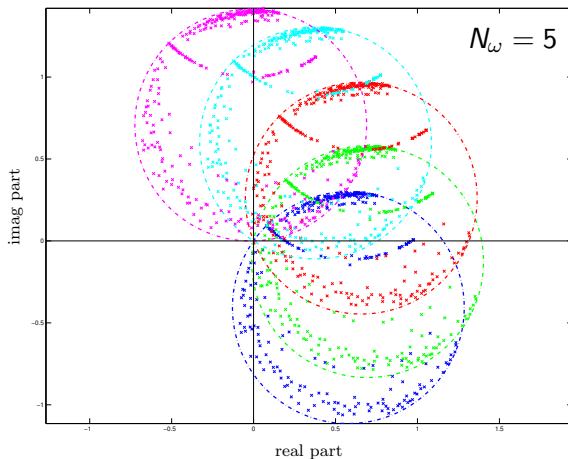
[Saad, Iter. Methods]

Let the eigenvalues of a matrix be enclosed by a circle with radius R_k and center c_k . Then the GMRES-residual norm after i iterations $\|\mathbf{r}_k^{(i)}\|$ satisfies,

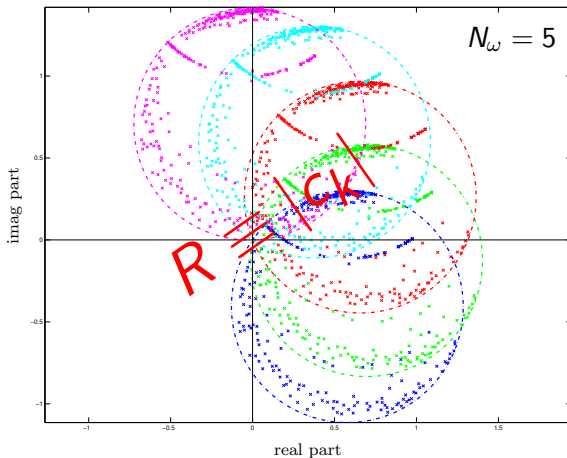
$$\frac{\|\mathbf{r}_k^{(i)}\|}{\|\mathbf{r}_k^{(0)}\|} \leq c_2(X) \left(\frac{R_k(\tau)}{|c_k(\tau)|} \right)^i, \quad k = 1, \dots, N_\omega,$$

where X is the matrix of eigenvectors, and $c_2(X)$ its condition number in the 2-norm.

The preconditioned spectra – no damping

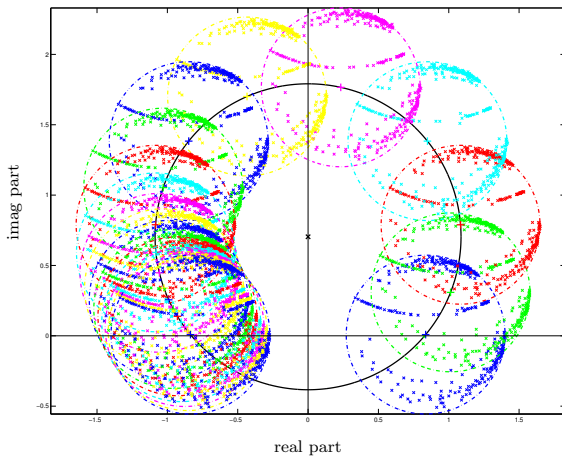


The preconditioned spectra – no damping



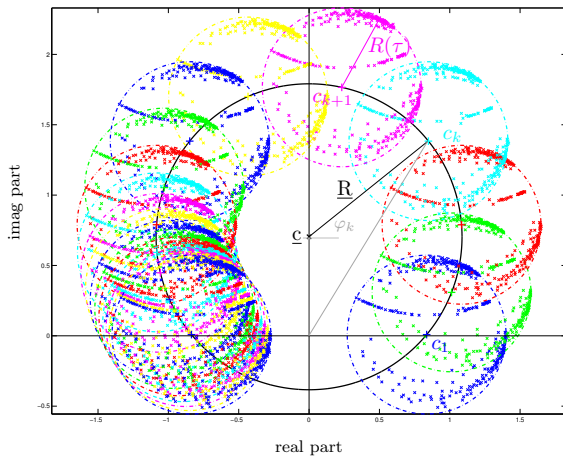
The preconditioned spectra – with damping $\epsilon > 0$

$$\hat{\omega}_k := (1 - \epsilon i)\omega_k$$



The preconditioned spectra – with damping $\epsilon > 0$

$$\hat{\omega}_k := (1 - \epsilon i)\omega_k$$



The preconditioned spectra

Lemma: Optimal seed shift for msGMRES

[B/vG, 2016]

- (i) For $\lambda \in \Lambda[\mathcal{A}\mathcal{B}^{-1}]$ it holds $\Im(\lambda) \geq 0$.
- (ii) The preconditioned spectra are enclosed by circles of radii R_k and center points c_k .
- (iii) The points $\{c_k\}_{k=1}^{N_\omega} \subset \mathbb{C}$ described in statement (ii) lie on a circle with center \underline{c} and radius \underline{R} .
- (iv) Consider the preconditioner $\mathcal{P}(\tau^*) = \mathcal{A} - \tau^*\mathcal{B}$. An optimal seed frequency τ^* for preconditioned multi-shift GMRES is given by,

$$\begin{aligned}\tau^*(\epsilon) &= \min_{\tau \in \mathbb{C}} \max_{k=1, \dots, N_\omega} \left(\frac{R_k(\tau)}{|c_k|} \right) = \dots = \\ &= \frac{2\omega_1\omega_{N_\omega}}{\omega_1 + \omega_{N_\omega}} - i \frac{\sqrt{[\epsilon^2(\omega_1 + \omega_{N_\omega})^2 + (\omega_{N_\omega} - \omega_1)^2] \omega_1\omega_{N_\omega}}}{\omega_1 + \omega_{N_\omega}}\end{aligned}$$

The preconditioned spectra – Proof (1/4)

Proof. (i) We have to show $\Im(\omega) \geq 0$ for,

$$\begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} x = \omega \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} x$$

or, alternatively ($\lambda = i\omega$),

$$(K + \lambda C + \lambda^2 M)v = 0$$

§3.8		come in pairs $(\lambda, \bar{\lambda})$	λ then x is a left eigenvector of $\bar{\lambda}$
P5 §3.8	M Hermitian positive definite, C, K Hermitian positive semidefinite	$\Re(\lambda) \leq 0$	
P6 §3.9	M, C symmetric positive definite, K symmetric	λ s are real and negative, gap between n largest and	n linearly independent eigenvectors associated with

$$\Re(\lambda) \leq 0 \Rightarrow \Im(\omega) \geq 0$$

The preconditioned spectra – Proof (1/4)

Proof. (i) We have to show $\Im(\omega) \geq 0$ for,

$$\begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} x = \omega \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} x$$

or, alternatively ($\lambda = i\omega$),

$$(K + \lambda C + \lambda^2 M)v = 0$$

§3.8		come in pairs $(\lambda, \bar{\lambda})$	λ then x is a left eigenvector of $\bar{\lambda}$
P5 §3.8	M Hermitian positive definite, C, K Hermitian positive semidefinite	$\Re(\lambda) \leq 0$	
P6 §3.9	M, C symmetric positive definite, K symmetric	λ s are real and negative, gap between n largest and	n linearly independent eigenvectors associated with

$$\Re(\lambda) \leq 0 \Rightarrow \Im(\omega) \geq 0$$

The preconditioned spectra – Proof (2/4)

(ii) *The preconditioned spectra are enclosed by circles.*

Factor out $\mathcal{A}\mathcal{B}^{-1}$,

$$\mathcal{C} - \eta_k I = \mathcal{A}(\mathcal{A} - \tau\mathcal{B})^{-1} - \eta_k I = \mathcal{A}\mathcal{B}^{-1}(\mathcal{A}\mathcal{B}^{-1} - \tau I)^{-1} - \eta_k I,$$

and note that

$$\Lambda[\mathcal{A}\mathcal{B}^{-1}] \ni \lambda \mapsto \frac{\lambda}{\lambda - \tau} - \frac{\omega_k}{\omega_k - \tau},$$

is a Möbius transformation^(*).

Reference

M.B. van Gijzen, Y.A. Erlangga, C. Vuik. *Spectral Analysis of the Discrete Helmholtz Operator Preconditioned with a Shifted Laplacian*. SIAM J. Sci. Comput., **29**(5), 1942–1958 (2007)

The preconditioned spectra – Proof (3/4)

(iii) *Spectra are bounded by circles (c_k, R) . These center point $\{c_k\}_{k=1}^{N_\omega}$ lie on a 'big circle' $(\underline{c}, \underline{R})$.*

1. Construct center:

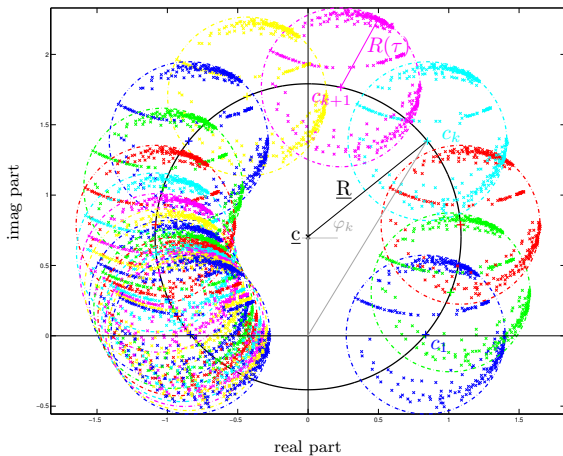
$$\underline{c} = \left(0, \frac{\epsilon |\tau|^2}{2\Im(\tau)(\Im(\tau) + \epsilon\Re(\tau))} \right) \in \mathbb{C}$$

2. A point c_k has constant distance to \underline{c} :

$$\underline{R}^2 = \|c_k - \underline{c}\|_2^2 = \frac{|\tau|^2(\epsilon^2 + 1)}{4(\Im(\tau) + \epsilon\Re(\tau))^2} \quad (\text{independent of } \omega_k)$$

The preconditioned spectra – with damping $\epsilon > 0$

$$\hat{\omega}_k := (1 - \epsilon i)\omega_k$$

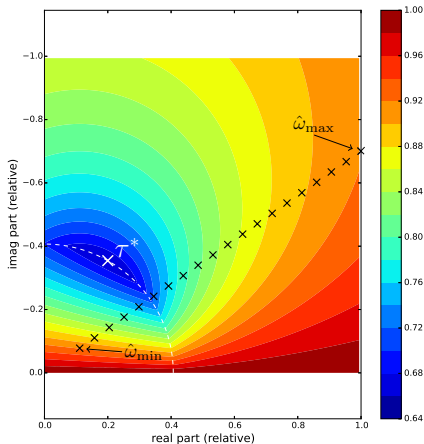


The preconditioned spectra – Proof (4/4)

(iv) Find optimal τ^* .

$$\tau^* = \min_{\tau \in \mathbb{C}} \max_{k=1, \dots, N_\omega} \left(\frac{R}{|c_k|} \right)$$

- ① $|c_k| = f(\underline{c}, \underline{R}, \varphi_k)$
- ② polar coordinates
- ③ $\frac{\partial \tau}{\partial \varphi} = 0$ (optimize along φ)

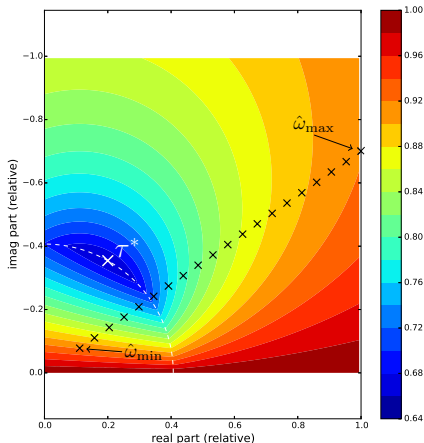


The preconditioned spectra – Proof (4/4)

(iv) Find optimal τ^* .

$$\tau^* = \min_{\tau \in \mathbb{C}} \max_{k \in \{1, N_\omega\}} \left(\frac{R}{|c_k|} \right)$$

- 1 $|c_k| = f(\underline{c}, \underline{R}, \varphi_k)$
- 2 polar coordinates
- 3 $\frac{\partial \tau}{\partial \varphi} = 0$ (optimize along φ)

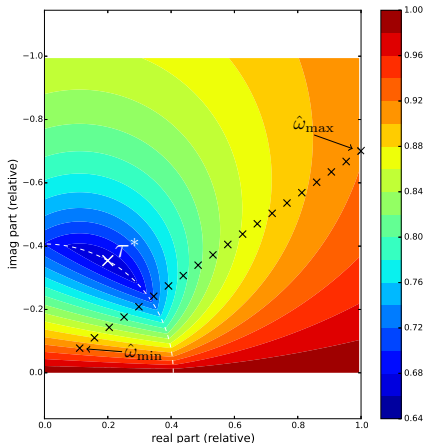


The preconditioned spectra – Proof (4/4)

(iv) Find optimal τ^* .

$$\tau^* = \min_{\tau \in \mathbb{C}} \max_{k \in \{1, N_\omega\}} \left(\frac{R}{|c_k|} \right)$$

- ① $|c_k| = f(\underline{c}, \underline{R}, \varphi_k)$
- ② polar coordinates
- ③ $\frac{\partial \tau}{\partial \varphi} = 0$ (optimize along φ)



$$\tau^* = \frac{2\omega_1\omega_{N_\omega}}{\omega_1 + \omega_{N_\omega}} - i \frac{\sqrt{[\epsilon^2(\omega_1 + \omega_{N_\omega})^2 + (\omega_{N_\omega} - \omega_1)^2]\omega_1\omega_{N_\omega}}}{\omega_1 + \omega_{N_\omega}}$$

- 1 The shift-and-invert preconditioner for GMRES
- 2 Optimization of seed frequency
- 3 Shifted Neumann preconditioners**
- 4 Numerical experiments

Second level: shifted polynomial preconditioners (1/2)

Polynomial preconditioners preserve shift-invariance:

$$(\mathcal{C} - \eta_k I) p_{n,k}(\mathcal{C}) = \mathcal{C} p_n(\mathcal{C}) - \tilde{\eta}_k I$$

- $\mathcal{C}^{-1} \approx p_n(\mathcal{C}) = \sum_{k=0}^n (I - \xi^* \mathcal{C})^k =: \sum_{i=0}^n \gamma_i \mathcal{C}^i$
 - $p_{n,k}(\mathcal{C}) = \sum_{i=0}^n \gamma_{i,k} \mathcal{C}^i$
 - $\tilde{\eta}_k = \eta_k \gamma_{0,k}$
- optimal: $\xi^* = \frac{1}{c_0(\tau^*)}$

Reference

M.I. Ahmad, D.B. Szyld, M.B. van Gijzen. *Preconditioned multishift BiCG for \mathcal{H}_2 -optimal model reduction*. Tech. report 12-06-15, Temple U (2013)

Second level: shifted polynomial preconditioners (2/2)

Substitution into,

$$(\mathcal{C} - \eta_k I) p_{n,k}(\mathcal{C}) = \mathcal{C} p_n(\mathcal{C}) - \tilde{\eta}_k I,$$

yields,

$$\sum_{i=0}^n \gamma_{i,k} \mathcal{C}^{i+1} - \sum_{i=0}^n \eta_k \gamma_{i,k} \mathcal{C}^i - \sum_{i=0}^n \gamma_i \mathcal{C}^{i+1} + \tilde{\eta}_k I = 0. \quad (*)$$

Difference equation (*) can be solved:

$$\begin{aligned} \gamma_{n,k} &= \gamma_n \\ \gamma_{i-1,k} &= \gamma_{i-1} + \eta_k \gamma_{i,k}, \quad \text{for } i = n, \dots, 1 \\ \tilde{\eta}_k &= \eta_k \gamma_{0,k} \end{aligned}$$

Second level: shifted polynomial preconditioners (2/2)

Substitution into,

$$(\mathcal{C} - \eta_k I) p_{n,k}(\mathcal{C}) = \mathcal{C} p_n(\mathcal{C}) - \tilde{\eta}_k I,$$

yields,

$$\sum_{i=0}^n \gamma_{i,k} \mathcal{C}^{i+1} - \sum_{i=0}^n \eta_k \gamma_{i,k} \mathcal{C}^i - \sum_{i=0}^n \gamma_i \mathcal{C}^{i+1} + \tilde{\eta}_k I = 0. \quad (*)$$

Difference equation (*) can be solved:

$$\begin{aligned} \gamma_{n,k} &= \gamma_n \\ \gamma_{i-1,k} &= \gamma_{i-1} + \eta_k \gamma_{i,k}, \quad \text{for } i = n, \dots, 1 \\ \tilde{\eta}_k &= \eta_k \gamma_{0,k} \end{aligned}$$

- 1 The shift-and-invert preconditioner for GMRES
- 2 Optimization of seed frequency
- 3 Shifted Neumann preconditioners
- 4 Numerical experiments**

The (damped) time-harmonic elastic wave equation

Continuous setting

Elastic wave equation

$$-\omega_k^2 \rho(\mathbf{x}) \mathbf{u}_k - \nabla \cdot \sigma(\mathbf{u}_k) = \mathbf{s}$$

with boundary conditions

$$\begin{aligned} i\omega_k \rho(\mathbf{x}) B \mathbf{u}_k + \sigma(\mathbf{u}_k) \hat{\mathbf{n}} &= \mathbf{0}, \\ \sigma(\mathbf{u}_k) \hat{\mathbf{n}} &= \mathbf{0}, \end{aligned}$$

on $\partial\Omega_a \cup \partial\Omega_r$.

Discrete setting

Solve

$$(K + i\omega_k C - \omega_k^2 M) \mathbf{u}_k = \mathbf{s}$$

$\hat{\omega}_k = (1 - \epsilon i)\omega_k$

with FEM matrices

$$K_{ij} = \int_{\Omega} \sigma(\varphi_i) : \nabla \varphi_j \, d\Omega,$$

$$M_{ij} = \int_{\Omega} \rho(\mathbf{x}) \varphi_i \cdot \varphi_j \, d\Omega,$$

$$C_{ij} = \int_{\partial\Omega_a} \rho(\mathbf{x}) B \varphi_i \cdot \varphi_j \, d\Gamma.$$

The (damped) time-harmonic elastic wave equation

Continuous setting

Elastic wave equation

$$-\omega_k^2 \rho(\mathbf{x}) \mathbf{u}_k - \nabla \cdot \sigma(\mathbf{u}_k) = \mathbf{s}$$

with boundary conditions

$$\begin{aligned} i\omega_k \rho(\mathbf{x}) B \mathbf{u}_k + \sigma(\mathbf{u}_k) \hat{\mathbf{n}} &= \mathbf{0}, \\ \sigma(\mathbf{u}_k) \hat{\mathbf{n}} &= \mathbf{0}, \end{aligned}$$

on $\partial\Omega_a \cup \partial\Omega_r$.

Discrete setting

Solve

$$(K + i\omega_k C - \omega_k^2 M) \mathbf{u}_k = \mathbf{s}$$

$\hat{\omega}_k = (1 - \epsilon i) \omega_k$

with FEM matrices

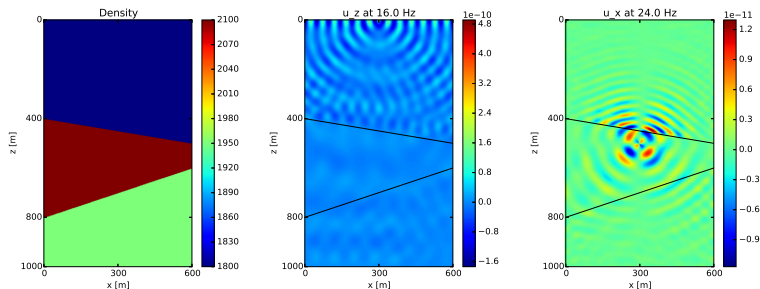
$$K_{ij} = \int_{\Omega} \sigma(\varphi_i) : \nabla \varphi_j \, d\Omega,$$

$$M_{ij} = \int_{\Omega} \rho(\mathbf{x}) \varphi_i \cdot \varphi_j \, d\Omega,$$

$$C_{ij} = \int_{\partial\Omega_a} \rho(\mathbf{x}) B \varphi_i \cdot \varphi_j \, d\Gamma.$$

Numerical experiments (1/5)

Set-up: An *elastic* wedge problem.



Numerical experiments (2/5)

$$\tau^*(\epsilon) = \sqrt{\omega_1 \omega_{N_\omega} (1 + \epsilon^2)} \cdot e^{i \arctan \left(-\sqrt{\frac{\epsilon^2 (\omega_1 + \omega_{N_\omega})^2 + (\omega_{N_\omega} - \omega_1)^2}{4 \omega_1 \omega_{N_\omega}}} \right)}$$

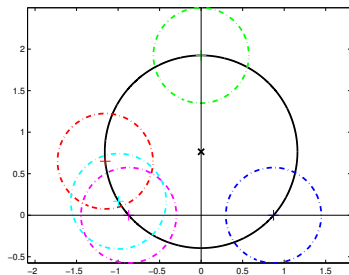
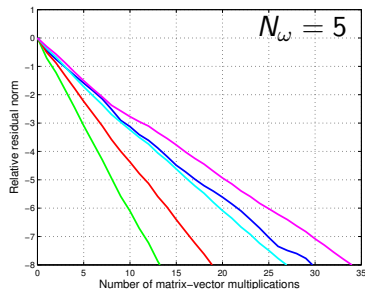
$\omega_1/2\pi$ [Hz]	$\omega_{N_\omega}/2\pi$ [Hz]	N_ω	# iterations	CPU time [s]
1	5	2	92	34.71
		10	92	36.43
		20	92	38.76
1	10	2	207	137.77
		10	207	151.17
		20	207	166.28

- damping factor $\epsilon = 0.07$
- #dofs = 48,642 (\mathcal{Q}_1 finite elements)
- no polynomial preconditioner ($n = 0$)

Numerical experiments (3/5)

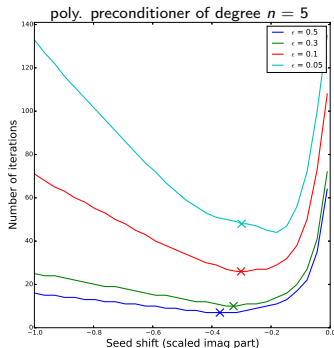
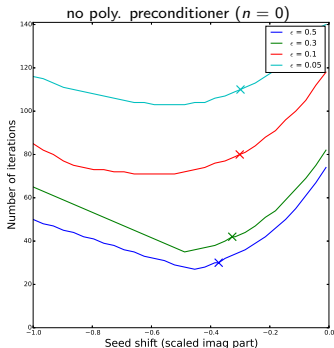
Convergence behavior:

- ω_{\min} and ω_{\max} converge slowest,
- smallest factor $R/|c_k|$ yields fastest convergence,
- 'inner' frequencies *for free*.

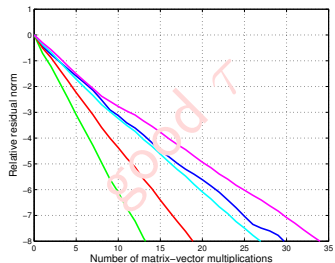
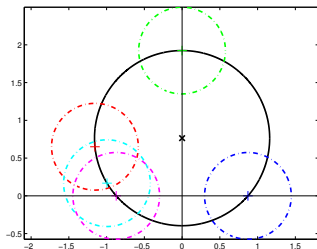
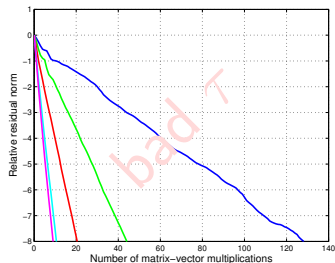
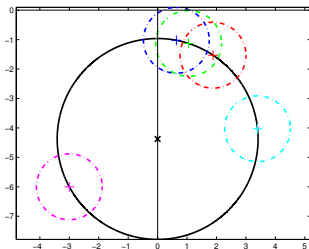


Numerical experiments (4/5)

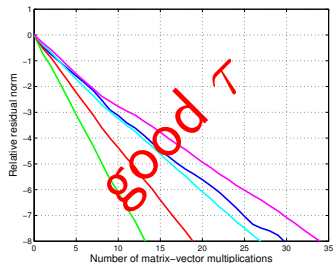
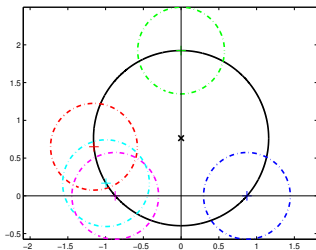
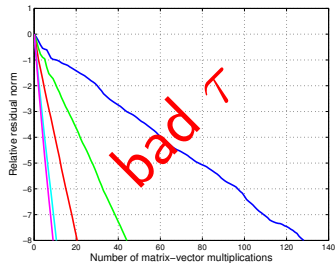
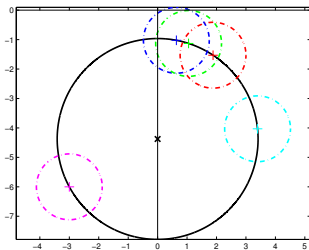
Optimality of τ^ in terms of no. iterations.*



Numerical experiments (5/5)



Numerical experiments (5/5)



Conclusions

- ✓ Optimal shift-and-invert preconditioner for msGMRES.
- ✓ Can be used for 'optimal' shifted polynomial preconditioner.
- ✗ Optimality for $\epsilon = 0$ only by continuity.
- ? For multi-core CPUs: Splitting strategy of frequency range.
- ? Relation to pole selection in rational Krylov methods.

Thank you for your attention!

Nice to be back at TU Berlin ☺

Conclusions

- ✓ Optimal shift-and-invert preconditioner for msGMRES.
- ✓ Can be used for 'optimal' shifted polynomial preconditioner.
- ✗ Optimality for $\epsilon = 0$ only by continuity.
- ? For multi-core CPUs: Splitting strategy of frequency range.
- ? Relation to pole selection in rational Krylov methods.

Thank you for your attention!

Nice to be back at TU Berlin ☺

References



M. Baumann and M.B. Van Gijzen. *Nested Krylov methods for shifted linear systems*. SIAM J. Sci. Comput., **37**(5), S90-S112 (2015).



M. Baumann, R. Astudillo, Y. Qiu, E. Ang, M.B. Van Gijzen, and R.-E. Plessix. *An MSSS-Preconditioned Matrix Equation Approach for the Time-Harmonic Elastic Wave Equation at Multiple Frequencies*. DIAM Technical Report 16-04, TU Delft [under review].



M. Baumann and M.B. Van Gijzen. *An Efficient Two-level Preconditioner for Multi-Frequency Wave Propagation Problems*. DIAM Technical Report 17-03, TU Delft [in preparation].



M. Baumann and M.B. Van Gijzen. *Efficient iterative methods for multi-frequency wave propagation problems: A comparison study*. Proceeding of ICCS 2017 [under review].

Research funded by Shell.

MSSS matrix computations “in a nutshell”

Definition: SSS matrix

[Chandrasekaran et al., 2005]

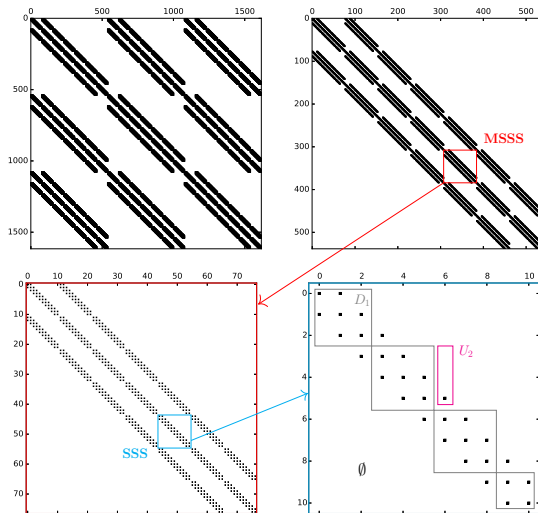
Let A be an $n \times n$ block matrix with **sequentially semi-seperable** structure. Then A can be written in the following block partitioned form

$$A_{i,j} = \begin{cases} U_i W_{i+1} \cdots W_{j-1} V_j^T, & \text{if } i < j; \\ D_i, & \text{if } i = j; \\ P_i R_{i-1} \cdots R_{j+1} Q_j^T, & \text{if } i > j. \end{cases}$$

- linear computational complexity for $(\cdot)^{-1}$
- limit off-diagonal rank with MOR
- **M**SSS: constructors are SSS matrices

D_1	$U_1 V_2^T$	\cdots	
$P_2 Q_1^T$	D_2	\ddots	
\vdots	\ddots	\ddots	
			D_n

The 3D elastic operator $(K + i\tau C - \tau^2 M) \rightsquigarrow (\cdot)^{-1}$



GMRES - Generalized minimal residual method

Solve large-scale linear system ($N \gg m$):

$$A\mathbf{x} = \mathbf{b}, \quad \text{where } A \in \mathbb{R}^{N \times N}$$

approximately in m -th Krylov subspace,

$$\mathbf{x}_m \in \mathcal{K}_m(A, \mathbf{b}) := \text{span} \{ \mathbf{b}, A\mathbf{b}, \dots, A^{m-1}\mathbf{b} \}.$$

Arnoldi relation yields,

$$AV_m = V_{m+1}\underline{H}_m,$$

and GMRES method minimizes residual:

$$\begin{aligned} \mathbf{x}_m &= \underset{\mathbf{x} \in \mathcal{K}_m(A, \mathbf{b})}{\operatorname{argmin}} \|\mathbf{b} - A\mathbf{x}\|_2 = \underset{\mathbf{y} \in \mathbb{R}^m}{\operatorname{argmin}} \|\mathbf{b} - AV_m\mathbf{y}\|_2 \\ &= \underset{\mathbf{y} \in \mathbb{R}^m}{\operatorname{argmin}} \|\mathbf{b} - V_{m+1}\underline{H}_m\mathbf{y}\|_2 = \dots = \underset{\mathbf{y} \in \mathbb{R}^m}{\operatorname{argmin}} \|\beta\mathbf{e}_1 - \underline{H}_m\mathbf{y}\|_2. \end{aligned}$$