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

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Motivation (1/3)

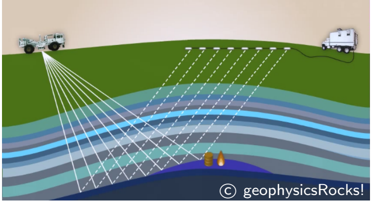
Seismic exploration:

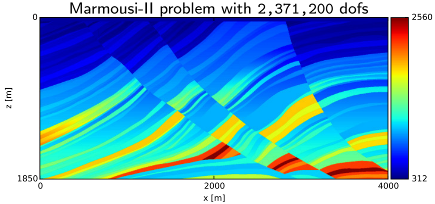
- elastic wave equation
- in frequency-domain
- 'only' forward problem

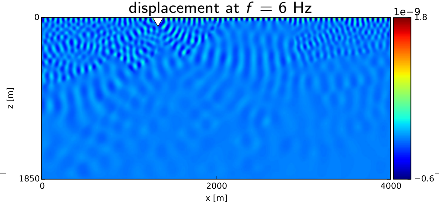
Solve

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

for multiple frequencies ω_k.







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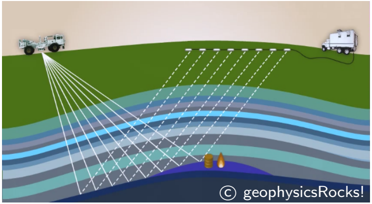

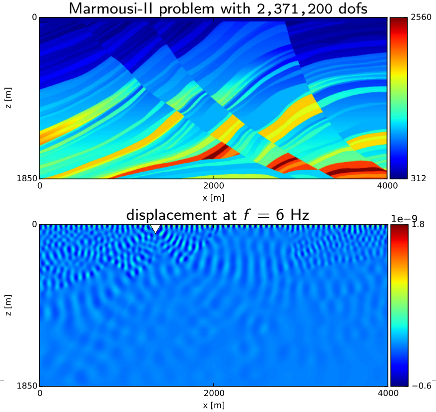

Solve

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

for multiple frequencies ω_k.

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

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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:

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

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

Motivation (2/3)

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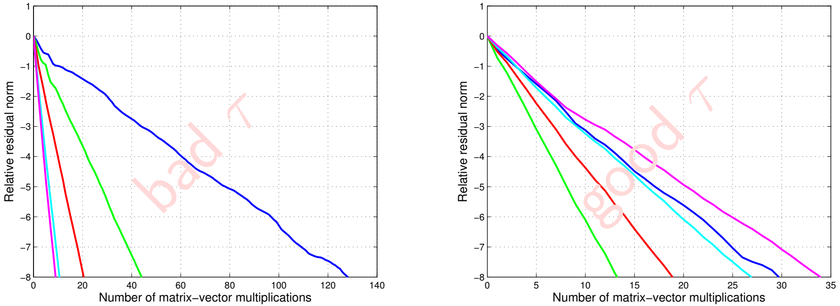
Single preconditioner:

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

Motivation (3/3)

Convergence behavior for two different τ.



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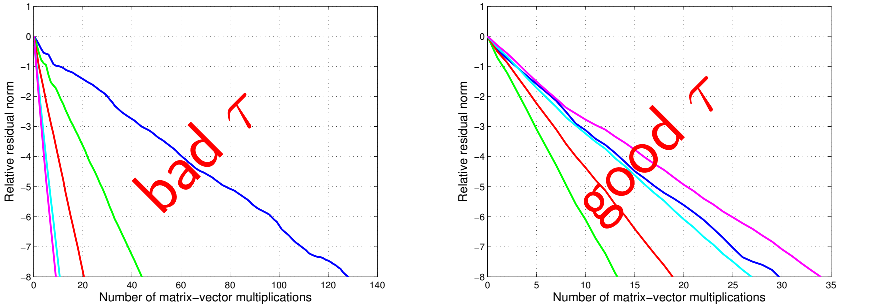

Outlook

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

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

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

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

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

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

Multi-shift GMRES... Did you know?

For shifted problems,

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

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:

$$(\mathcal{C} - \eta_k I)V_m = V_{m+1}(\underline{\mathrm{H}}_m - \eta_k \underline{\mathrm{I}})$$

Reference

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

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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

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

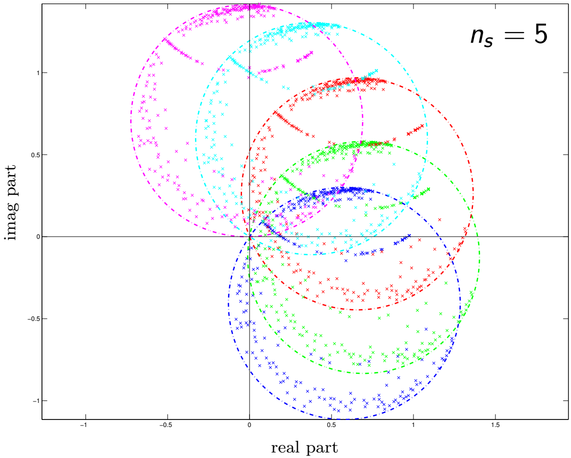
Theorem: msGMRES convergence bound [Saad, Iter. Methods]

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,

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

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

The preconditioned spectra – no damping



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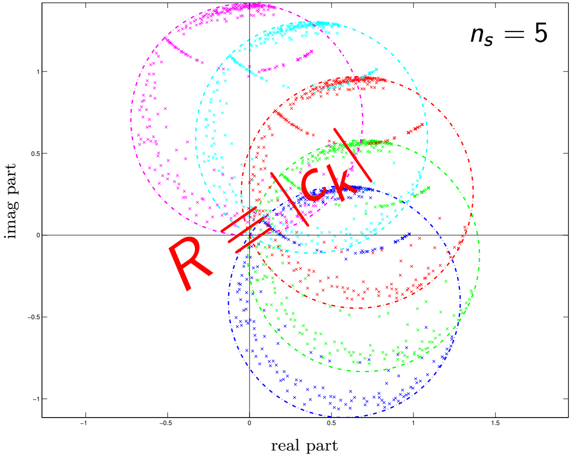
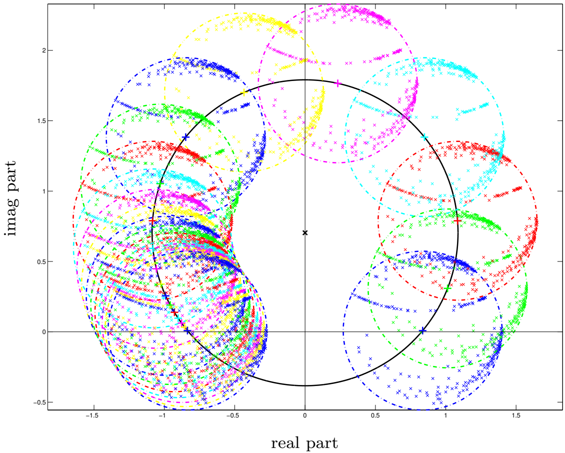


The preconditioned spectra – with damping $\epsilon > 0$

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



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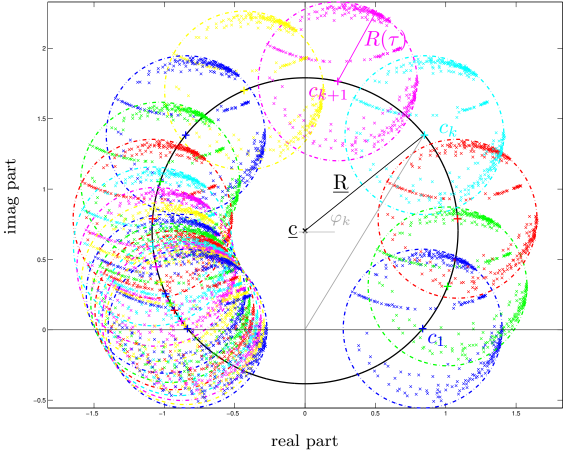

The preconditioned spectra

Lemma: Optimal seed shift for msGMRES [B/vG, 2016]

(i) For $\lambda \in \mathbf{\Lambda}[\mathcal{A}\mathcal{B}^{-1}]$ 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 $\underline{\mathrm{c}}$ and radius $\underline{\mathrm{R}}$.

(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,

$$\tau^*(\epsilon) = \min_{\tau \in \mathbb{C}} \max_{k=1,..,n_s} \left(\frac{R_k(\tau)}{|c_k|} \right) = \ldots =$$

$$= \frac{2\omega_1 \omega_{n_s}}{\omega_1 + \omega_{n_s}} - i \frac{\sqrt{\left[\epsilon^2(\omega_1 + \omega_{n_s})^2 + (\omega_{n_s} - \omega_1)^2\right] \omega_1 \omega_{n_s}}}{\omega_1 + \omega_{n_s}}$$

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	$\mathrm{Re}(\lambda) \leq 0$	
P6 §3.9	M, C symmetric positive definite, K symmetric	λs are real and negative, gap between n largest and	n linearly independent eigenvectors associated with

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

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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

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

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)

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$(*)\ :\ z \mapsto \frac{az+b}{cz+d}$

The preconditioned spectra – Proof (3/4)

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

1. Construct center:

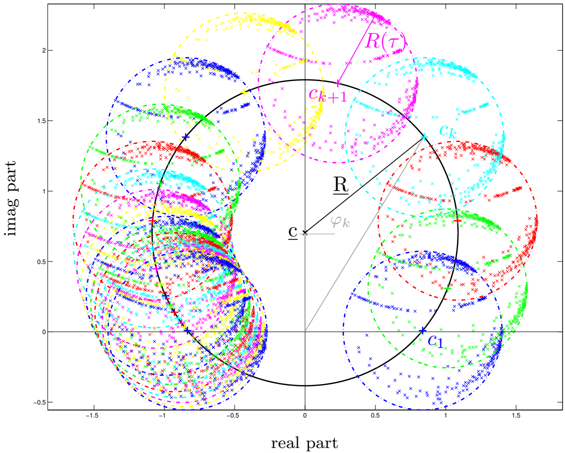
$$\underline{c} = \left(0, \frac{\epsilon|\tau|^2}{2\Im(\tau)(\Im(\tau) + \epsilon\Re(\tau))}\right) \in \mathbb{C}$$

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

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

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

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

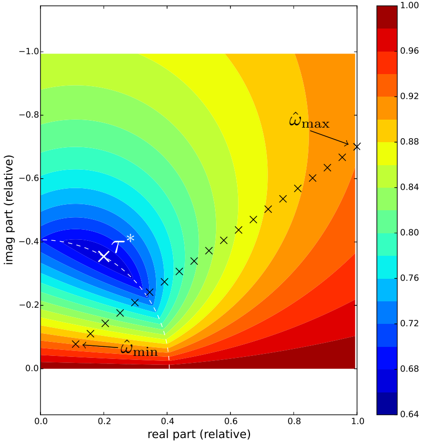


The preconditioned spectra – Proof (4/4)

(iv) *Find optimal τ^*.*

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

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



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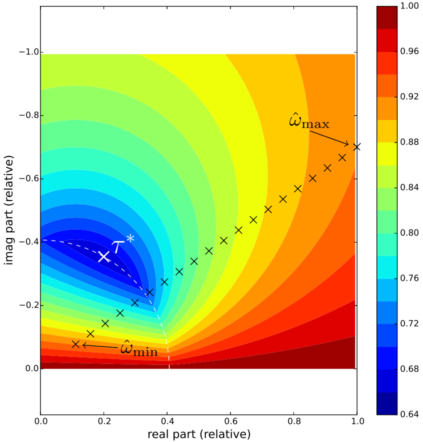

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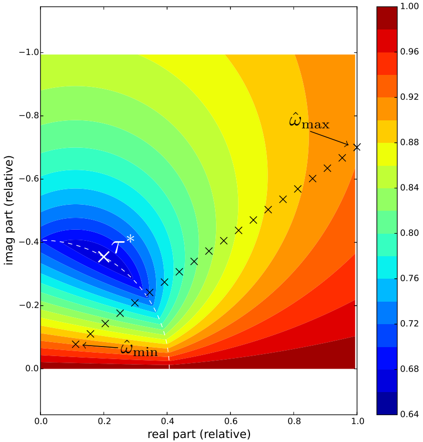

$$\tau^* = \frac{2\omega_1\omega_{n_s}}{\omega_1+\omega_{n_s}} - i\frac{\sqrt{[\epsilon^2(\omega_1+\omega_{n_s})^2+(\omega_{n_s}-\omega_1)^2]\omega_1\omega_{n_s}}}{\omega_1+\omega_{n_s}}$$

Second level: shifted polynomial preconditioners (1/2)

Polynomical 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,

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

Difference equation $(*)$ can be solved:

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

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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

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

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

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

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with FEM matrices

$$\begin{aligned} K_{ij} &= \int_\Omega \sigma(\varphi_i) : \nabla\varphi_j \, d\Omega, \\ M_{ij} &= \int_\Omega \rho(\mathbf{x})\varphi_i \cdot \varphi_j \, d\Omega, \\ C_{ij} &= \int_{\partial\Omega_a} \rho(\mathbf{x}) B\varphi_i \cdot \varphi_j \, d\Gamma. \end{aligned}$$

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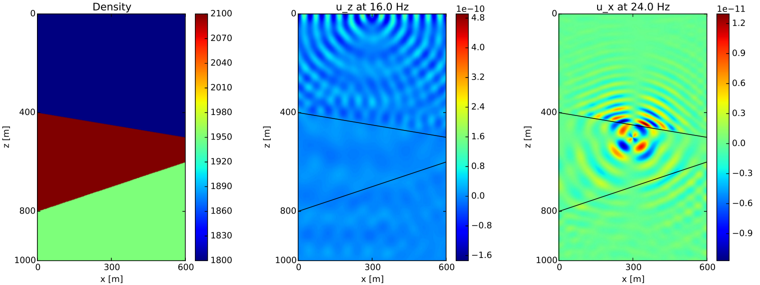
Numerical experiments (1/5)

Set-up: An *elastic* wedge problem.



Numerical experiments (2/5)

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

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

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

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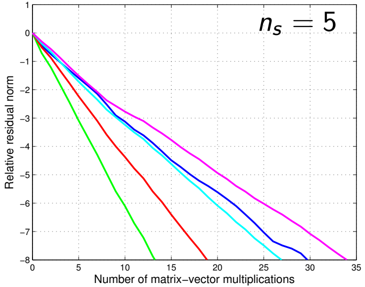
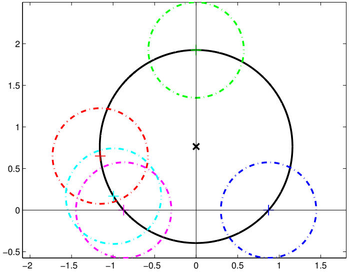
Numerical experiments (3/5)

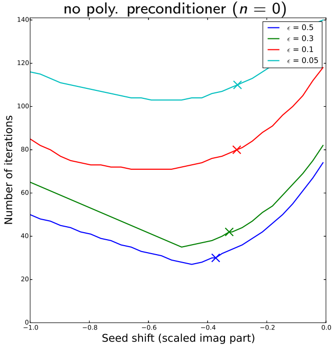


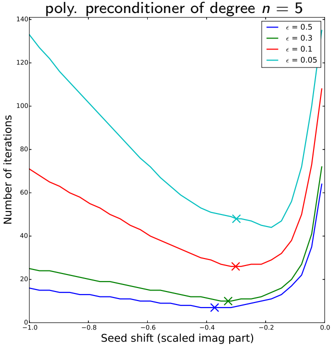
Convergence behavior:

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

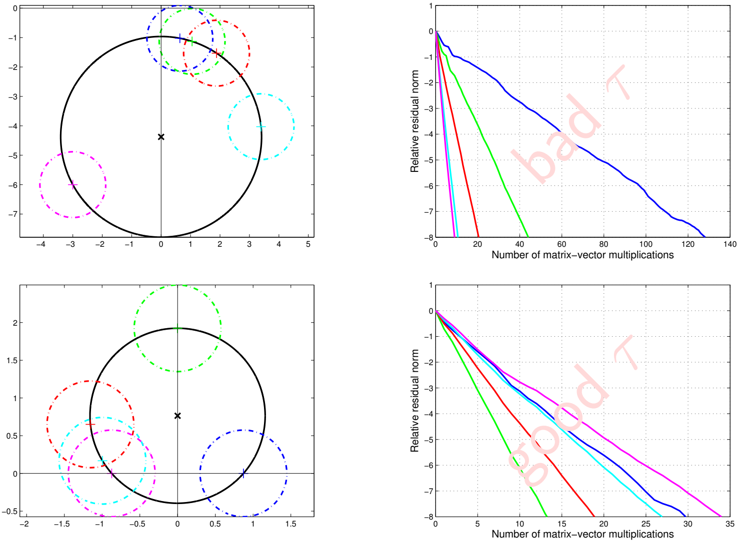


Optimality of τ^* in terms of no. iterations.

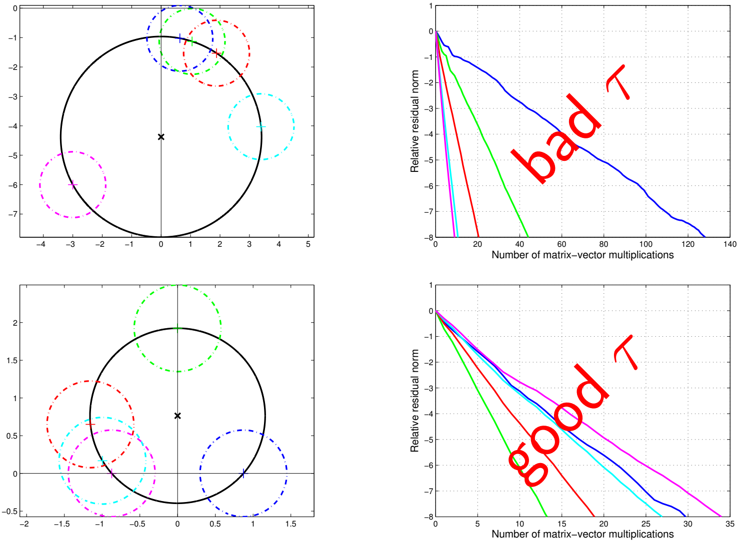




Numerical experiments (5/5)



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 ☺

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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].

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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].

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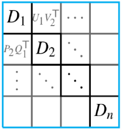
MSSS matrix computations "in a nutshell"

Definition: SSS matrix [Chandrasekaran et al., 2005]

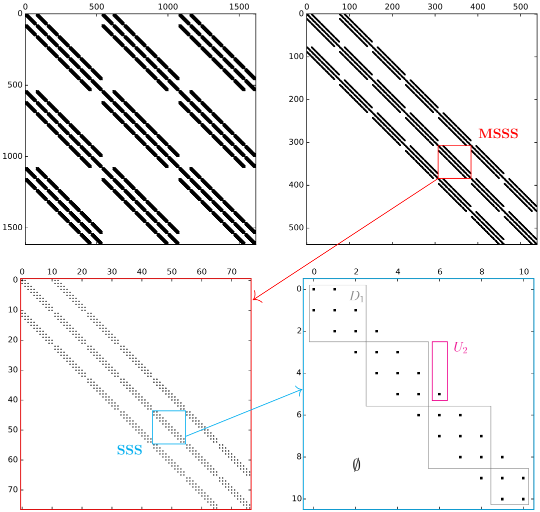
Let A be an $n \times n$ block matrix with **s**equentially **s**emi-**s**eperable structure. Then A can be written in the following block partitioned form

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

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



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



GMRES - Generalized minimal residual method

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

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

approximately in m-th Krylov subspace,

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

Arnoldi relation yields,

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

and GMRES method minimizes residual:

$$\mathbf{x}_m = \underset{x \in \mathcal{K}_m(A,\mathbf{b})}{\text{argmin}} \|\mathbf{b} - A\mathbf{x}\|_2 = \underset{\mathbf{y} \in \mathbb{R}^m}{\text{argmin}} \|\mathbf{b} - AV_m\mathbf{y}\|_2$$

$$= \underset{\mathbf{y} \in \mathbb{R}^m}{\text{argmin}} \|\mathbf{b} - V_{m+1}\underline{\mathrm{H}}_m\mathbf{y}\|_2 = \ldots = \underset{\mathbf{y} \in \mathbb{R}^m}{\text{argmin}} \|\beta\mathbf{e}_1 - \underline{\mathrm{H}}_m\mathbf{y}\|_2.$$

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