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

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January 31, 2017

Motivation (1/3)

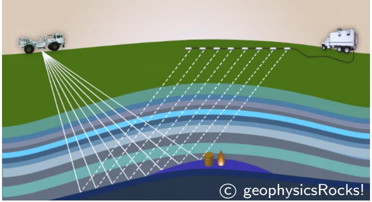
Seismic exploration:

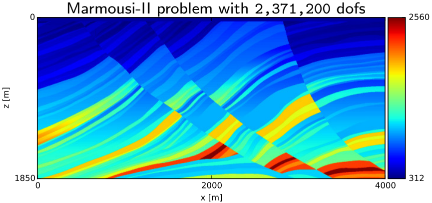
- elastic wave equation
- in frequency-domain
- 'only' forward problem

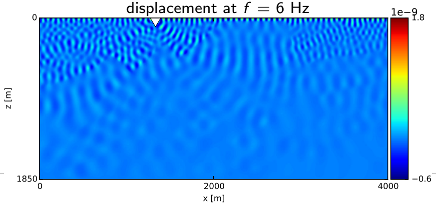
Solve

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

for multiple frequencies ω_k.







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Motivation (2/3)

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

Linearization:

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

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)

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Linearization:

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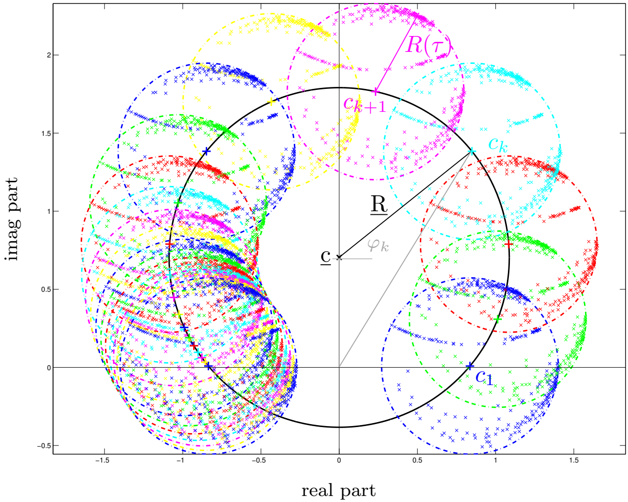
Motivation (3/3)



Outlook

1. The shift-and-invert preconditioner for GMRES
2. Optimization of seed frequency
3. 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

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

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

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

Shift-and-invert preconditioner for GMRES

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

Multi-shift GMRES... Did you know?

For shifted problems,

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

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:

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

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

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

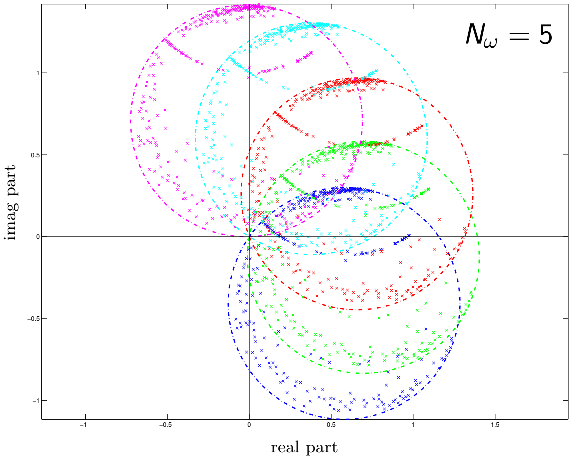
Theorem: msGMRES convergence bound [Saad, Iter. Methods]

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,

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

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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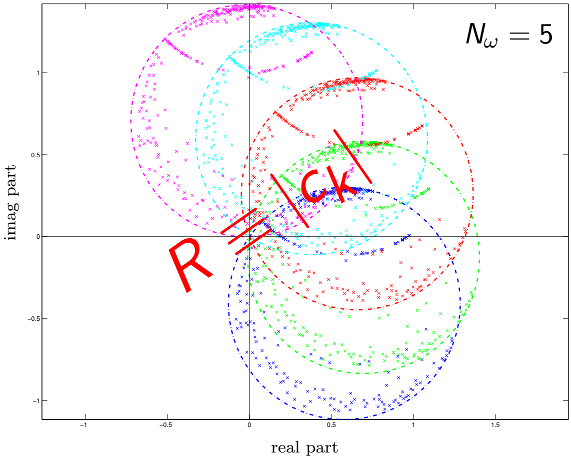
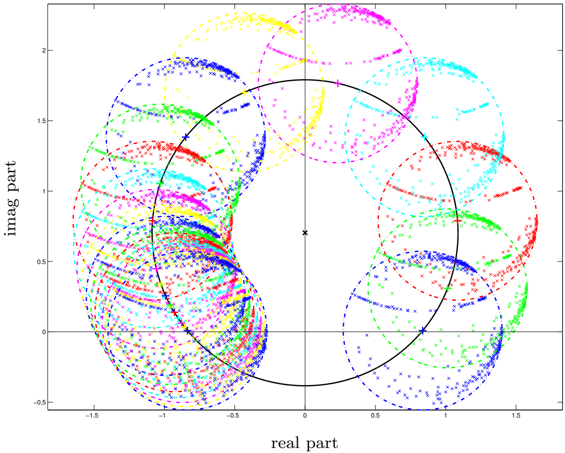


The preconditioned spectra – with damping $\epsilon > 0$

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



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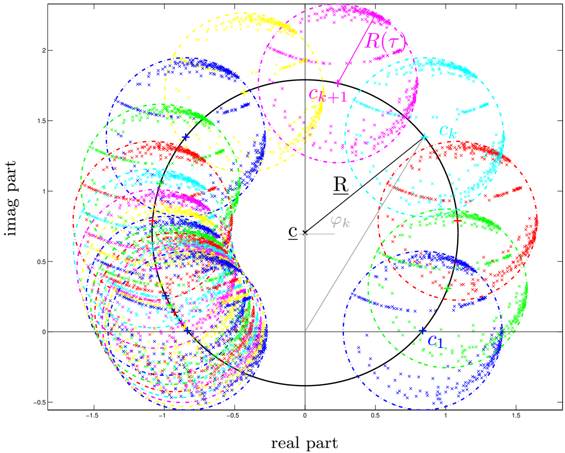

The preconditioned spectra

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 $\underline{c}$ 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,

$$\tau^*(\epsilon) = \min_{\tau \in \mathbb{C}} \max_{k=1,..,N_\omega} \left(\frac{R_k(\tau)}{|\hat{c}_k|} \right) = \ldots =$$

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

The preconditioned spectra – Proof (1/4)

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

$$\begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} x = \lambda \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} x \quad :\Leftrightarrow \quad \bar{\mathcal{A}} x = \lambda \bar{\mathcal{B}} x \;\Leftrightarrow\; \lambda = \frac{x^{\mathrm{H}} \bar{\mathcal{A}} x}{x^{\mathrm{H}} \bar{\mathcal{B}} x}.$$

Based on the splitting,

$$\bar{\mathcal{A}} := \begin{bmatrix} iC & K \\ K & 0 \end{bmatrix} = \begin{bmatrix} 0 & K \\ K & 0 \end{bmatrix} + i \begin{bmatrix} C & 0 \\ 0 & 0 \end{bmatrix},$$

the bound follows from Bendixon's theorem.

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the bound follows from Bendixon's theorem.

Thm: Bendixon's theorem [taken from Householder, 1964]

$$A = \frac{1}{2}(A + A^{\mathsf{H}}) + i \frac{1}{2i}(A - A^{\mathsf{H}}) \equiv \Re(A) + i\Im(A),$$

For this splitting holds: $\lambda_{\min}^{\Im(A)} \leq \Im(\lambda^A) \leq \lambda_{\max}^{\Im(A)}$.

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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)

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

The preconditioned spectra – Proof (3/4)

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

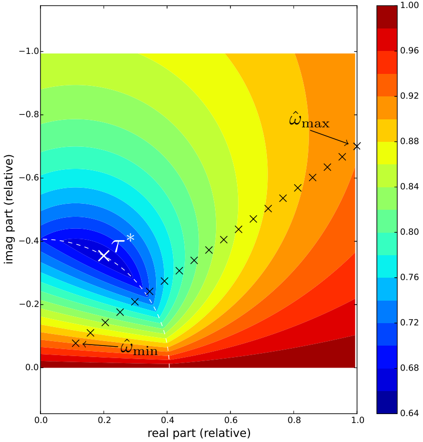
$$\underline{R}^2 = \|c_k - \underline{c}\|_2^2 = \frac{|\tau|^2(\epsilon^2 + 1)}{4(\Im(\tau) + \epsilon\Re(\tau))^2} \quad \text{(independent of } \omega_k\text{)}$$

The preconditioned spectra – Proof (4/4)

(iv) *Find optimal τ^*.*

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

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



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:

$$\gamma_{n,k} = \gamma_n$$
$$\gamma_{i-1,k} = \gamma_{i-1} + \eta_k\gamma_{i,k}, \quad \text{for } i = n, \ldots, 1$$
$$\tilde{\eta}_k = \eta_k\gamma_{0,k}$$

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1. The shift-and-invert preconditioner for GMRES
2. Optimization of seed frequency
3. 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

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

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

with FEM matrices

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

The (damped) time-harmonic elastic wave equation

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

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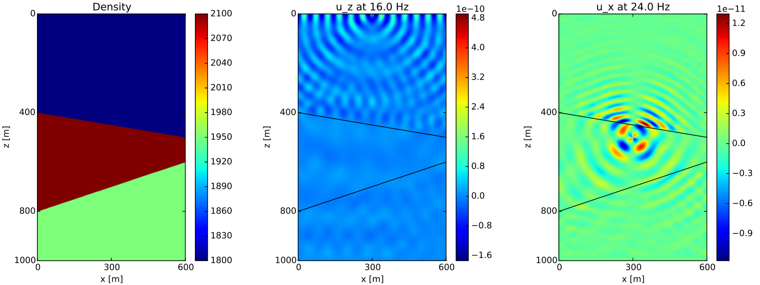
$$C_{ij} = \int_{\partial\Omega_a} \rho(\mathbf{x}) B\varphi_i \cdot \varphi_j \, d\Gamma.$$

Numerical experiments (1/5)

Set-up: An *elastic* wedge problem.



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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]`
		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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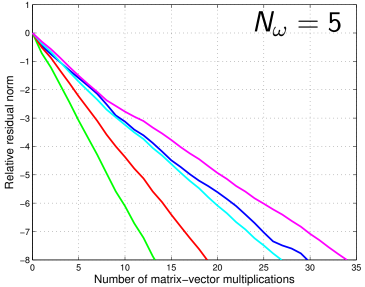
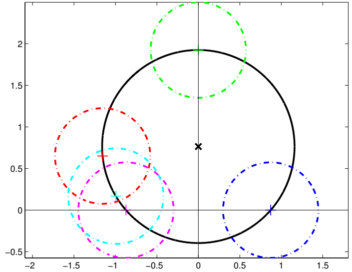
Numerical experiments (3/5)



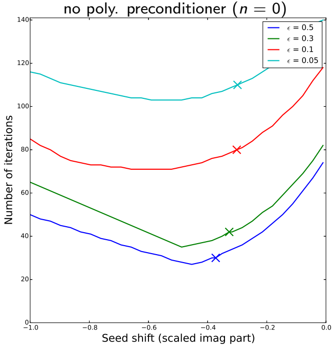
Convergence behavior:

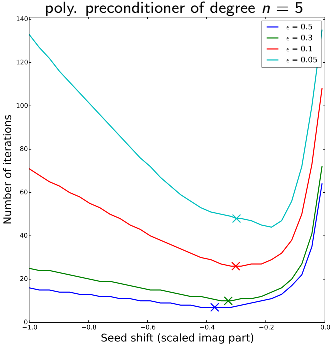
- ω_{min} and ω_{max} converge slowest,
- smallest factor $R/|c_k|$ yields fastest convergence,
- 'inner' frequencies *for free*.



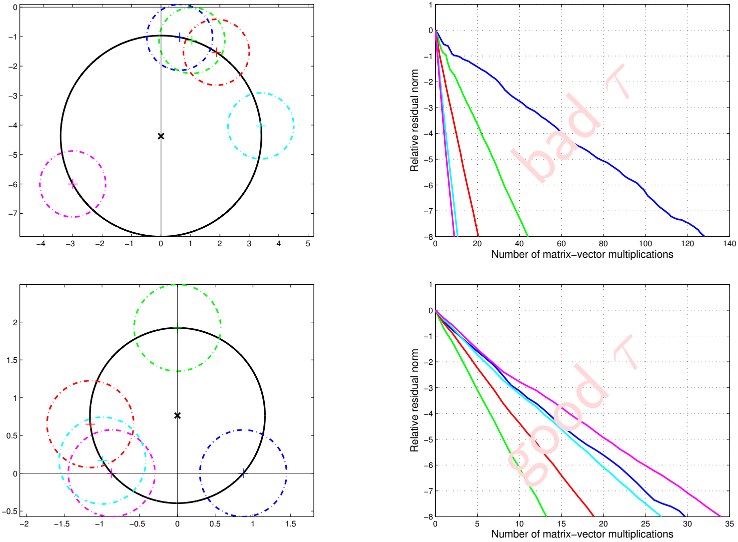
Numerical experiments (4/5)

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

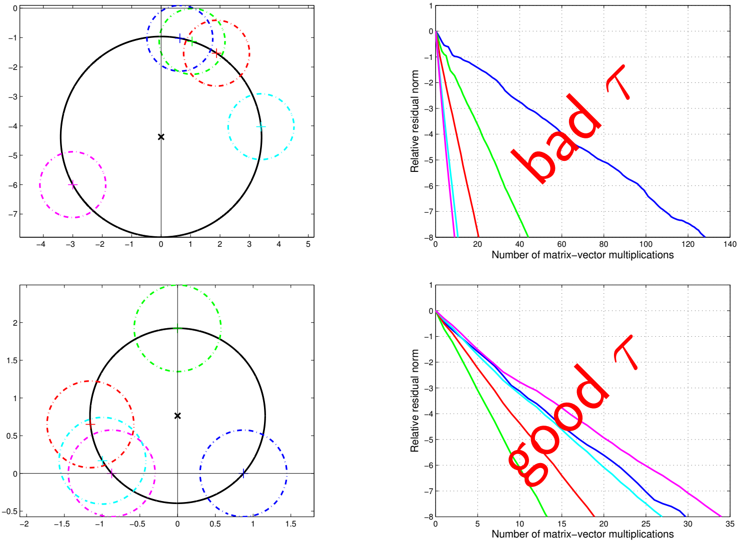




Numerical experiments (5/5)



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 ☺

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✓ 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).
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Research funded by Shell.

MSSS matrix computations "in a nutshell"

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

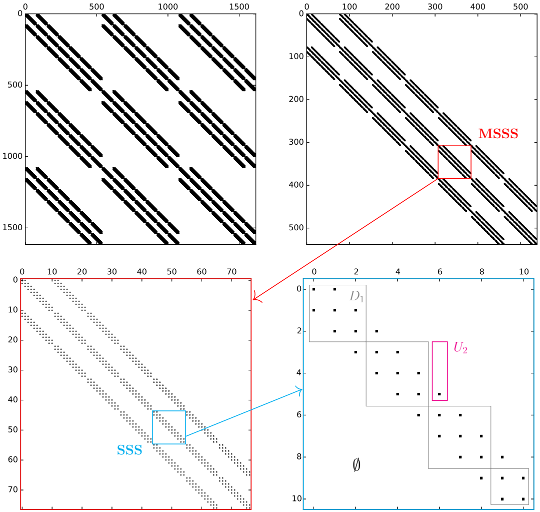
Let A be an $n \times n$ block matrix with **s**equentially **s**emi-**s**eperable structure. Then A can be written in the following block partitioned form

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

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

$$\begin{bmatrix} D_1 & U_1V_2^T & \cdots & \\ P_2Q_1^T & D_2 & \ddots & \\ \vdots & \ddots & \ddots & \\ & & & D_n \end{bmatrix}$$

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,

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

Arnoldi relation yields,

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

and GMRES method minimizes residual:

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

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