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

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Motivation (1/3)

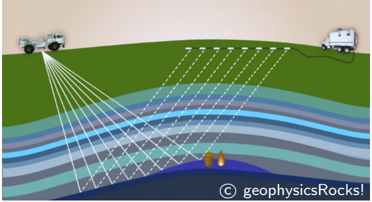
Seismic exploration:

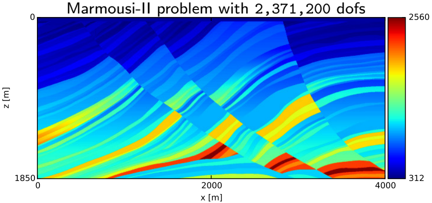
- elastic wave equation
- in frequency-domain
- 'only' forward problem

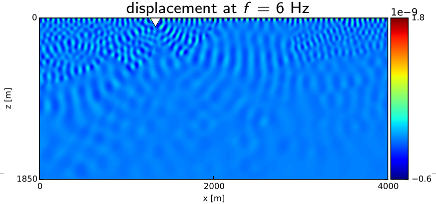
Solve

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

for multiple frequencies ω_k.







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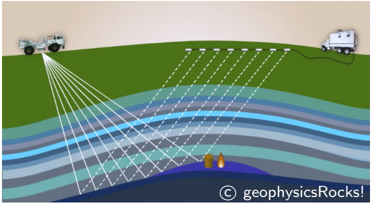
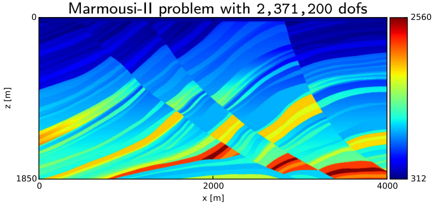
Solve

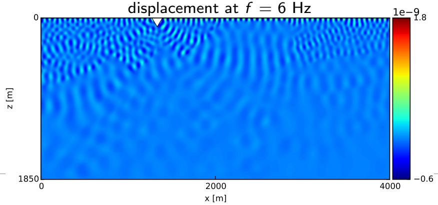
$$(K + i\omega_k C - \omega_k^2 M)\mathbf{x}_k = \mathbf{b}$$

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:

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

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

Motivation (2/3)

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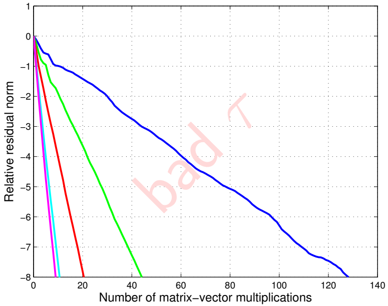
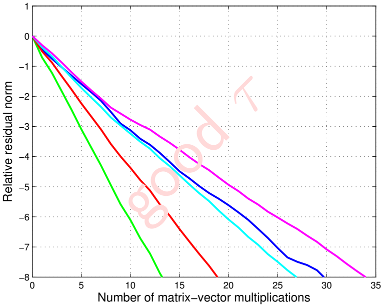
Motivation (3/3)

Convergence behavior for two different τ.





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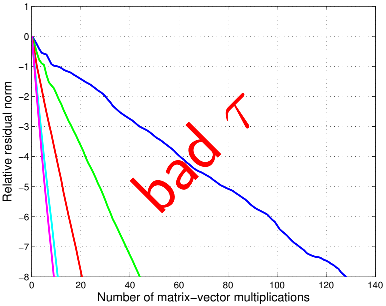

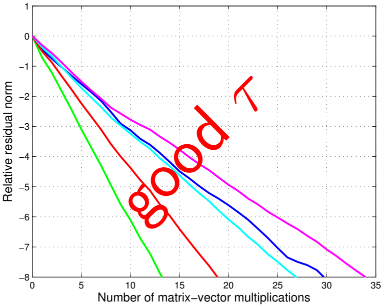

Outlook

1. The shift-and-invert preconditioner within multi-shift GMRES
2. Optimization of seed frequency τ
3. Numerical experiments
   - Validations
   - Shifted Neumann preconditioner
   - Matrix equation with rotation

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,

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

Krylov spaces are shift-invariant

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

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.

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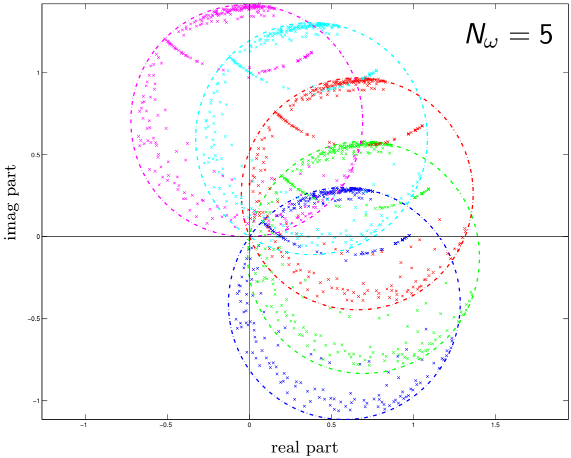
The preconditioned spectra – no damping



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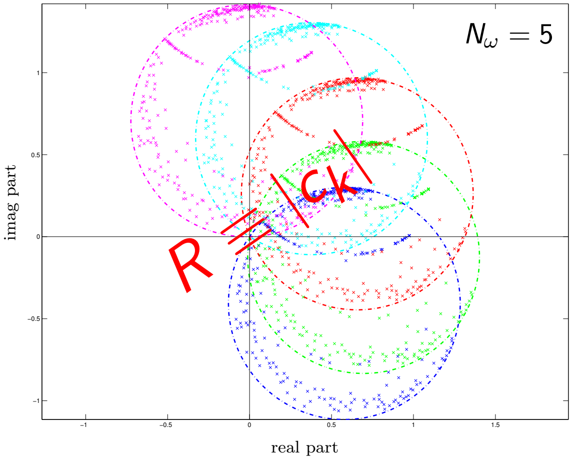
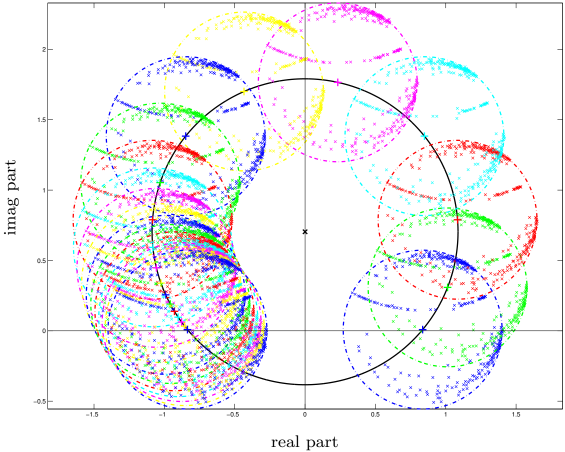


The preconditioned spectra – with damping $\epsilon > 0$

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



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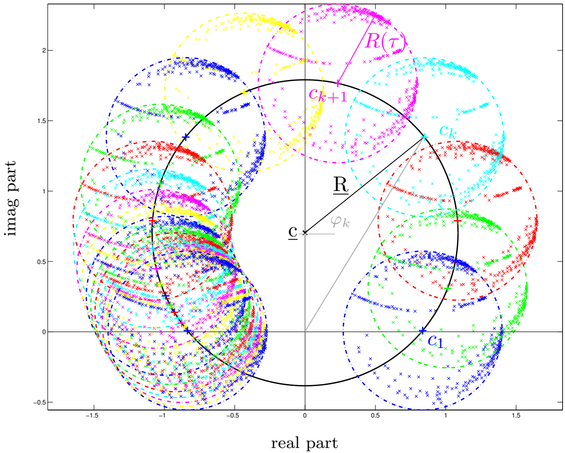

The preconditioned spectra

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,

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

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

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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 ($\lambda = i\omega$), consider the QEP,

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

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

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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* $\{c_k\}_{k=1}^{N_\omega}$ *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 $\underline{c}$:

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

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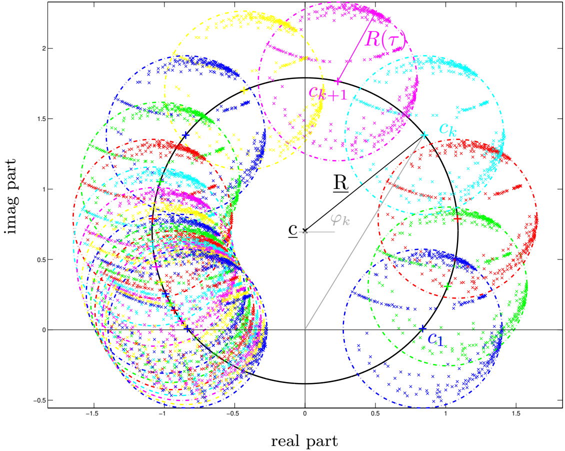
The preconditioned spectra – with damping $\epsilon > 0$

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

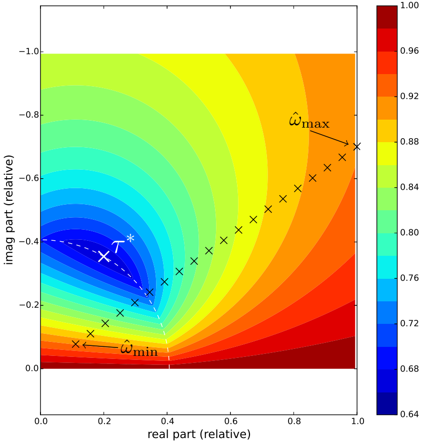


The preconditioned spectra – Proof (4/4)

(iv) *Find optimal τ^*.*

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

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



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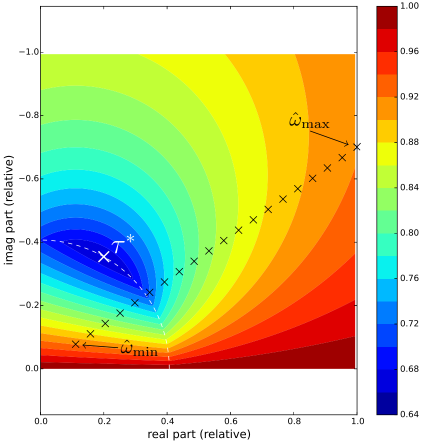

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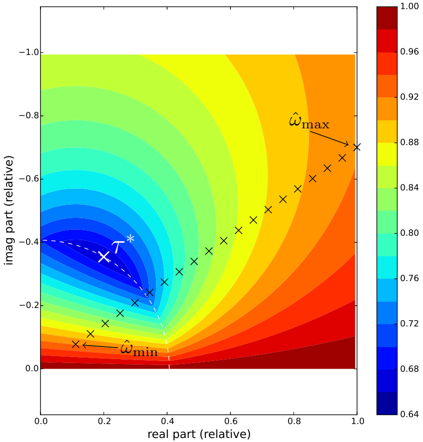

$$\tau^* = \frac{2\omega_1 \omega_{N_\omega}}{\omega_1 + \omega_{N_\omega}} - i \frac{\sqrt{[\epsilon^2(\omega_1 + \omega_{N_\omega})^2 + (\omega_{N_\omega} - \omega_1)^2]\omega_1 \omega_{N_\omega}}}{\omega_1 + \omega_{N_\omega}}$$

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2 Optimization of seed frequency τ

3 Numerical experiments
- Validations
- Shifted Neumann preconditioner
- Matrix equation with rotation

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

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

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nutils

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

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

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

Discrete setting

Solve

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

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

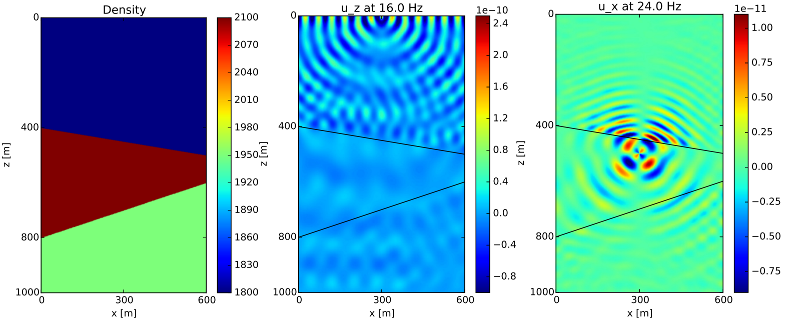
with FEM matrices

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

Numerical experiments

Validations and second-level preconditioners

Set-up: An *elastic* wedge problem.



Numerical experiments (1/4)

Validations I

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

$\omega_{\min}/2\pi$ [Hz]	$\omega_{\max}/2\pi$ [Hz]	N_ω	# iterations	CPU time [s]
		5	106	45.6
1	5	10	106	48.7
		20	106	47.3
		5	251	205.1
1	10	10	252	223.7
		20	252	243.5

- damping factor $\epsilon = 0.05$
- $\#$dofs $= 48,642$ ($\mathcal{Q}_1$ finite elements)

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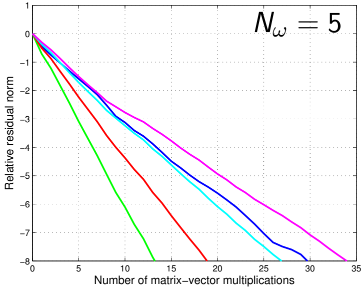
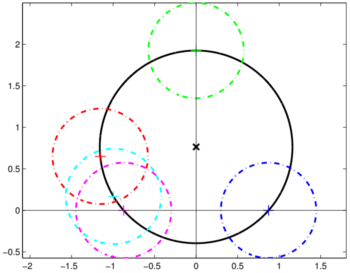
Numerical experiments (2/4)

Validations II



Convergence behavior:

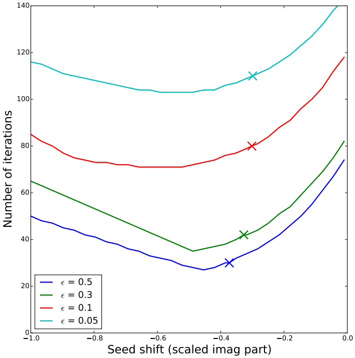
- ω_{min} and ω_{max} converge slowest,
- smallest factor $R/|c_k|$ yields fastest convergence,
- 'inner' frequencies *for free*.



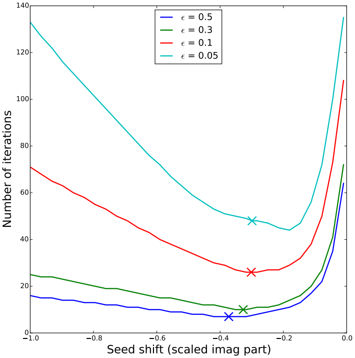
Numerical experiments (3/4)

Shifted Neumann preconditioner

Apply a Neumann polynomial preconditioner of degree n.



case $n = 0$



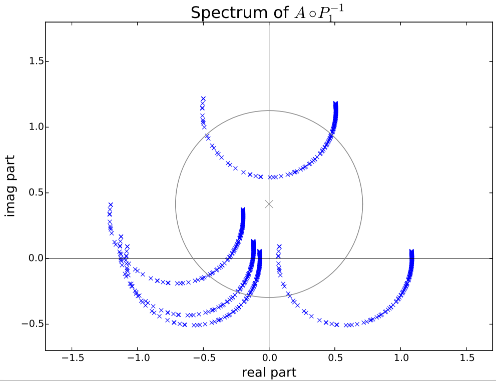
case $n = 5$

Numerical experiments (4/4)

Matrix equation with rotation

Solve matrix equation,

$$A(\mathbf{X}) := K\mathbf{X} + iC\mathbf{X}\Omega - M\mathbf{X}\Omega^2 = B.$$



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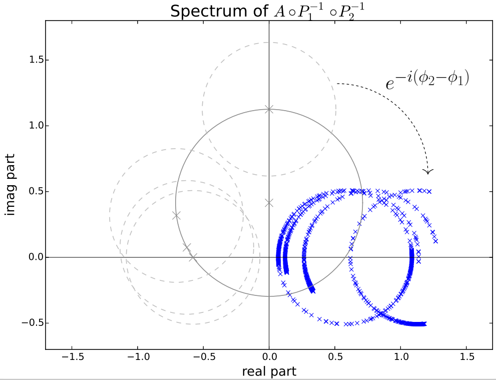
Numerical experiments (4/4)

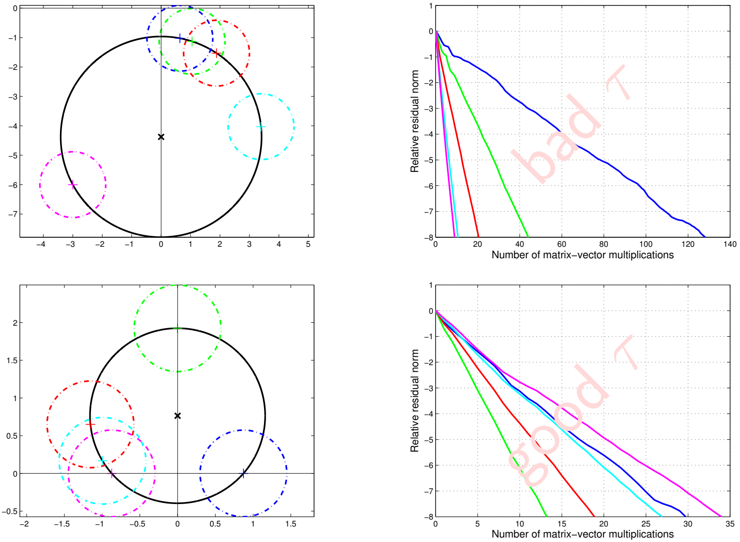
Matrix equation with rotation

Solve matrix equation,

$$A(\mathbf{X}) := K\mathbf{X} + iC\mathbf{X}\Omega - M\mathbf{X}\Omega^2 = B.$$

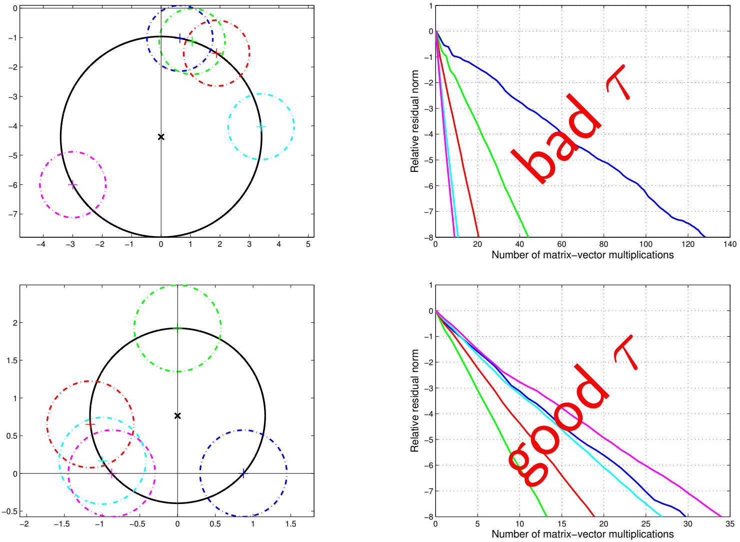


Summary



Relative residual norm
Number of matrix−vector multiplications
bad τ
Relative residual norm
Number of matrix−vector multiplications
good τ

Summary


Relative residual norm
Number of matrix−vector multiplications
bad τ
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Conclusions

- ✓ Optimal shift-and-invert preconditioner for msGMRES.
- ✓ Second level: Shifted Neumann preconditioner & rotations in matrix equation approach.
- ✓ For multi-core CPUs: Splitting strategy of frequency range.
- ✗ Optimality for $\epsilon = 0$ only by continuity.
- ? Relation to pole selection in rational Krylov methods.

Thank you for your attention!

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References

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Finite element discretization in Python

FEM discretization of stiffness matrix K,

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

$$\sigma(\varphi_i) = \lambda(\mathbf{x}) div(\varphi_i) I_3 + \mu(\mathbf{x}) \left(\nabla \varphi_i + (\nabla \varphi_i)^T \right),$$

becomes in nutils:

```
ndims  = 3
phi    = domain.splinefunc(degree=2).vector(ndims)
stress = lambda u: lam*u.div(geom)[:,_,_]*function.eye(ndims)
                    + mu*u.symgrad(geom)
elast  = function.outer(
         stress(phi), phi.grad(geom) ).sum([2,3])
K = domain.integrate(elast, geometry=geom, ischeme='gauss2')
```

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