

Fast Iterative Solution of the Time-Harmonic Elastic Wave Equation at Multiple Frequencies

Manuel M. Baumann

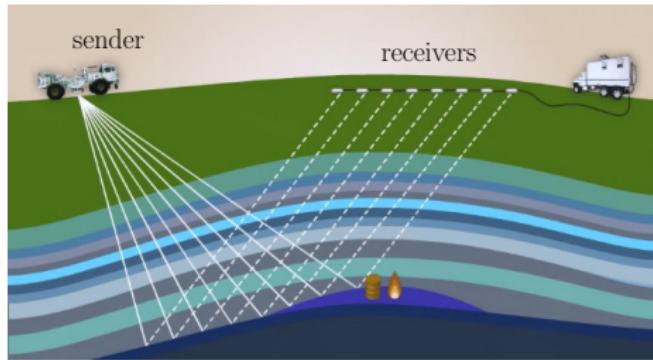
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Royal Institute of Technology in Stockholm - February 1, 2018



Nice to be back!

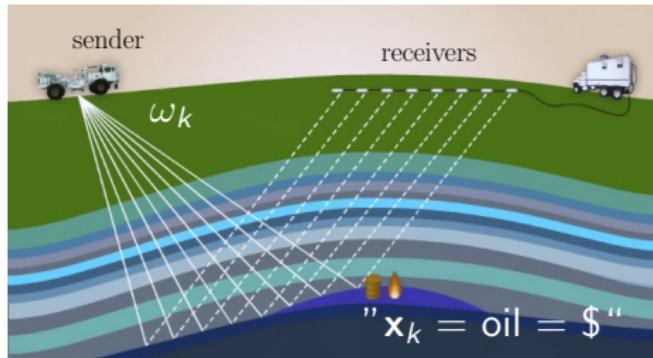
Seismic Full-Waveform Inversion



Inverse problem:

- least-squares fit of measurements and simulations,
- requires *fast* forward solves.

Seismic Full-Waveform Inversion



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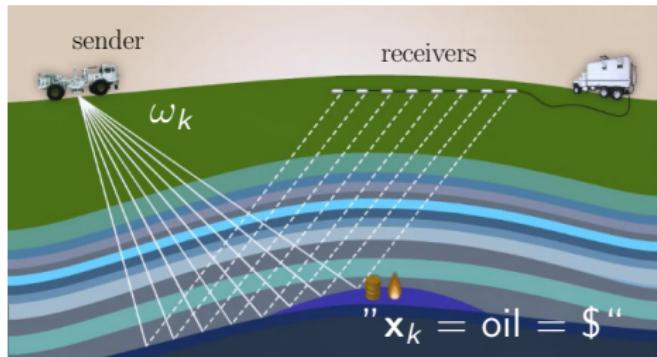
- least-squares fit of measurements and simulations,
- requires *fast* forward solves.

"Solve the linear systems of equations,

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

efficiently (= fast and at low memory) for multiple frequencies."

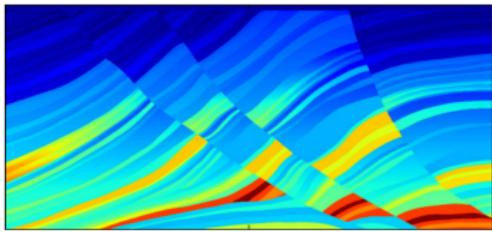
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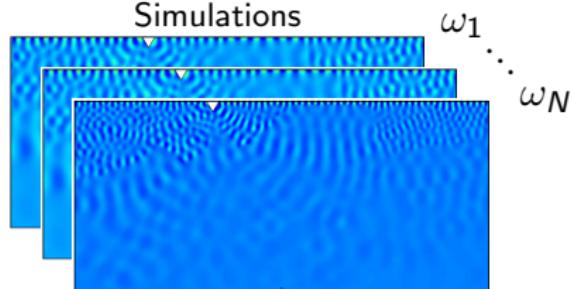
Inverse problem:

- least-squares fit of measurements and simulations,
- requires *fast* forward solves.

Density distribution



Simulations



The 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

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

with FEM matrices

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

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

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

Shifted systems vs. matrix equation

Two main approaches for solving,

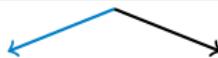
$$(K + i\omega_k C - \omega_k^2 M)\mathbf{x}_k = \mathbf{b}, \quad k > 1.$$



Shifted systems vs. matrix equation

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Shifted systems

$$\left(\begin{bmatrix} iC & K \\ I & 0 \end{bmatrix} - \omega_k \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} \right) \begin{bmatrix} \omega_k \mathbf{x}_k \\ \mathbf{x}_k \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}$$

- Most work for \mathbf{x}_0 (at $\omega = 0$)
- Requires preconditioning

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Matrix equation

$$K\mathbf{X} + iC\mathbf{X}\Omega - M\mathbf{X}\Omega^2 = \mathbf{B}$$

- Most work for \mathbf{x}_0 (at $\omega = 0$)
- Requires preconditioning
- Solve for $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_N]$ *all-at-once*
- Requires preconditioning

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- 1 Multi-shift GMRES
- 2 Optimal preconditioner for ms-GMRES
- 3 Nested multi-shift Krylov methods
- 4 Conclusions

What's a shifted linear system?

Definition

Shifted linear systems are of the form

$$(A - \omega I)\mathbf{x}^{(\omega)} = \mathbf{b},$$

where $\omega \in \mathbb{C}$ is the *shift*.

For the simultaneous solution, **Krylov methods** are well-suited because of the *shift-invariance* property:

$$\mathcal{K}_m(A, \mathbf{b}) \equiv \text{span}\{\mathbf{b}, A\mathbf{b}, \dots, A^{m-1}\mathbf{b}\} = \mathcal{K}_m(A - \omega I, \mathbf{b}).$$

"Proof" (shift-invariance)

$$\text{For } m = 2: \quad \mathcal{K}_2(A, \mathbf{b}) = \text{span}\{\mathbf{b}, A\mathbf{b}\}$$

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

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For shifted systems, we get

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The shift-and-invert preconditioner

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

The multi-frequency problem reads,

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

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

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

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

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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.

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Theorem: msGMRES convergence bound

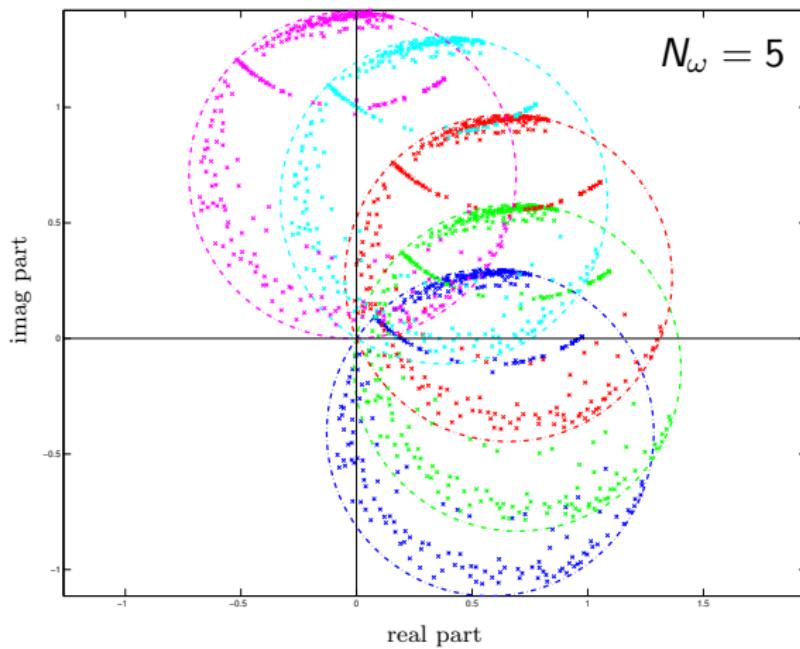
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Let the eigenvalues of a matrix be enclosed by a circle with radius R_k and center c_k . Then the GMRES-residual norm after i iterations $\|\mathbf{r}_k^{(i)}\|$ satisfies,

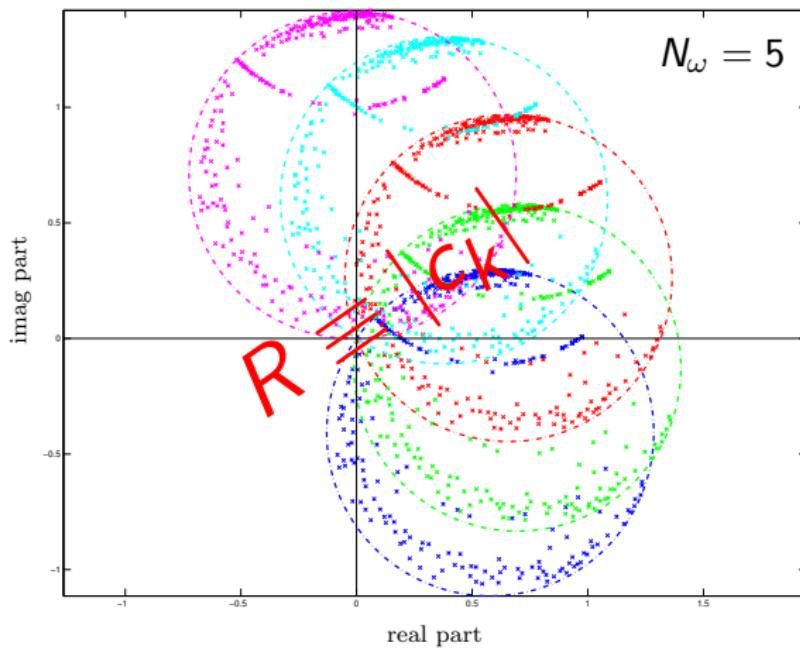
$$\frac{\|\mathbf{r}_k^{(i)}\|}{\|\mathbf{r}^{(0)}\|} \leq c_2(X) \left(\frac{R_k(\tau)}{|c_k(\tau)|} \right)^i, \quad k = 1, \dots, N_\omega,$$

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The preconditioned spectra – no damping

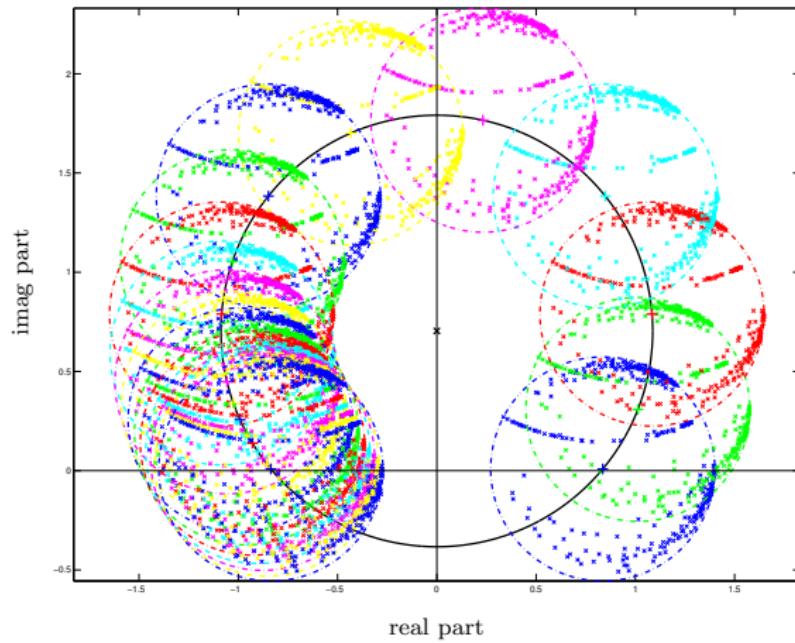


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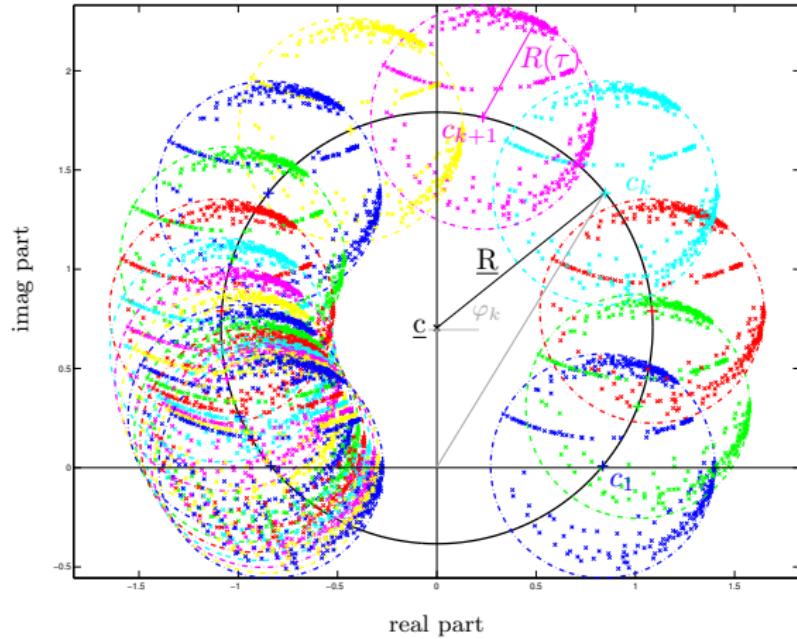
The preconditioned spectra – with damping $\epsilon > 0$

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



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The preconditioned spectra

Lemma: Optimal seed shift for ms-GMRES

[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,

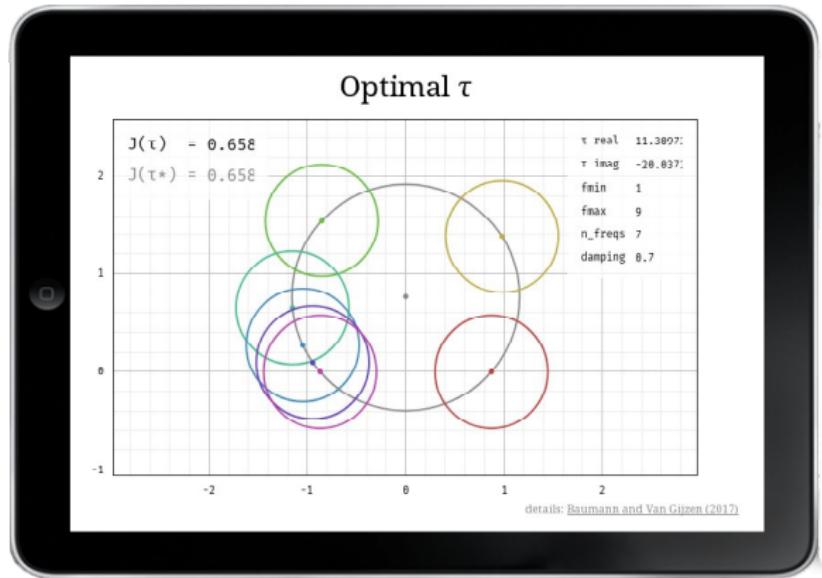
$$\begin{aligned}\tau^*(\epsilon) &= \min_{\tau \in \mathbb{C}} \max_{k=1,..,N_\omega} \left(\frac{R_k(\tau)}{|c_k|} \right) = \dots = \\ &= \frac{2\omega_1 \omega_{N_\omega}}{\omega_1 + \omega_{N_\omega}} - i \frac{\sqrt{[\epsilon^2(\omega_1 + \omega_{N_\omega})^2 + (\omega_{N_\omega} - \omega_1)^2]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

The preconditioned spectra

Proof: Maybe later.

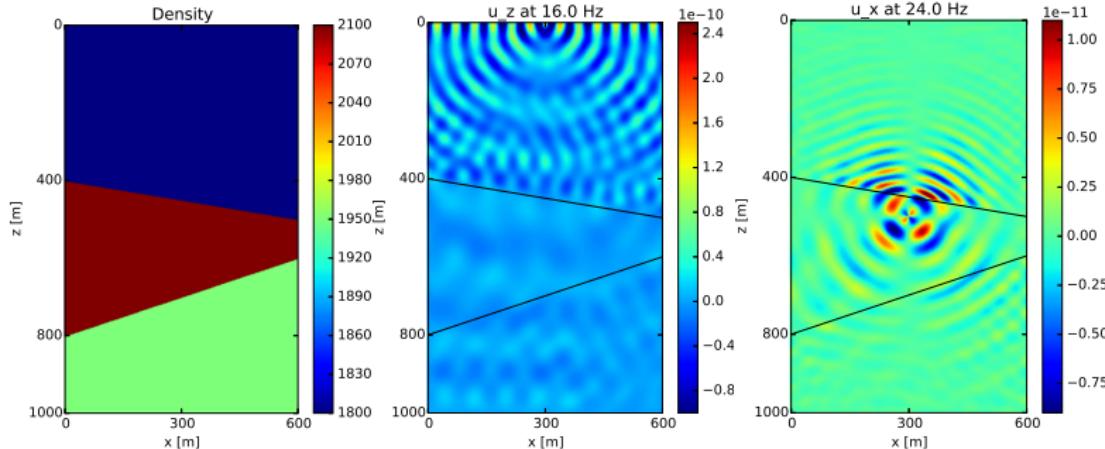
The preconditioned spectra

Proof: There is an App for that.



Numerical experiments I

Set-up: An *elastic wedge* problem.

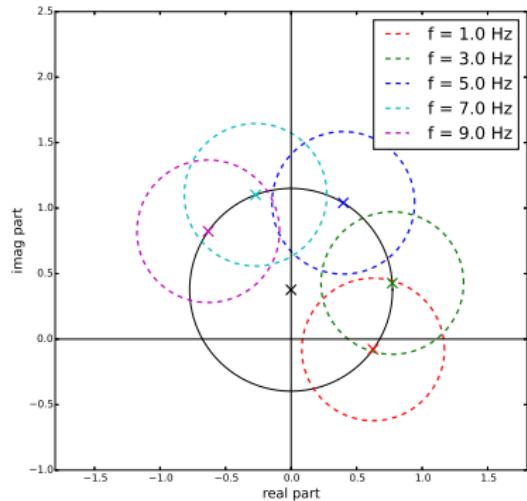
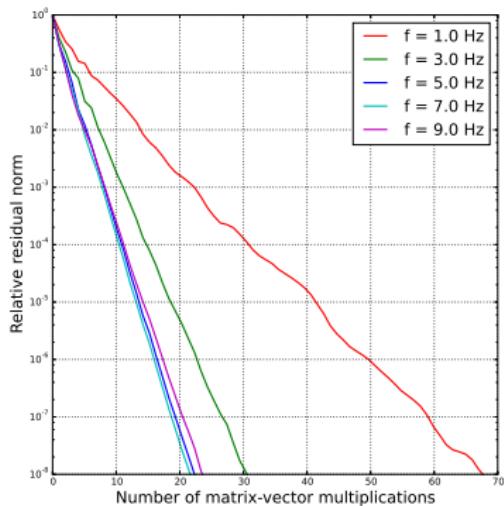


Reference

M. Baumann and M.B. van Gijzen (2017). *An Efficient Two-Level Preconditioner for Multi-Frequency Wave Propagation Problems*. DIAM Technical Report 17-03, TU Delft.

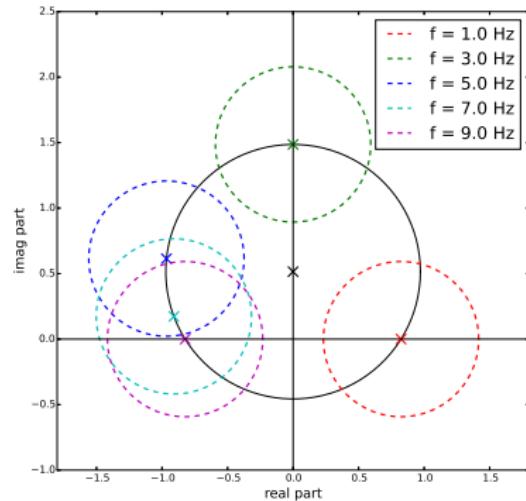
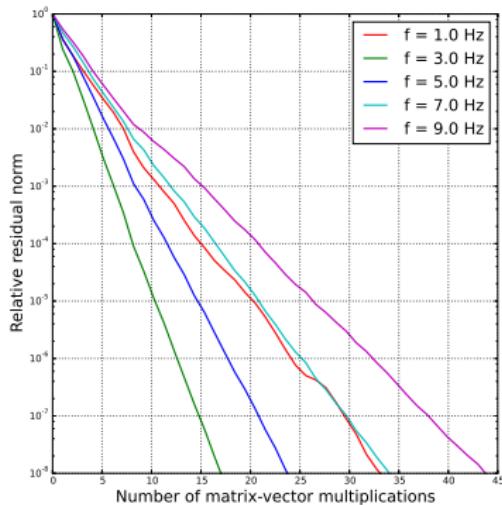
Convergence behavior and spectral bounds

For any τ ...



Convergence behavior and spectral bounds

For the optimal τ^* ...



An interval splitting strategy

Suppose $n_p \geq 2$ parallel processors are available.

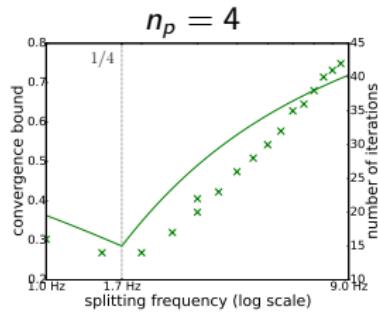
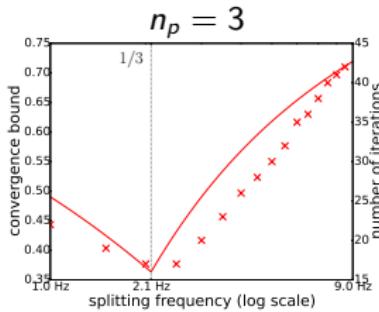
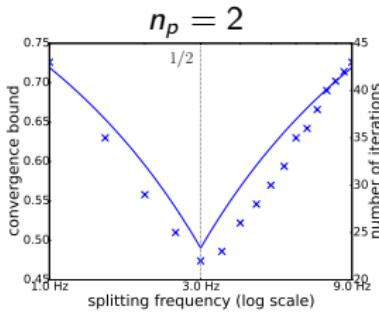
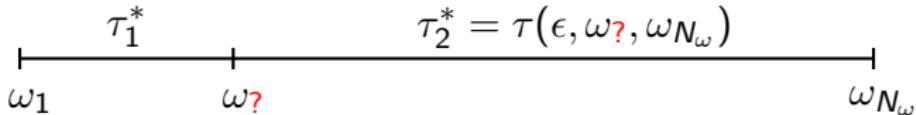


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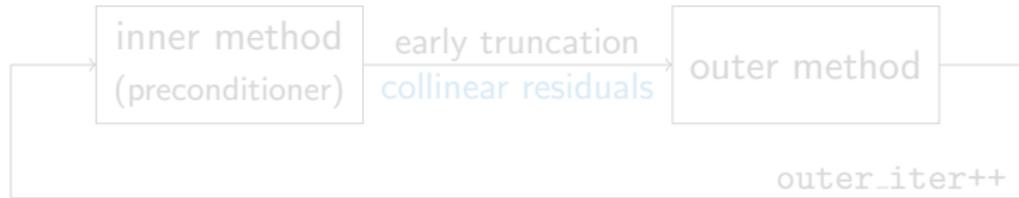
Nested (inner-outer) multi-shift Krylov methods

Solve the shifted linear systems

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

with a nested Krylov method, and preserve,

$$\mathcal{K}_m(A, \mathbf{r}_0) = \mathcal{K}_m(A - \omega I, \mathbf{r}_0) \quad \forall \omega.$$



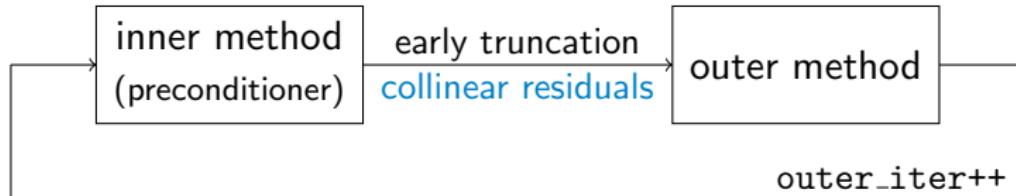
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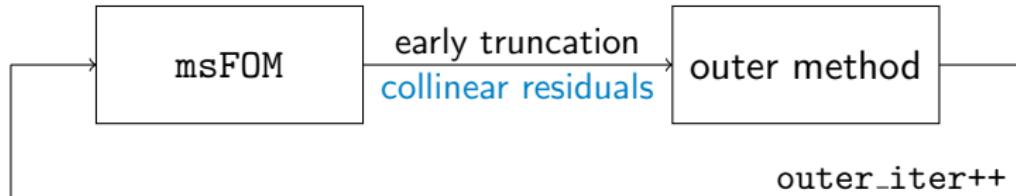
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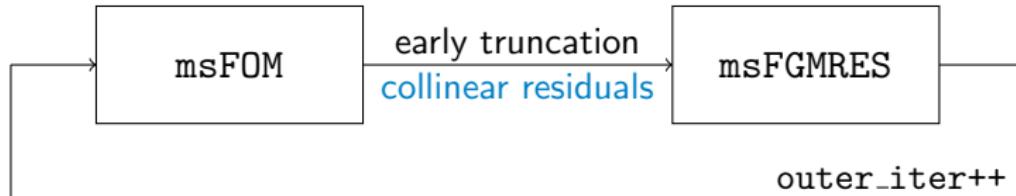
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Multi-shift FOM as inner method

Classical result: In FOM, the residuals are

$$\mathbf{r}_j = \mathbf{b} - A\mathbf{x}_j = \dots = -h_{j+1,j}\mathbf{e}_j^T \mathbf{y}_j \mathbf{v}_{j+1}.$$

Thus, for the shifted residuals it holds:

$$\mathbf{r}_j^{(\omega)} = \mathbf{b} - (A - \omega I)\mathbf{x}_j^{(\omega)} = \dots = -h_{j+1,j}^{(\omega)}\mathbf{e}_j^T \mathbf{y}_j^{(\omega)} \mathbf{v}_{j+1},$$

which gives $\gamma = y_j^{(\omega)} / y_j$.

Reference

V. Simoncini, *Restarted full orthogonalization method for shifted linear systems*. BIT Numerical Mathematics, 43 (2003).

Flexible multi-shift GMRES as outer method

Use flexible GMRES in the outer loop,

$$(A - \omega I) \widehat{\mathcal{V}}_m = V_{m+1} \underline{H}_m^{(\omega)},$$

where one column yields

$$(A - \omega I) \underbrace{\mathcal{P}(\omega)_j^{-1} \mathbf{v}_j}_{\text{inner loop}} = V_{m+1} \underline{\mathbf{h}}_j^{(\omega)}, \quad 1 \leq j \leq m.$$

The “inner loop” is the truncated solution of $(A - \omega I)$ with right-hand side \mathbf{v}_j using msFOM.

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The “inner loop” is the truncated solution of $(A - \omega I)$ with right-hand side \mathbf{v}_j using `msFOM`.

Flexible multi-shift GMRES

Thus, the inner residuals are:

$$\begin{aligned}\mathbf{r}_j^{(\omega)} &= \mathbf{v}_j - (A - \omega I)\mathcal{P}(\omega)_j^{-1}\mathbf{v}_j, \\ \mathbf{r}_j &= \mathbf{v}_j - A\mathcal{P}_j^{-1}\mathbf{v}_j,\end{aligned}$$

Imposing $\mathbf{r}_j^{(\omega)} = \gamma \mathbf{r}_j$ yields:

$$(A - \omega I)\mathcal{P}(\omega)_j^{-1}\mathbf{v}_j = \gamma A\mathcal{P}_j^{-1}\mathbf{v}_j - (\gamma - 1)\mathbf{v}_j \quad (*)$$

Note that the right-hand side in (*) is a preconditioned shifted system!

Flexible multi-shift GMRES

Thus, the inner residuals are:

$$\begin{aligned}\mathbf{r}_j^{(\omega)} &= \mathbf{v}_j - (A - \omega I) \mathcal{P}(\omega)_j^{-1} \mathbf{v}_j, \\ \mathbf{r}_j &= \mathbf{v}_j - A \mathcal{P}_j^{-1} \mathbf{v}_j,\end{aligned}$$

Imposing $\mathbf{r}_j^{(\omega)} = \gamma \mathbf{r}_j$ yields:

$$(A - \omega I) \mathcal{P}(\omega)_j^{-1} \mathbf{v}_j = \gamma A \mathcal{P}_j^{-1} \mathbf{v}_j - (\gamma - 1) \mathbf{v}_j \quad (*)$$

Note that the right-hand side in (*) is a preconditioned shifted system!

Flexible multi-shift GMRES

Altogether,

$$(A - \omega I) \mathcal{P}(\omega)_j^{-1} \mathbf{v}_j = V_{m+1} \underline{\mathbf{h}}_j^{(\omega)}$$

$$\gamma A \mathcal{P}_j^{-1} \mathbf{v}_j - (\gamma - 1) \mathbf{v}_j = V_{m+1} \underline{\mathbf{h}}_j^{(\omega)}$$

$$\gamma V_{m+1} \underline{\mathbf{h}}_j - V_{m+1} (\gamma - 1) \underline{\mathbf{e}}_j = V_{m+1} \underline{\mathbf{h}}_j^{(\omega)}$$

$$V_{m+1} (\gamma \underline{\mathbf{h}}_j - (\gamma - 1) \underline{\mathbf{e}}_j) = V_{m+1} \underline{\mathbf{h}}_j^{(\omega)}$$

which yields:

$$\underline{\mathbf{H}}_m^{(\omega)} = (\underline{\mathbf{H}}_m - \underline{\mathbf{I}}_m) \Gamma_m + \underline{\mathbf{I}}_m,$$

with $\Gamma_m := \text{diag}(\gamma_1, \dots, \gamma_m)$.

Flexible multi-shift GMRES

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Flexible multi-shift GMRES

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with $\Gamma_m := \text{diag}(\gamma_1, \dots, \gamma_m)$.

Summary: Nested FOM-FGMRES

In nested FOM-FGMRES, we solve the following (small) optimization problems,

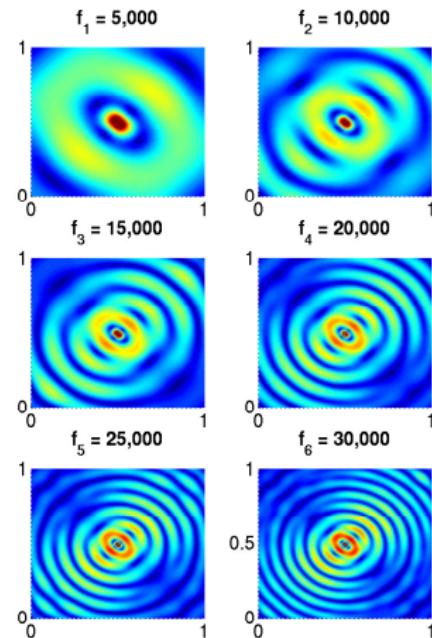
$$\begin{aligned}\mathbf{x}_m^{(\omega)} &= \underset{\mathbf{x} \in \widehat{\mathcal{V}}_m}{\operatorname{argmin}} \|\mathbf{b} - (A - \omega I)\mathbf{x}\| \\&= \underset{\mathbf{y} \in \mathbb{C}^m}{\operatorname{argmin}} \left\| \mathbf{b} - (A - \omega I)\widehat{V}_m \mathbf{y} \right\| \\&= \underset{\mathbf{y} \in \mathbb{C}^m}{\operatorname{argmin}} \left\| \mathbf{b} - V_{m+1} \underline{H}_m^{(\omega)} \mathbf{y} \right\| \\&= \underset{\mathbf{y} \in \mathbb{C}^m}{\operatorname{argmin}} \left\| \beta \mathbf{e}_1 - \left((\underline{H}_m - \underline{I}_m) \Gamma_m^{(\omega)} + \underline{I}_m \right) \mathbf{y} \right\|,\end{aligned}$$

where the entries of $\Gamma_m^{(\omega)}$ are **collinearity factors of inner FOM**.

Numerical experiments II

Test case from literature:

- $\Omega = [0, 1] \times [0, 1]$
- $h = 0.01$ implying
 $n = 10.201$ grid points
- system size:
 $4n = 40.804$
- $N = 6$ frequencies
- point source at center



Reference

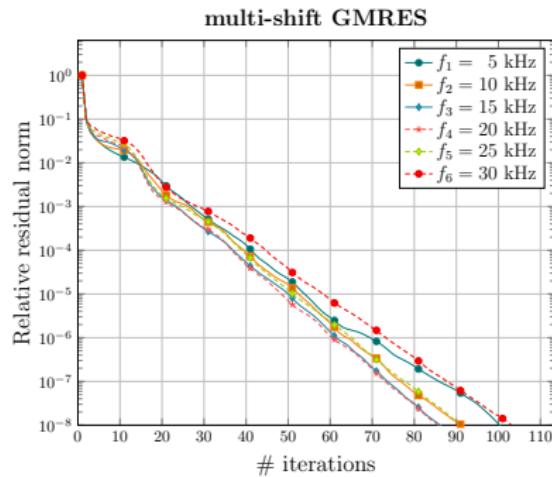
M. Baumann and M.B. van Gijzen (2015). *Nested Krylov methods for shifted linear systems*. SIAM J. Sci. Comput., **37**(5), S90-S112.

Numerical experiments II

as presented in [B./vG., 2015]

Preconditioned **multi-shift** GMRES:

- simultaneous solve
- linear convergence rates
- $\tau = \tau^* = (0.3 - 0.7i)\omega_{max}$
- CPU time: 17.71s

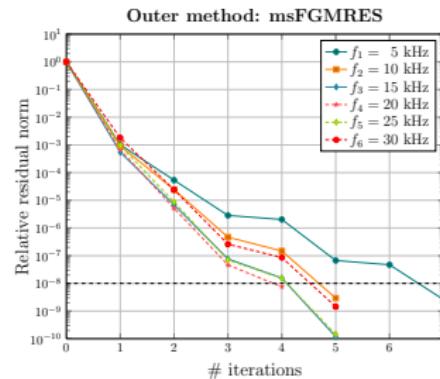
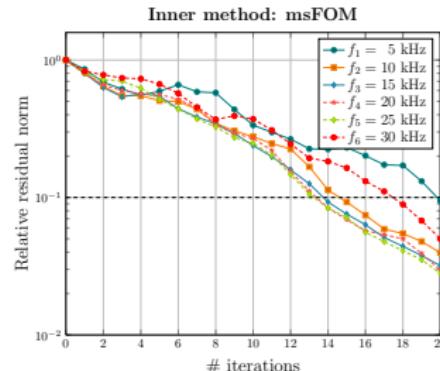


Numerical experiments II

as presented in [B./vG., 2015]

Preconditioned nested FOM-FGMRES:

- 20 inner iterations
- truncate when inner residual norm ~ 0.1
- very few outer iterations
- CPU time: **9.12s**



Numerical experiments II

as presented in [B./vG., 2015]

Various combinations of inner/outer methods *possible*:

	msGMRES	msGMRESr	multi-shift Krylov methods	
# inner iterations	-	20	QMRIDR(4)	msIDR(4)
# outer iterations	103	7	136	134
CPU time	17.71s	6.13s	22.35s	22.58s
nested multi-shift Krylov methods				
	FOM-FGMRES	IDR(4)-FGMRES	FOM-FQMRIDR(4)	IDR(4)-FQMRIDR(4)
# inner iterations	20	25	30	30
# outer iterations	7	9	5	15
CPU time	9.12s	32.99s	8.14s	58.36s

Different combination (CMRH-FCMRH) is exploited in:

X.-M. Gu, T.-Z. Huang, B. Carpentieri, A. Imakura, K. Zhang, L. Du.
Variants of the CMRH method for solving multi-shifted non-Hermitian linear systems. Technical Report, University of Groningen (2016).

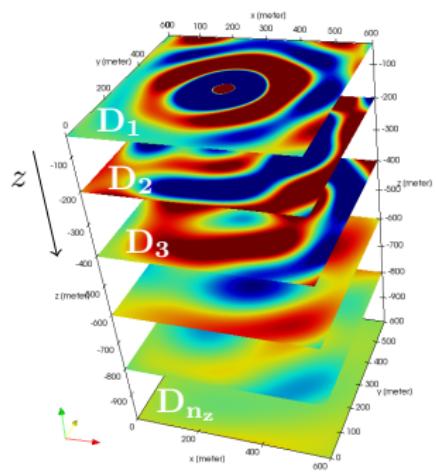
Conclusions

What I have shown today:

- ✓ Optimal τ^* for multi-shift GMRES
- ✓ Nested multi-shift FOM-FGMRES

What I have not shown today:

- ✓ MSSS preconditioning techniques
- ✓ matrix equation (global GMRES)
- ✓ large-scale 3D examples
- ✗ deflation, model-order reduction, ...



References

-  M. Baumann and M.B. van Gijzen (2015). *Nested Krylov methods for shifted linear systems*. SIAM J. Sci. Comput., **37**(5), S90-S112.
-  M. Baumann, R. Astudillo, Y. Qiu, E. Ang, M.B. van Gijzen, and R.-E. Plessix (2017). *An MSSS-Preconditioned Matrix Equation Approach for the Time-Harmonic Elastic Wave Equation at Multiple Frequencies*. Springer Computat. Geosci., DOI: 10.1007/s10596-017-9667-7.
-  M. Baumann and M.B. van Gijzen (2017). *Efficient iterative methods for multi-frequency wave propagation problems: A comparison study*. Procedia Comput. Sci., Vol. **108**, pp. 645-654.
-  M. Baumann and M.B. van Gijzen (2017). *An Efficient Two-Level Preconditioner for Multi-Frequency Wave Propagation Problems*. DIAM Technical Report **17-03**, TU Delft. [under review]

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,

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

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 ($\lambda = i\omega$), 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	$\text{Re}(\lambda) \leq 0$	
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

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

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

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:

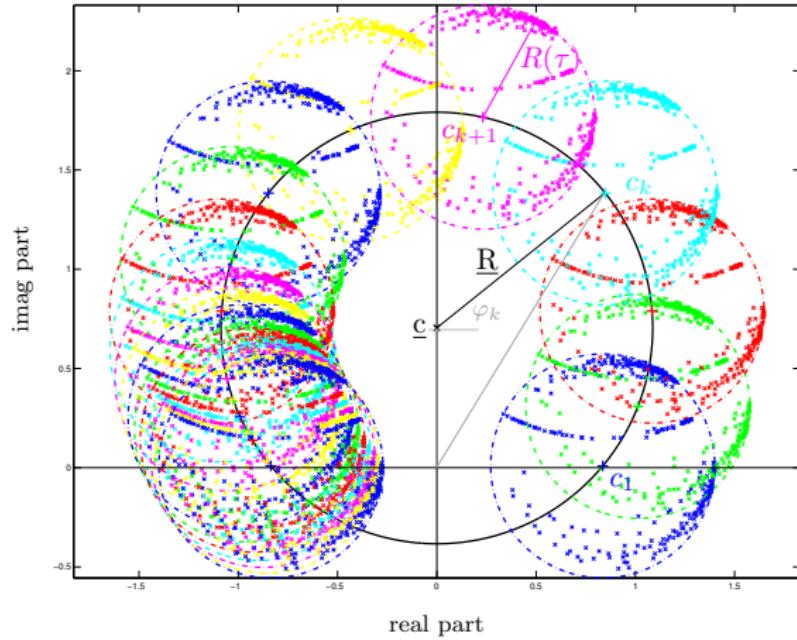
$$\underline{c} = \left(0, \frac{\epsilon |\tau|^2}{2\Im(\tau)(\Im(\tau) + \epsilon \Re(\tau))} \right) \in \mathbb{C}$$

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 $\epsilon > 0$

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

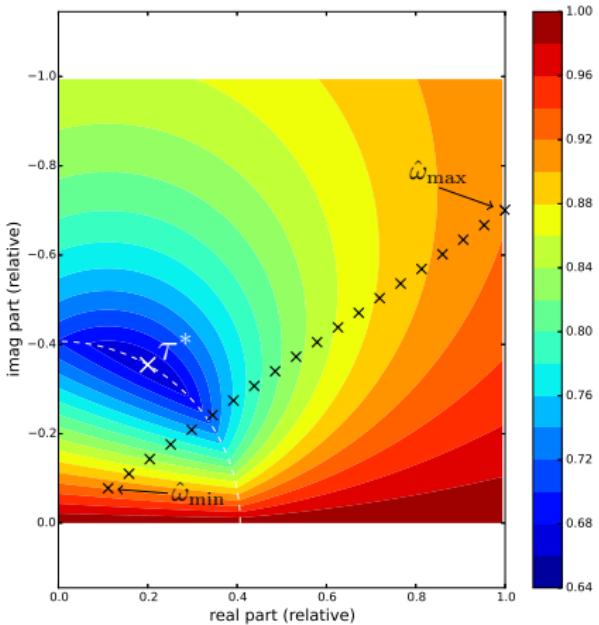


The preconditioned spectra – Proof (4/4)

(iv) Find optimal τ^* .

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

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

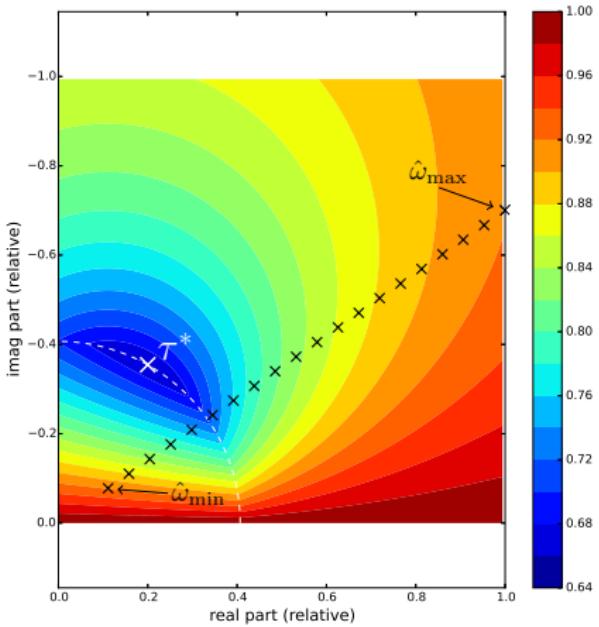


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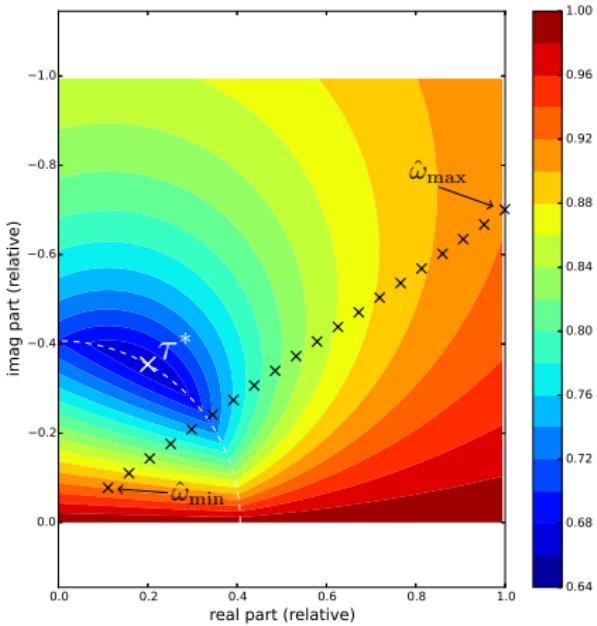


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$$\tau^* = \frac{2\omega_1\omega_{N_\omega}}{\omega_1 + \omega_{N_\omega}} - i \frac{\sqrt{[\epsilon^2(\omega_1 + \omega_{N_\omega})^2 + (\omega_{N_\omega} - \omega_1)^2]\omega_1\omega_{N_\omega}}}{\omega_1 + \omega_{N_\omega}}$$