Efficient iterative methods for multi-frequency wave propagation problems

A comparison study

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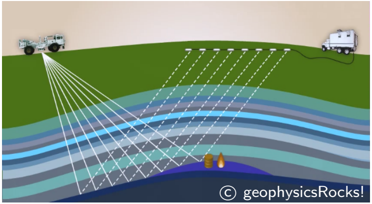
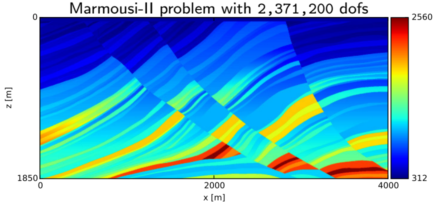
June 14, 2017

Full-waveform inversion



Seismic exploration:

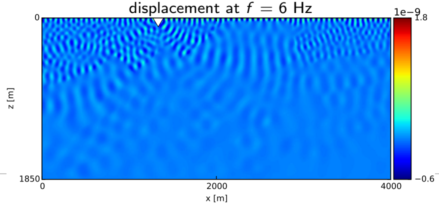
- elastic wave equation
- in frequency-domain
- 'only' forward problem



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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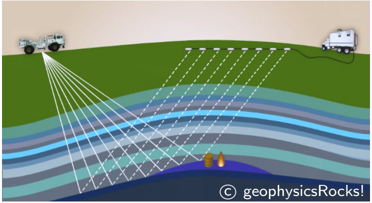
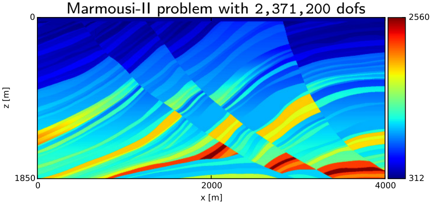
Solve

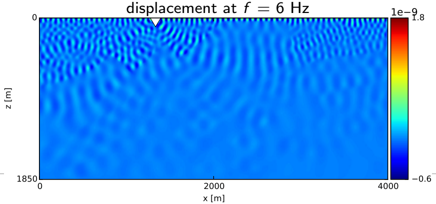
$$\boxed{(K + i\omega_k C - \omega_k^2 M)\mathbf{x}_k = \mathbf{b}}$$

for multiple frequencies ω_k.

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







Different approaches

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

1. Shifted systems:

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

   - Multi-shift GMRES
   - Nested multi-shift FOM-FGMRES

2. Matrix equation:

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

   - Global GMRES

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- Multi-shift GMRES + preconditioning
- Nested multi-shift FOM-FGMRES + preconditioning

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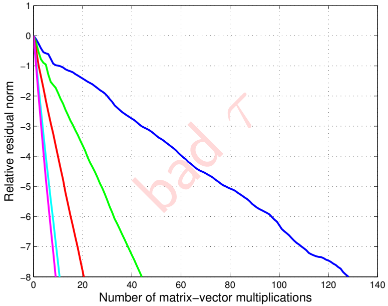
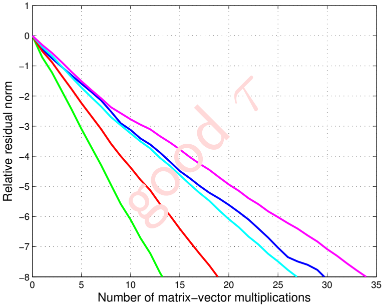
- Global GMRES + preconditioning

First example - preconditioned multi-shift GMRES

Convergence behavior for two different $\mathcal{P}(\tau)$.





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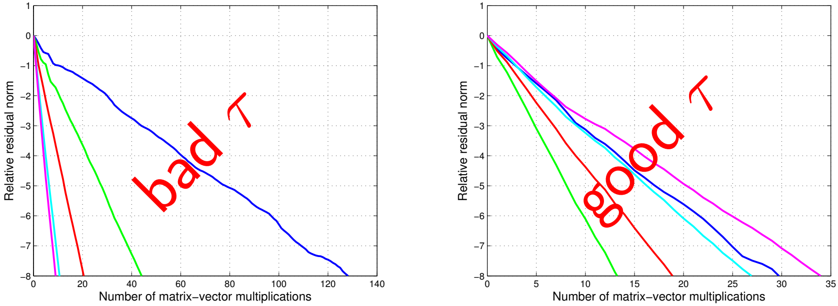

Outlook

1. The three approaches – in a nutshell
   - Multi-shift GMRES
   - Nested multi-shift FOM-FGMRES
   - Global GMRES
2. Preconditioner design
3. Numerical examples

Alg. 1: Multi-shift GMRES (1/2)

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

Want to solve

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

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

Alg. 1: Multi-shift GMRES (2/2)

For shifted problems,

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

Krylov spaces are shift-invariant, i.e.,

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

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

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Alg. 2: Nested multi-shift FOM-FGMRES (1/2)

Consider, again, shifted problems,

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

- Inner method = preconditioner
- Outer method: Multi-shift Krylov
- Preserve shift-invariance!

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Consider, again, shifted problems,

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

- Inner method = preconditioner $\rightarrow$ msFOM
- Outer method: Multi-shift Krylov $\rightarrow$ msGMRES
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Alg. 2: Nested multi-shift FOM-FGMRES (2/2)

Inner method: Residuals in multi-shift FOM are collinear, i.e. for

$$\mathbf{r}_j^{(0)} = \mathbf{b} - \mathcal{C}\mathbf{y}_j^{(0)},$$
$$\mathbf{r}_j^{(k)} = \mathbf{b} - (\mathcal{C} - \eta_k I)\mathbf{y}_j^{(k)},$$

it holds $\mathbf{r}_j^{(k)} = \gamma_j^{(k)} \mathbf{r}_j^{(0)}$ (after j inner iterations).

Outer method: Collinearity factors appear in the Hessenberg matrix,

$$\underline{\mathrm{H}}_m^{(k)} = (\underline{\mathrm{H}}_m - \underline{\mathrm{I}}_m)\Gamma_k + \underline{\mathrm{I}}_m, \quad \Gamma_k := \mathrm{diag}(\gamma_1^{(k)}, \ldots, \gamma_m^{(k)}),$$

of multi-shift GMRES applied to the system with shift η_k.

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of multi-shift GMRES applied to the system with shift η_k.

Alg. 3: Global GMRES (1/2)

Consider, on the other hand, the matrix equation,

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

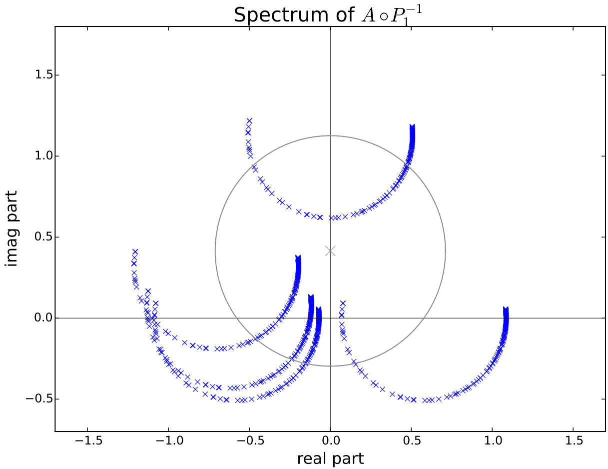
- Frequencies appear in $\Omega \equiv \text{diag}(\omega_1, ..., \omega_N)$.
- Global Krylov methods for $\mathcal{A}(\mathbf{X}) = \mathbf{B}$.
- Efficient block MatVec's via BLAS-3.

Reference

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.

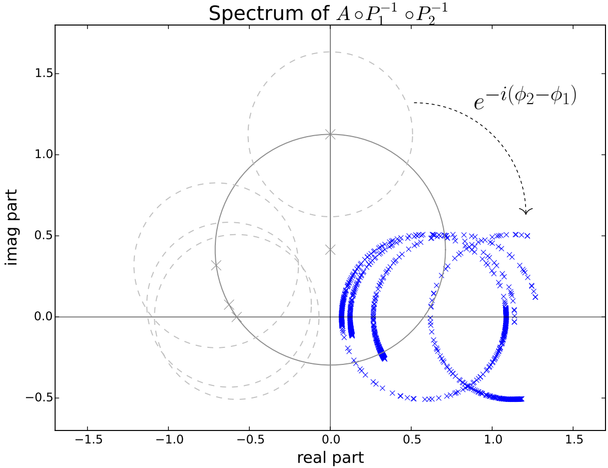
Alg. 3: Global GMRES (2/2)

Spectral analysis



Alg. 3: Global GMRES (2/2)

Spectral analysis



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3. Numerical examples

Optimization of seed frequency τ

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

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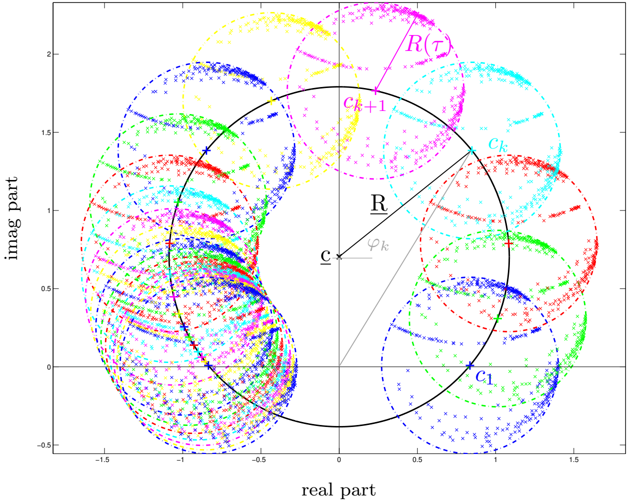
Theorem: msGMRES convergence bound [Saad, Iter. Methods]

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,

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

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

The preconditioned spectra



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,

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

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

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Applet

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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

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

nutils

The (damped) time-harmonic elastic wave equation

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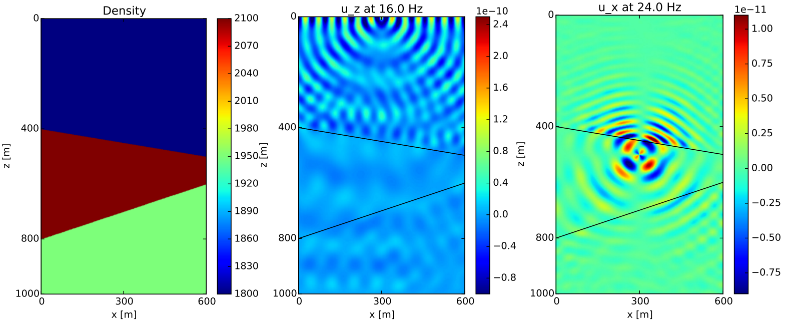
nutils

Numerical experiments

Set-up: An *elastic* wedge problem.

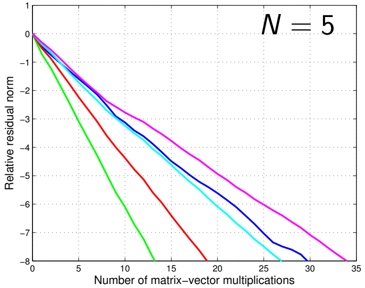


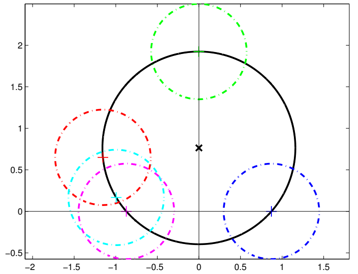
Numerical experiments (1/3)

Optimal τ^* – Validations

Convergence behavior:

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





Numerical experiments (2/3)

Multi-shift vs. matrix equation

CPU times and iteration numbers for a typical 2D problem:

problem size	frequency range	n_ω	Gl-GMRES	poly-msGMRES	FOM-FGMRES
$2 \times 200 \times 200$	$\omega_k \in 2\pi[12, 16]$Hz	5	29.3 (48)	12.65 (12)	12.63 $(7 \cdot 8)$
$2 \times 200 \times 200$	$\omega_k \in 2\pi[10, 16]$Hz	5	46.6 (75)	15.31 (19)	16.04 $(12 \cdot 8)$
$2 \times 200 \times 200$	$\omega_k \in 2\pi[8, 16]$Hz	5	79.9 (112)	19.80 (29)	19.90 $(17 \cdot 8)$
$2 \times 200 \times 200$	$\omega_k \in 2\pi[12, 16]$Hz	15	64.8 (47)	15.71 (12)	13.41 $(7 \cdot 8)$
$2 \times 200 \times 200$	$\omega_k \in 2\pi[10, 16]$Hz	15	115.9 (73)	18.37 (19)	16.86 $(12 \cdot 8)$
$2 \times 200 \times 200$	$\omega_k \in 2\pi[8, 16]$Hz	15	198.9 (109)	22.49 (29)	20.71 $(17 \cdot 8)$

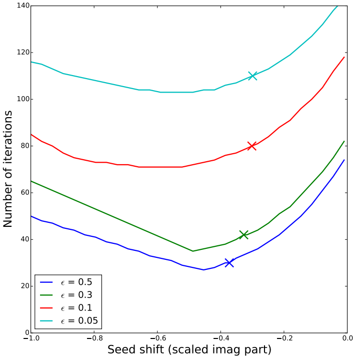
Reference

M. Baumann and M.B. van Gijzen (2017). *Efficient iterative methods for multi-frequency wave propagation problems: A comparison study.* Procedia Computer Science, Vol. **108**, pp. 645–654.

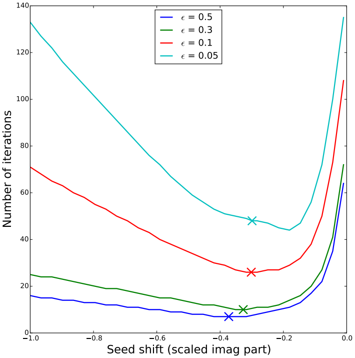
Numerical experiments (3/3)

Shifted Neumann preconditioner

Apply a Neumann polynomial preconditioner of degree n.

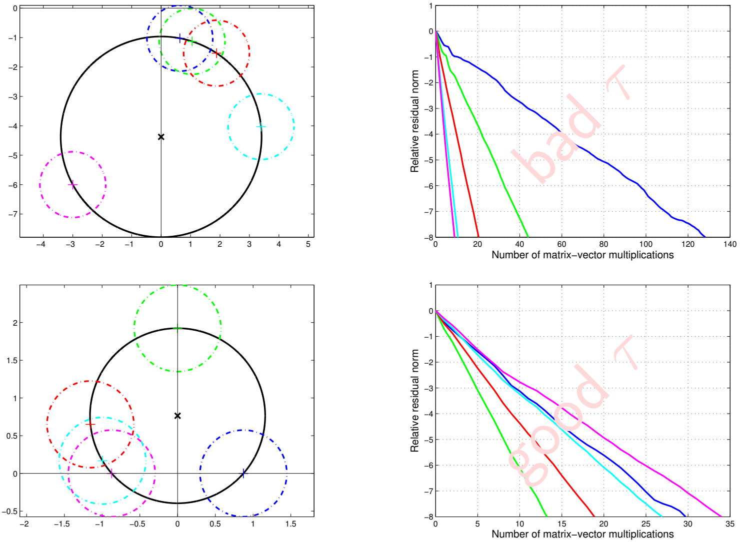


case $n = 0$



case $n = 5$

Summary



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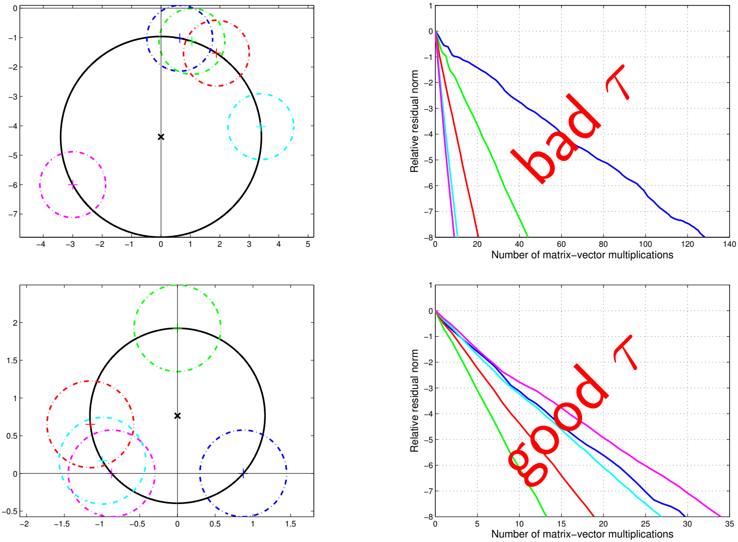
Summary


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

Conclusions

What have we learnt?

- ✓ Spectral analysis yields optimal τ^*
- ✓ Multi-shift approaches: Exact solves for $\mathcal{P}(\tau^*)^{-1}$,
  but τ^* has (a lot of) damping
- ✓ Matrix equation: Spectral rotation improves convergence
- ? SSOR + coarse grid correction for large 3D problems

Thank you for your attention!

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M. Baumann and M.B. van Gijzen (2017). *Efficient iterative methods for multi-frequency wave propagation problems: A comparison study.* Procedia Computer Science, 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].

Research funded by Shell.

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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