Nested Krylov Methods for Solving the Time-Harmonic Elastic Wave Equation at Multiple Frequencies

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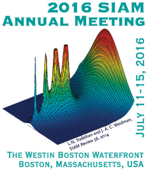

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Context of this work (1/3)

Why are we here?

Definition: Shifted linear systems

We want to *efficiently* solve

$$(\mathcal{A} - \sigma_k I)\mathbf{x}_k = \mathbf{b}$$

for multiple shifts $\sigma_1, ..., \sigma_{N_\sigma}, N_\sigma \in \mathbb{N}$.

The *efficiency* of our numerical method heavily relies on the shift-invariance property of Krylov subspaces,

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

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Context of this work (2/3)

Who works in this area?

Recent work

- A. Saibaba, T. Bakhos, and P. Kitanidis. *A flexible Krylov solver for shifted systems with application to oscillatory hydraulic tomography.* SIAM J. Sci. Comput. **35**:3001-3023 (2013).
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What does the present work contribute?

We present a nested Krylov solver for shifted linear systems:

1. Use a multi-shift Krylov method as an inner method (the preconditioner),
2. use a flexible multi-shift Krylov method as an outer method,
3. apply a single *shifted Laplace* preconditioner as a first layer.

In this talk, we will concentrate on 1-2, and comment on 3 when presenting numerical tests.

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Outlook

1. Nested Krylov methods for shifted systems
2. The time-harmonic elastic wave equation
3. Numerical examples
   - Example 1: Academic test case
   - Example 2: Marmousi-II

Nested (inner-outer) multi-shift Krylov methods

Solve the shifted linear systems

$$(\mathcal{A} - \sigma_k I)\,\mathbf{x}_k = \mathbf{b}, \quad k = 1, \ldots, N_\sigma,$$

with a nested Krylov method based on

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

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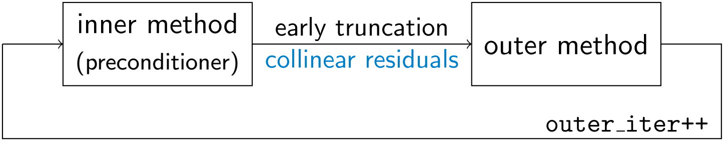

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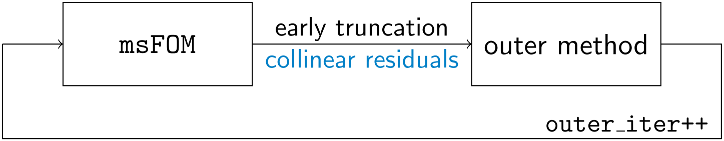

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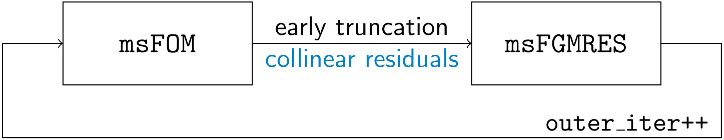

Inner method: multi-shift FOM

Classical result: In FOM, the residuals are:

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

Thus, for the shifted residuals it holds:

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

Hence, we obtain collinear residuals,

$$\mathbf{r}_j^{(\sigma)} = \gamma_j \mathbf{r}_j,$$

with factor $\gamma_j = y_j^{(\sigma)}/y_j$.

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Outer method: flexible multi-shift GMRES (1/3)

Use flexible GMRES in the outer loop,

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

where one column yields:

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

Recap: The "inner loop" is the truncated solution of $(\mathcal{A} - \sigma I)$ with right-hand side $\mathbf{v}_j$ using `msFOM`.

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The inner residuals are:

$$\mathbf{r}_j^{(\sigma)} = \mathbf{v}_j - (\mathcal{A} - \sigma I)\mathcal{P}(\sigma)_j^{-1}\mathbf{v}_j,$$
$$\mathbf{r}_j = \mathbf{v}_j - \mathcal{A}\mathcal{P}_j^{-1}\mathbf{v}_j.$$

Imposing collinearity, $\mathbf{r}_j^{(\sigma)} = \gamma_j \mathbf{r}_j$, yields:

$$(\mathcal{A} - \sigma I)\mathcal{P}(\sigma)_j^{-1}\mathbf{v}_j = \gamma_j \mathcal{A}\mathcal{P}_j^{-1}\mathbf{v}_j - (\gamma_j - 1)\mathbf{v}_j$$

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Outer method: flexible multi-shift GMRES (3/3)

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with $\Gamma_m := diag(\gamma_1, ..., \gamma_j, ..., \gamma_m)$.

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Summary: Nested FOM-FGMRES

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

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

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

Relation to Rational Krylov methods

The FOM-FGMRES Hessenberg matrix,

$$\underline{\mathrm{H}}_m^{(\sigma)} = (\underline{\mathrm{H}}_m - \underline{\mathrm{I}}_m)\,\Gamma_m^{(\sigma)} + \underline{\mathrm{I}}_m, \quad \Gamma_m^{(\sigma)} := diag(\gamma_1^{(\sigma)}, \dots, \gamma_m^{(\sigma)}),$$

is closely related to the formula,

$$\underline{\mathrm{H}}(\sigma; T_m) = (\underline{\mathrm{H}}_m(T_m - \sigma I_m) + \underline{\mathrm{I}}_m), \quad T_m := diag(\tau_1, \dots, \tau_m),$$

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2. The time-harmonic elastic wave equation

3. Numerical examples
   - Example 1: Academic test case
   - Example 2: Marmousi-II

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 $\partial\Omega_a \,\dot\cup\, \partial\Omega_r$.

Discrete setting

Solve

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

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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The time-harmonic elastic wave equation

The discretized problem

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

can be re-formulated to

$$\left[\begin{pmatrix} iC & K \\ I & 0 \end{pmatrix} - \omega_k \begin{pmatrix} M & 0 \\ 0 & I \end{pmatrix}\right]\begin{pmatrix} \omega_k \mathbf{u}_k \\ \mathbf{u}_k \end{pmatrix} = \begin{pmatrix} \mathbf{s} \\ 0 \end{pmatrix},$$

which is of block form:

$$(\mathcal{A} - \omega_k \mathcal{M})\mathbf{x}_k = \mathbf{b}.$$

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The time-harmonic elastic wave equation

Right-preconditioning yields,

$$(\mathcal{A} - \omega_k \mathcal{M})\mathcal{P}_{\omega}^{-1}\mathbf{y}_k = \mathbf{b} \quad \Leftrightarrow \quad \boxed{(\mathcal{A}\mathcal{P}^{-1} - \sigma_k I)\mathbf{y}_k = \mathbf{b},}$$

with $\mathcal{P}^{-1} \equiv (\mathcal{A} - \tau\mathcal{M})^{-1}, \sigma_k = \omega_k/(\omega_k - \tau)$.

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

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The time-harmonic elastic wave equation

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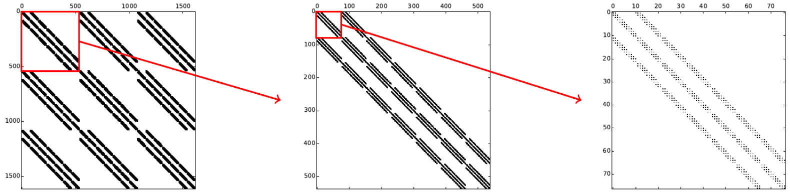

Reference

M. Baumann, R. Astudillo, Y. Qiu, E. Ang, M.B. Van Gijzen, and R.-É. Plessix. *An MSSS-Preconditioned Matrix Equation Approach for the Time-Harmonic Elastic Wave Equation at Multiple Frequencies.* Technical Report 16-04, Delft University of Technology (2016).

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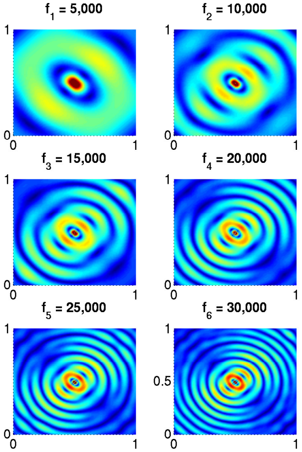
Numerical example # 1

as presented in [B./vG., 2014]

Test case from literature:

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



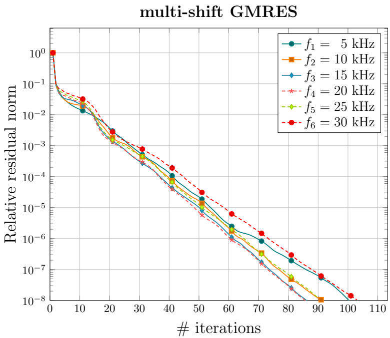
Reference

T. Airaksinen, A. Pennanen, and J. Toivanen. *A damping preconditioner for time-harmonic wave equations in fluid and elastic material.* J. Comput. Phys., **228**:1466-1479 (2009).

Numerical example # 1
as presented in [B./vG., 2014]

Preconditioned **multi-shift GMRES**:

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

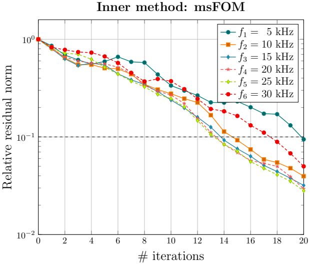


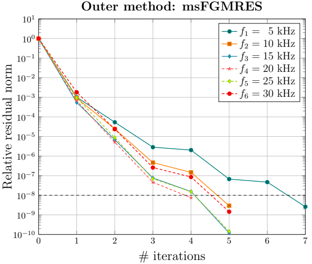
Numerical example # 1

as presented in [B./vG., 2014]

Preconditioned **nested FOM-FGMRES**:

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





Numerical example # 1

as presented in [B./vG., 2014]

Various combinations of inner/outer methods *possible*:

	multi-shift Krylov methods			
	`msGMRES`	`msGMRESr`	`QMRIDR(4)`	`msIDR(4)`
# inner iterations	-	20	-	-
# 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).

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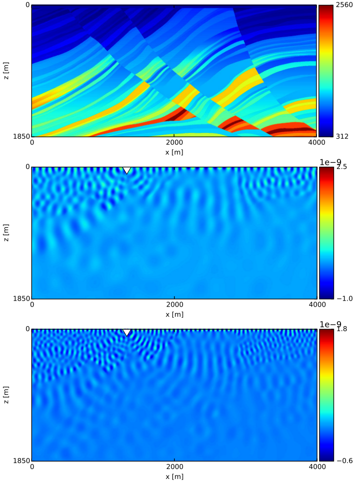
Numerical example # 2

The Marmousi-II test case:

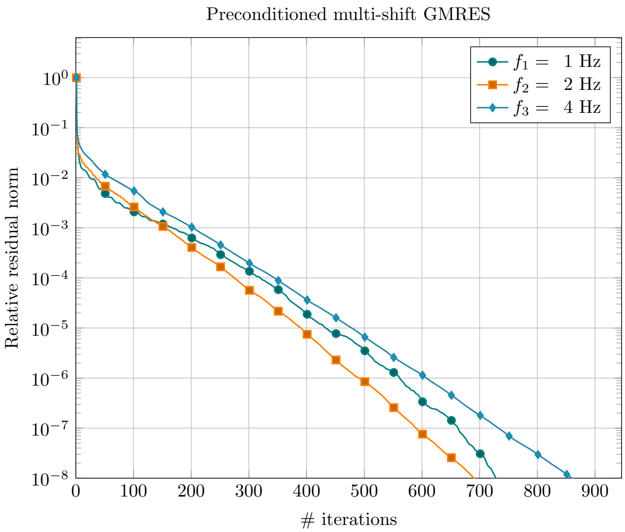
- 2D benchmark problem
- $f_k = \{1, 2, 4\} Hz$
- $\tau \in \mathbb{C}$ *"optimal"*
- 593,600 # dofs
- 20 ppw
- single source



Reference

G. Rizzuti and W. Mulder. *Multigrid-based 'shifted-Laplacian' preconditioning for the time-harmonic elastic wave equation.* J. Comput. Phys., **317**:47-65 (2016).

Numerical example # 2



Numerical example # 2

	# inner	# outer	CPU time
`msGMRES`	-	871	2:37:01
`msGMRESr`	100	18	4:43:41
`FOM-FGMRES`	100	14	3:27:35

References

- A. Frommer and U. Glässner. *Restarted GMRES for Shifted Linear Systems.* SIAM J. Sci. Comput., **19**:15-26, (1998).
- 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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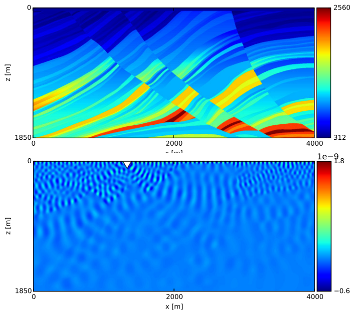
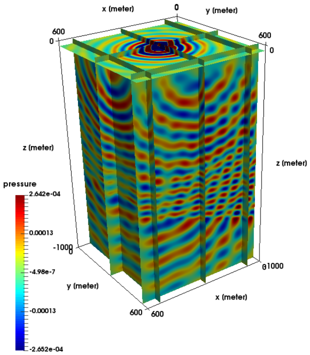
Conclusions and future work

- ✓ inner-outer Krylov method for shifted systems
- ✓ single preconditioner based on MSSS structure
- ? optimal parameter choice for τ $\rightarrow$ Rational Krylov





Thank you for your attention!

Further reading:

- 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.* Technical report 16-04, TU Delft, 2016.

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