Nested Krylov methods for shifted linear systems

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Context of this work (1/3)

Why are we all 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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References

- 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).
- M. Ahmad, D. Szyld, and M. van Gijzen. *Preconditioned multishift BiCG for $\mathcal{H}_2$-optimal model reduction.* Report 12-06-15, Temple University (2013).

Their combined message is:

- Many shifted Laplace preconditioners can be used in a flexible multi-shift Krylov method (*Tania et al.*)
- Polynomial preconditioners preserve shift-invariance (*Mian et al.*)

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Context of this work (3/3)

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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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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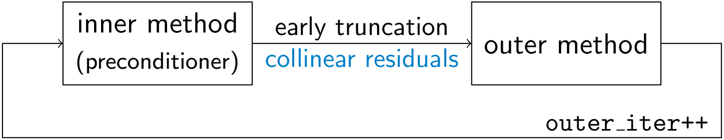

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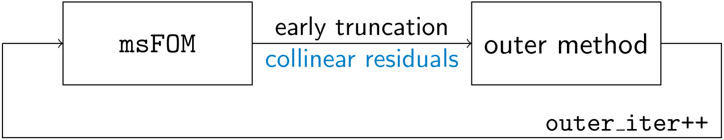

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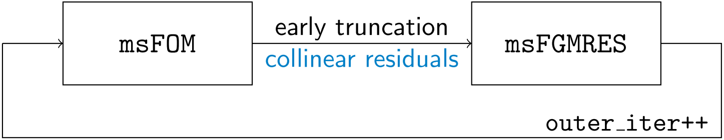

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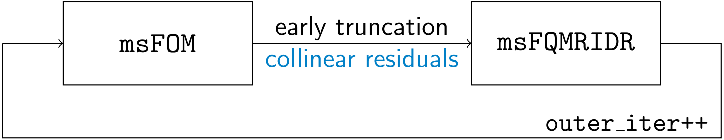

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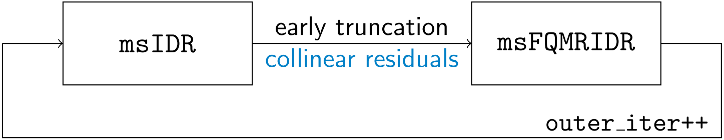

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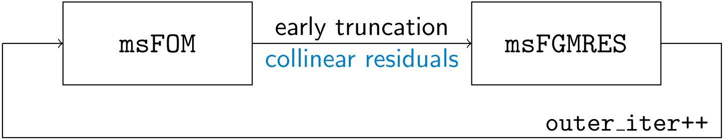

Inner method: multi-shift FOM

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,

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

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

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

Use flexible GMRES in the outer loop,

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

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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Outer method: flexible multi-shift GMRES (2/3)

The inner residuals are:

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$$\mathbf{r}_j = \mathbf{v}_j - \mathcal{A}\mathcal{P}_j^{-1}\mathbf{v}_j.$$

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

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

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which yields:

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

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

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

Summary: Nested FOM-FGMRES

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

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

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

By the way...

Our key findings,

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

are closely related to the formula,

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

which is taken from [Bakhos et al, 2013] and adapted in notation.

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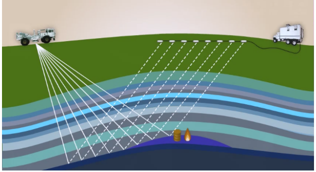
Application & numerical tests

Application (1/3)

Full-waveform inversion

PDE-constrained optimization:

$$\min_{\rho(\mathbf{x}),c_p(\mathbf{x}),c_s(\mathbf{x})} \left\| \mathbf{u}_{sim} - \mathbf{u}_{meas} \right\|,$$



where in our application:

- $\mathbf{u}_{sim}$ is the (numerical) solution of the elastic wave equation,
- $\mathbf{u}_{meas}$ is obtained from measurements,
- ρ, c_p, c_s are properties of earth layers we are interested in.

The modeling is done in frequency-domain.

Application (2/3)

The discrete forward model

An FEM discretization of the time-harmonic, inhomogeneous elastic wave equation at multiple frequencies σ_k is given by:

$$(K + i\sigma_k C - \sigma_k^2 M)\mathbf{u}_k = \mathbf{s}, \quad k = 1, ..., N_\sigma,$$

where

- M, K are mass and stiffness matrix, respectively,
- C encounters Sommerfeld boundary conditions,
- $\mathbf{s}$ usually models a point source,
- we need to compute the displacement vector $\mathbf{u}_k$ for multiple frequencies (shifts) σ_k.

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Application (3/3)

Reformulation to shifted linear systems

We can reformulate the previous problem to:

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

which is of the form:

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

Apply shifted Laplace preconditioner

$$\mathcal{P} = (\mathcal{A} - \tau \mathcal{M}), \quad \text{with } \Im(\tau) > 0.$$

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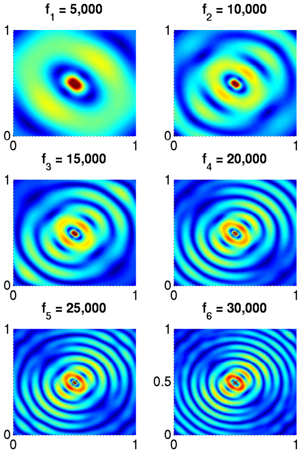
Numerical experiments (1/4)

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, J. Toivanen. *A damping preconditioner for time-harmonic wave equations in fluid and elastic material.* Journal of Computational Physics, 2009.

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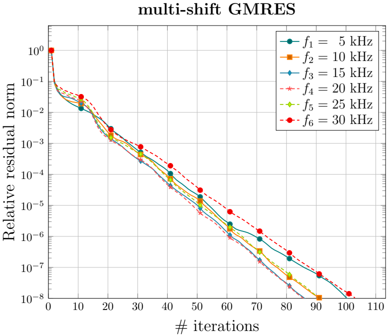
Numerical experiments (2/4)

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

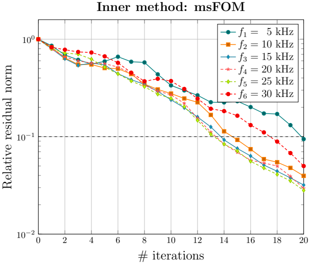


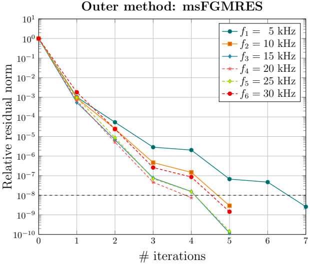
Numerical experiments (3/4)

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





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Numerical experiments (4/4)

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

Various combinations of nested algorithms:

	multi-shift Krylov methods			
	msGMRES	rest_msGMRES	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

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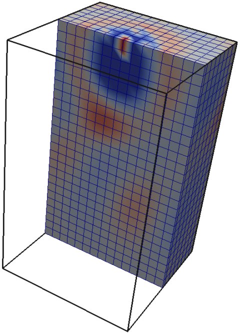
Conclusions and future work

✓ Inner-outer Krylov methods for $\mathcal{A}\mathbf{x} = \mathbf{b}$ are widely used
$\rightsquigarrow$ We present an extension to shifted linear systems

✓ Multiple combinations of inner-outer methods possible, e.g. `FOM-FGMRES`, `IDR-FQMRIDR`, ...

? Future work: 3D problems

- discretization using TU/e package `nutils` (high-order FEM)
- approximate shifted Laplacian with $\mathcal{MSSS}$ preconditioner
- nested solver in a coupled `Python - Fortran` framework



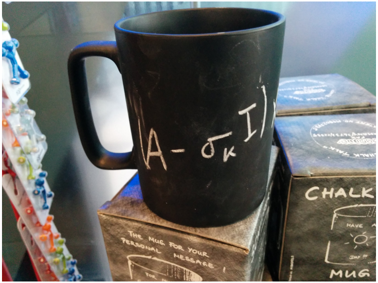
Thank you for your attention!

Further reading:

M. Baumann and M. B. van Gijzen. *Nested Krylov methods for shifted linear systems.* SIAM J. Sci. Comput. [in press]

Research funded by Shell.

Shifted systems appear a lot in practice...



...which is why we meet again for PART II at 3:00 pm.