Nested Krylov methods for shifted linear systems

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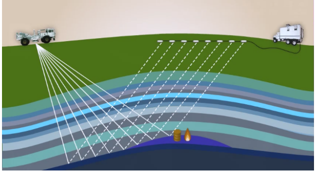
Motivation (1/3)

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.

Motivation (2/3)

The discrete forward model

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

$$(K + i\omega_k C - \omega_k^2 M)\mathbf{u}_k = \mathbf{s}, \quad k = 1, \ldots, N,$$

where

- K, C, M are sparse and symmetric,
- $\mathbf{s}$ usually models a point source,
- we need to compute the displacement vector $\mathbf{u}_k$ for multiple frequencies (shifts) ω_k.

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Motivation (3/3)

Multi-shift Krylov methods

We can re-formulate the previous problem 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 the form:

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

Shift-invariance of Krylov subspaces:

$$\mathcal{K}_m(\mathcal{A}, \mathbf{r}_0) \equiv \text{span}\{\mathbf{r}_0, \mathcal{A}\mathbf{r}_0, \ldots, \mathcal{A}^{m-1}\mathbf{r}_0\} = \mathcal{K}_m(\mathcal{A} - \omega I, \mathbf{r}_0)$$

is challenging to *preserve* when preconditioning!

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Preconditioners for shifted linear systems

2004 (Complex) shifted Laplace preconditioner:

$$\mathcal{P} = (\mathcal{A} - \tau\mathcal{M}), \quad \tau \approx \{\omega_1, ..., \omega_N\}$$

2007 Many shifted Laplace preconditioners:

$$\mathcal{P}_j = (\mathcal{A} - \tau_j\mathcal{M})$$

2013 Polynomial preconditioners [Plenary talk at PRECON13]

2014 Question: Can we use a Krylov method as preconditioner?
$\rightsquigarrow$ Nested Krylov methods

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Outline

The shifted Laplacian

The *generalized* shifted Laplace preconditioner,

$$\mathcal{P} = (\mathcal{A} - \tau \mathcal{M}), \quad \tau \in \mathbb{C}, \qquad (*)$$

has two benefits:

1. it transforms our problem to shifted linear systems and, hence, enables the benefits of shift-invariant Krylov spaces,
2. it maps the original spectrum to circles of known center and radius.

Moreover, $(*)$ is easy to apply because $\tau \in \mathbb{C}$ leads to a damped problem $\rightsquigarrow$ multigrid works!

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The shifted Laplacian

For $\mathcal{P} = (\mathcal{A} - \tau\mathcal{M})$, the following relation holds:

$$(\mathcal{A} - \omega_k\mathcal{M})\mathcal{P}_k^{-1} = \mathcal{A}\mathcal{P}^{-1} - \eta_k(\omega)I, \qquad (**)$$

with

- $\mathcal{P}_k^{-1} = \frac{\tau}{\tau - \omega_k}\mathcal{P}^{-1}$
- $\eta_k = \omega_k/(\omega_k - \tau)$
- τ is a free parameter (seed shift)

For the spectrum of the RHS in $(**)$, we see:

$$\sigma\left(\mathcal{A}\mathcal{M}^{-1}\right) \ni \lambda \mapsto \frac{\lambda}{\lambda - \tau} - \eta_k$$

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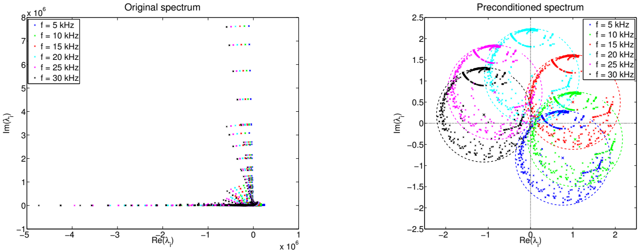
The shifted Laplacian - Spectral analysis

Compare:

$$\sigma(\mathcal{A} - \omega_k \mathcal{M}) \qquad \text{vs.} \qquad \sigma\left((\mathcal{A} - \omega_k \mathcal{M})\mathcal{P}_k^{-1}\right)$$



Open question: What's the optimal τ for equidistantly spaced frequencies $\omega_1, ..., \omega_N$???

Nested (inner-outer) multi-shift Krylov methods

Solve the preconditioned shifted problem, $\mathcal{B} := \mathcal{A}\mathcal{P}^{-1}$,

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

with a nested Krylov method based on

$$\mathcal{K}_k(\mathcal{B}, \mathbf{r}_0) = \mathcal{K}_k(\mathcal{B} - \eta I, \mathbf{r}_0) \quad \forall \eta.$$

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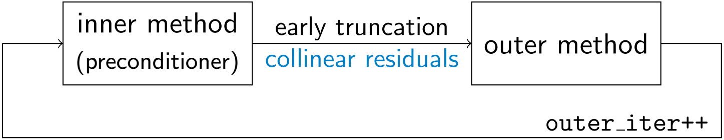

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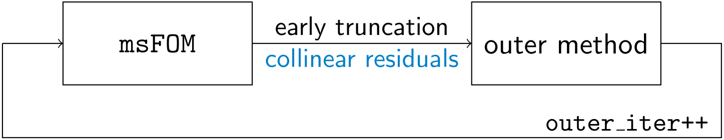

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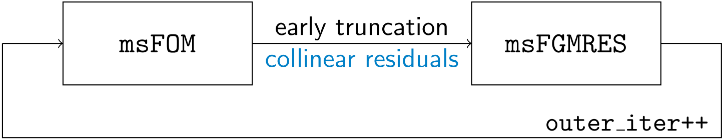

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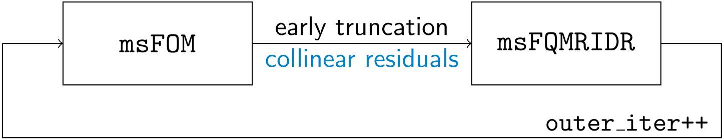

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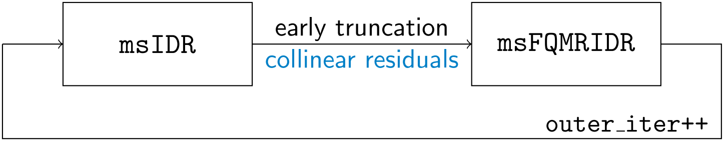

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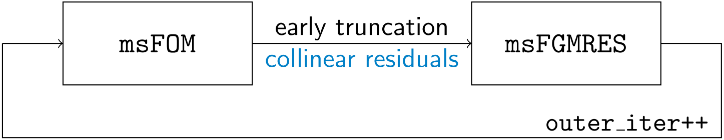

Inner method: multi-shift FOM

Classical result: In FOM, the residuals are:

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

Thus, for the shifted residuals it holds:

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Hence, we obtain collinear residuals,

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

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

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

Use flexible GMRES in the outer loop,

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

where one column yields:

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

Recap: The "inner loop" is the truncated solution of $(\mathcal{B} - \eta I)$ 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:

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

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

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

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which yields:

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\underline{\mathrm{H}}_m^{(\eta)} = (\underline{\mathrm{H}}_m - \underline{\mathrm{I}}_m)\,\Gamma_m + \underline{\mathrm{I}}_m,
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with $\Gamma_m := diag(\gamma_1, ..., \gamma_m)$.

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Summary: Nested FOM-FGMRES

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

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

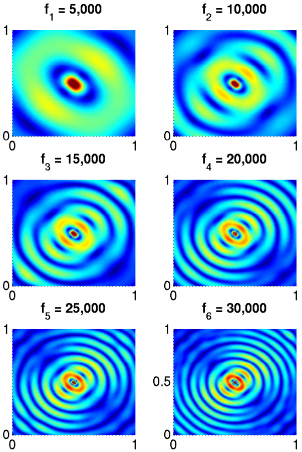
where the entries of $\Gamma_m^{(\eta)}$ are collinearity factors of inner FOM.

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:
  $4n = 40.804$
- $N = 6$ 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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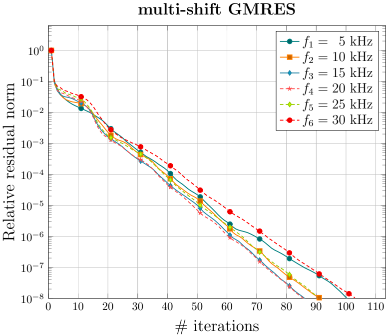
Numerical experiments (2/4)

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

Preconditioned **multi-shift GMRES**:

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

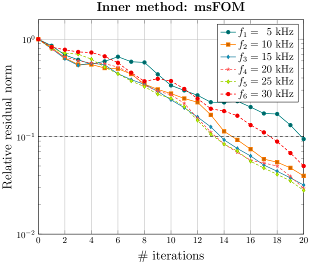


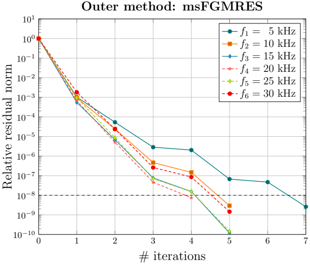
Numerical experiments (3/4)

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





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

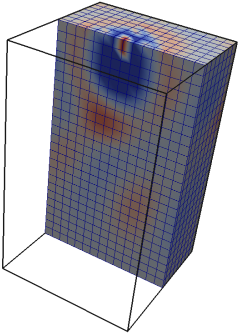
Conclusions and future work

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

✓ The shifted Laplace preconditioner is applied as a *first layer*

? Future work: 3D problems

- discretization using TU/e package `nutils` (high-order FEM)
- approximate shifted Laplacian with `AGMG`
- nested solver in `Fortran90`



Thank you for your attention!

Further reading:

M. Baumann and M. B. van Gijzen. *Nested Krylov methods for shifted linear systems.* SIAM Journal on Scientific Computing (SISC), Special Issue Copper Mountain Conference 2014 [in press].

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