Krylov Model-Order Reduction Techniques for Time- and Frequency-Domain Wavefield Problems

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Acknowledgment

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- Mikhail Zaslavsky, Schlumberger-Doll Research
- Jörn Zimmerling, Delft University of Technology
- Vladimir Druskin, Schlumberger-Doll Research

Outline

- Basic equations and symmetry properties
- Polynomial Krylov reduction 1
- Perfectly matched layers
- Polynomial Krylov reduction 2
- Laurent polynomial (extended) Krylov reduction
- Introducing rational and preconditioned rational Krylov reduction

  More on this in J. Zimmerling's talk

Basic equations

- First-order wavefield system
  acoustics, seismics, electrodynamics

$$(\mathcal{D} + \mathcal{M}\partial_t)\,\mathcal{F} = -w(t)\mathcal{Q}$$

- Plus initial conditions
- Dirichlet boundary conditions
- Signature matrix δ^-

$$\delta^- = \mathrm{diag}(1, -1, -1, -1) \qquad \text{(acoustics)}$$

Basic equations

- Spatial discretization

$$(D + M\partial_t)\, f = -w(t)q$$

- Order of this system can be very large especially in 3D
- Discretized counterpart of δ^- is denoted by d^-

Basic equations

- Solution

$$f(t) = -w(t) * \eta(t) \exp(-At) M^{-1} q$$

- $\eta(t)$ Heaviside unit step function
- System matrix

$$A = M^{-1} D$$

Symmetry

- System matrix A is skew-symmetric w.r.t. WM
- Evolution operator $\exp(-At)$ is orthogonal w.r.t. WM
- Inner product and norm

$$\langle x, y \rangle = y^H W M x \qquad \|x\| = \langle x, x \rangle^{1/2}$$

- Stored field energy in the computational domain (sum of field energies)

$$\frac{1}{2}\|f\|^2$$

- Initial-value problem: norm of f is preserved

Symmetry

- System matrix A is symmetric w.r.t. WMd^-
- Bilinear form

$$\langle x, y \rangle = y^H WMd^- x$$

- Free field Lagrangian
  (difference of field energies)

$$\frac{1}{2}\langle f, f \rangle$$

- Symmetry property related to reciprocity

Symmetry

- Introduce

$$d^{\mathrm{p}} = \frac{1}{2}(I + d^{-}) \quad \text{and} \quad d^{\mathrm{m}} = \frac{1}{2}(I - d^{-})$$

- Write $f = f(q)$ to indicate that the field is generated by a source q
- Reciprocity
- Source vector: $q = d^{\mathrm{p}} q$, receiver vector $r = d^{\mathrm{p}} r$

$$\langle f(q), r \rangle = \langle q, f(r) \rangle$$

- Source vector: $q = d^{\mathrm{p}} q$, receiver vector $r = d^{\mathrm{m}} r$

$$\langle f(q), r \rangle = -\langle q, f(r) \rangle$$

Polynomial Krylov reduction

- Exploit symmetry of system matrix in a Lanczos reduction algorithm
- For lossless media both symmetry properties lead to the same reduction algorithm
- First symmetry property is lost for lossy media with a system matrix of the form $A = M^{-1}(D + S)$
- Second symmetry property still holds

Polynomial Krylov reduction

- For lossless media, FDTD can be written in a similar form as Lanczos algorithm

$$\text{recurrence relation for FDTD} \\ = \\ \text{recurrence relation for Fibonacci polynomials}$$

- Stability of FDTD and numerical dispersion can be studied using this connection

Polynomial Krylov reduction

- Lanczos recurrence coefficients: β_i
- Comparison with FDTD: $1/\beta_i =$ time step of Lanczos
- Automatic time step adaptation – no Courant condition
- Lanczos reduction hardly provides any speedup compared with FDTD
- Both are polynomial field approximations
  - **Lanczos:** field is approximated by a Lanczos polynomial in A
  - **FDTD:** field is approximated by a Fibonacci polynomial in A

PML

- No outward wave propagation has been included yet
- Implementation via Perfectly Matched Layers (PML)
- Coordinate stretching (Laplace domain)

$$\partial_k \longleftrightarrow \chi_k^{-1}\partial_k \qquad k = x, y, z$$

- Stretching function

$$\chi_k(k, s) = \alpha_k(k) + \frac{\beta_k(k)}{s}$$

PML

- Stretched first-order system

$$\left[\mathcal{D}(s) + \mathcal{S} + s\mathcal{M}\right]\hat{\mathcal{F}} = -\hat{w}(s)\mathcal{Q}$$

- Direct spatial discretization

$$\left[D(s) + S + sM\right]\hat{f} = -\hat{w}(s)q$$

- Leads to nonlinear eigenproblems for spatial dimensions > 1

PML

- Linearization of the PML
- Spatial finite-difference discretization using *complex* PML step sizes

$$(D_{cs} + S + sM)\, f_{cs} = -w(s)q$$

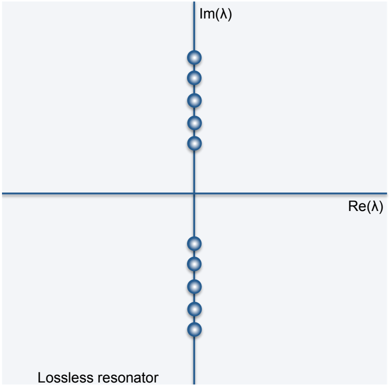
- System matrix

$$A_{cs} = M^{-1}(D_{cs} + S)$$

- V. Druskin and R. F. Remis, "A Krylov stability-corrected coordinate stretching method to simulate wave propagation in unbounded domains," *SIAM J. Sci. Comput.*, Vol. 35, 2013, pp. B376 – B400.
- V. Druskin, S. Güttel, and L. Knizhnerman, "Near-optimal perfectly matched layers for indefinite Helmholtz problems," SIAM Rev. 58-1 (2016), pp. 90 – 116.

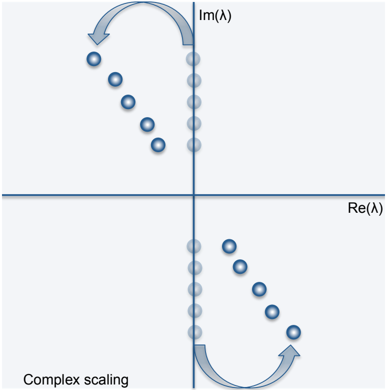
PML

- Spectrum of the system matrix A_{cs}



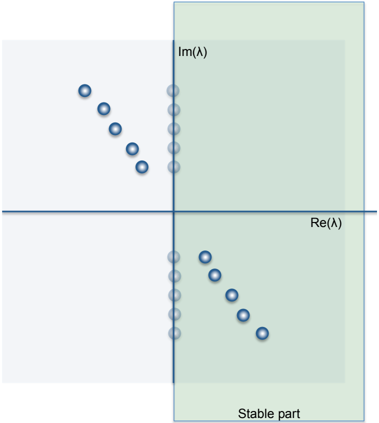
PML

- Eigenvalues move into the complex plane



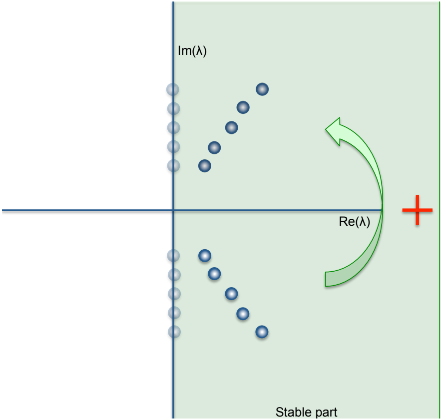
PML

- Stable part of the spectrum



PML

- Stability correction



PML

- Time-domain stability-corrected wave function

$$f(t) = -w(t) * 2\eta(t)\mathrm{Re}\left[\eta(A_{\mathrm{cs}})\exp(-A_{\mathrm{cs}}t)q\right]$$

- Complex Heaviside unit step function

$$\eta(z) = \begin{cases} 1 & \mathrm{Re}(z) > 0 \\ 0 & \mathrm{Re}(z) < 0 \end{cases}$$

PML

- Frequency-domain stability-corrected wave function

$$\hat{f}(s) = -\hat{w}(s)\left[r(A_{\text{cs}}, s) + r(\bar{A}_{\text{cs}}, s)\right] q$$

with

$$r(z,s) = \frac{\eta(z)}{z+s}$$

- Note that $\hat{f}(\bar{s}) = \bar{\hat{f}}(s)$ and the stability-corrected wave function is a nonentire function of the system matrix A_{cs}

PML

- Symmetry relations are preserved
- With a step size matrix W that has complex entries
- These entries correspond to PML locations

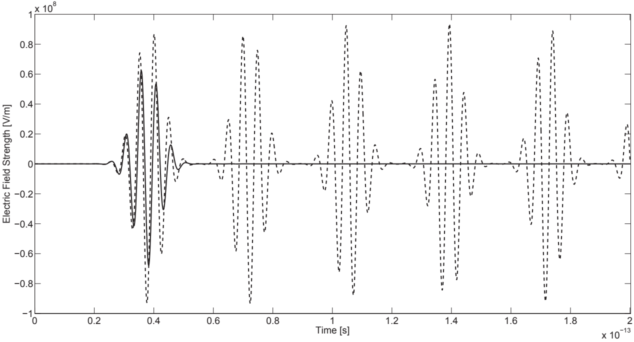
Polynomial Krylov Reduction

- Stability-corrected wave function cannot be computed by FDTD
- SLDM field approximations via modified Lanczos algorithm
- Reduced-order model

$$f_m(t) = -w(t) * 2\|M^{-1}\mathrm{q}\|\eta(t)\mathrm{Re}\left[V_m \eta(H_m)\exp(-H_m t)e_1\right]$$

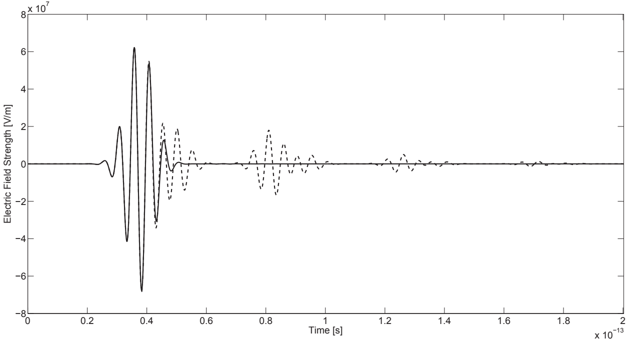
Polynomial Krylov Reduction

- $m = 300$



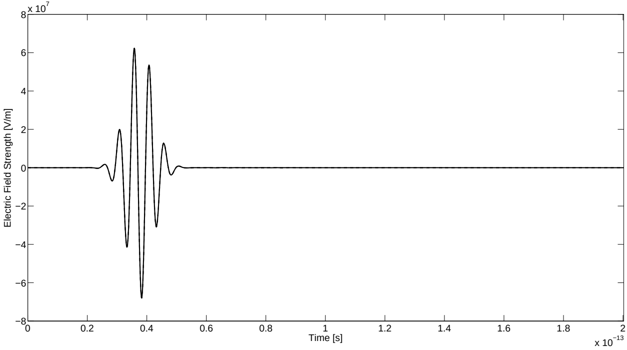
Polynomial Krylov Reduction

- $m = 400$



Polynomial Krylov Reduction

- $m = 500$



Extended Krylov reduction

- Stability-corrected wave function is approximated by a Lanczos polynomial in A_{cs}
- The wave function is a nonentire function of the system matrix
- Idea: approximate the stability-corrected function by a Laurent polynomial
- Perhaps an even better idea: approximate the stability-corrected wave function by rational functions (more on this later)

Extended Krylov reduction

- Extended Krylov subspace

$$\mathbb{K}_{m_1,m_2} = \mathrm{span}\{A^{-m_1+1}q, \ldots, A^{-1}q, q, Aq, \ldots, A^{m_2-1}q\}$$

- Elements from this space: Laurent polynomials in matrix A acting on the source vector q

Extended Krylov reduction

- Original extended Krylov method of Druskin and Knizhnerman generates the sequence of subspaces

$$\mathbb{K}_{m_1,1} \subset \mathbb{K}_{m_1,2} \subset \ldots \subset \mathbb{K}_{m_1,m_2}$$

via short-term recurrence relations

- A more general approach was proposed by Jagels and Reichel
- Efficiently generate the sequence of subspaces

$$\mathbb{K}_{1,i+1} \subset \mathbb{K}_{2,2i+1} \subset \ldots \subset \mathbb{K}_{k,ki+1}$$

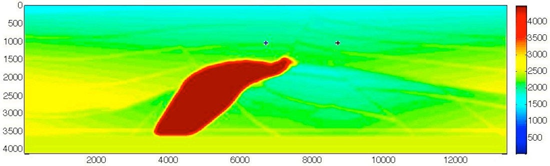
again via short term recurrence relations

- i is an integer

$$\#\text{ matvec with } A = i \cdot \#\text{ matvec with } A^{-1}$$

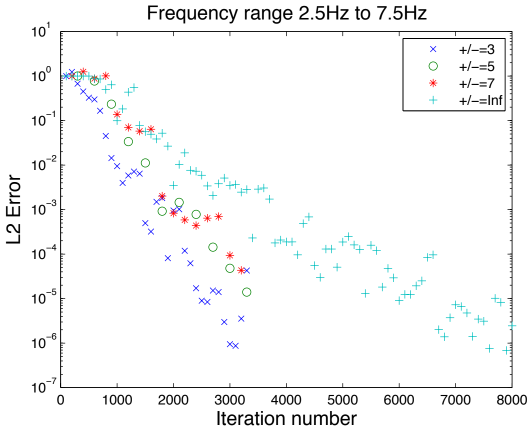
Extended Krylov reduction

- SEG Salt model/velocity profile – 3D acoustics, frequency-domain, order $\approx$ 93 million



Extended Krylov reduction

- SEG Salt model - generalized EKS implementation



Extended Krylov reduction

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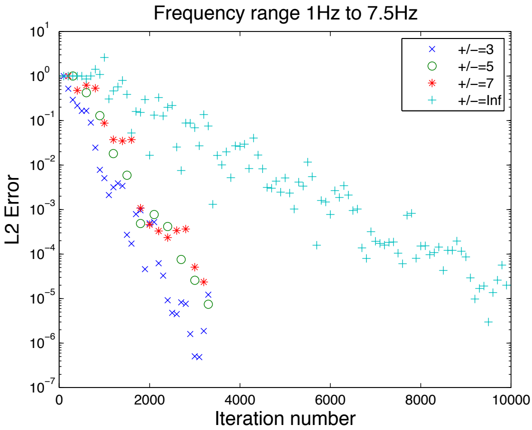
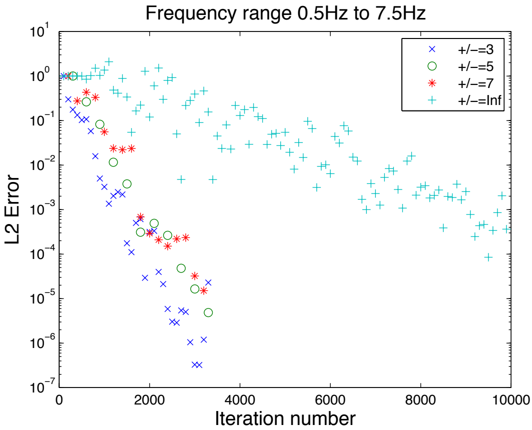


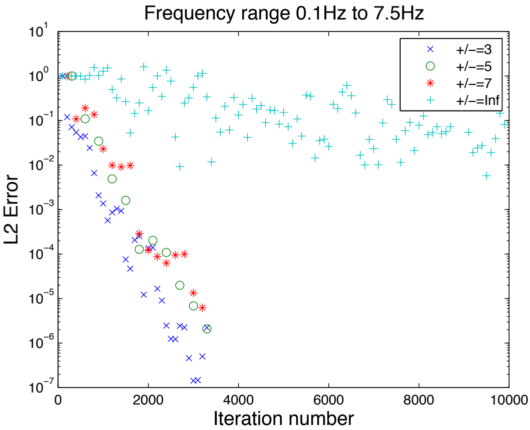
Extended Krylov reduction

- SEG Salt model - generalized EKS implementation



Extended Krylov reduction

- SEG Salt model - generalized EKS implementation



Rational Krylov reduction

- In a rational Krylov method, we approximate the field by the span of snapshots

$$\hat{f}(s_1), \hat{f}(s_2), ..., \hat{f}(s_m)$$

for different frequencies s_i, $i = 1, 2, ..., m$

- The snapshots are obtained by solving discretized wavefield systems of the form

$$[D(s_i) + s_i M]\, \hat{f}(s_i) = -q$$

Rational Krylov reduction

- No PML linearization is necessary!
- When using a rational Krylov method, we deal with the above system directly and not with the stability-corrected system/wave function

Rational Krylov reduction

- Return to the system

$$[D(s) + sM]\, f = -q$$

- Symmetry relation

$$D^T(s)\tilde{W}(s) = \tilde{W}(s)D(s)$$

- $\tilde{W}(s) = W(s)d^-$ is a nonsingular diagonal s-dependent step size matrix

Rational Krylov approximations

- Multiply by $\tilde{W}$ to obtain

$$A(s)\hat{f}(s) = \tilde{q}$$

- System matrix

$$A(s) = \tilde{W}(s)\,[D(s) + sM]$$

- Properties

$$A^T(s) = A(s) \quad \text{and} \quad A^*(s) = A(s^*)$$

Rational Krylov approximations

- Solve system for $m \geq 1$ different frequencies
- Construct the subspace

$$\mathcal{K}_m = \operatorname{span}\{\hat{f}(s_1), \hat{f}(s_2), \ldots, \hat{f}(s_m)\}$$

- and take

$$\mathcal{K}_m^{\mathrm{R}} = \operatorname{span}\{\operatorname{Re}\mathcal{K}_m, \operatorname{Im}\mathcal{K}_m\}$$

  as an expansion and projection space
- Note that

$$\hat{f}(s_i) \in \mathcal{K}_m^{\mathrm{R}} \quad \text{and} \quad \hat{f}(s_i^*) \in \mathcal{K}_m^{\mathrm{R}} \quad i = 1, 2, \ldots, m$$

Rational Krylov approximations

- Let V_m be a basis matrix of $\mathcal{K}_m^{\mathrm{R}}$
- Field approximation

$$f_m(s) = V_m \hat{a}_m(s)$$

- Expansion coeffcients are determined from Galerkin condition
- Structure-preserving reduced-order model

$$\hat{f}_m(s) = V_m \hat{R}_m^{-1}(s) V_m^T \tilde{q} \qquad R_m(s) = V_m^T A(s) V_m$$

Rational Krylov approximations

- Interpolation properties

$$\hat{f}_m(s_i) = \hat{f}(s_i) \quad \text{and} \quad \hat{f}_m(s_i^*) = \hat{f}(s_i^*) \qquad i = 1, 2, \ldots, m$$

- For coinciding source/receiver pairs

$$\frac{\mathrm{d}}{\mathrm{d}s} \tilde{q}^T \hat{f}_m(s) \Big|_{s=s_i, s_i^*} = \frac{\mathrm{d}}{\mathrm{d}s} \tilde{q}^T \hat{f}(s) \Big|_{s=s_i, s_i^*} \qquad i = 1, 2, \ldots, m$$

Rational Krylov approximations

- Large travel times: frequency-domain wavefield highly oscillatory in frequency domain
- Rational Krylov method requires many sampling/interpolation points
- Phase-preconditioned rational Krylov method: factor out the strongly oscillating part using high-frequency asymptotics
- Much more on this in talk of J. Zimmerling

Literature

- Complex PML step sizes and stability-correction:

  - V. Druskin and R. F. Remis, "A Krylov stability-corrected coordinate stretching method to simulate wave propagation in unbounded domains," *SIAM J. Sci. Comput.*, Vol. 35, 2013, pp. B376 – B400.
  - V. Druskin, S. Güttel, and L. Knizhnerman, "Near-optimal perfectly matched layers for indefinite Helmholtz problems," SIAM Rev. 58-1 (2016), pp. 90 – 116.
  - J. Zimmerling, L. Wei, P. Urbach, and R. Remis, "A Lanczos model-order reduction technique to efficiently simulate electromagnetic wave propagation in dispersive media," *J. Comp. Phys.*, Vol. 315, 2016, pp. 348 – 362.

Literature

- Extended Krylov subspace method:

  - V. Druskin and L. Knizhnerman, "Extended Krylov subspaces: approximation of the matrix square root and related functions," *SIAM* J. Matrix Anal. Appl., Vol. 19, 1998, pp. 755 – 771.
  - C. Jagels and L. Reichel, "Recursion relations for the extended Krylov subspace method," *Linear Algebra Appl.*, Vol. 434, pp. 1716 – 1732, 2011.
  - V. Druskin, R. Remis, and M. Zaslavsky, "An extended Krylov subspace model-order reduction technique to simulate wave propagation in unbounded domains," *J. Comp. Phys.*, Vol. 272, 2014, pp. 608 – 618.

Literature

- Phase-preconditioned rational Krylov method
  - V. Druskin, R. Remis, M. Zaslavsky, and J. Zimmerling, "Compressing large-scale wave propagation via phase-preconditioned rational Krylov subspaces," *to appear on ArXiv*, 2017. See also Jörn Zimmerling's talk.