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

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- 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
  \[ (\mathcal{D} + \mathcal{M} \partial_t) \mathcal{F} = -w(t)Q \]
- Plus initial conditions
- Dirichlet boundary conditions
- Signature matrix \( \delta^- \)
  \[ \delta^- = \text{diag}(1, -1, -1, -1) \quad (\text{acoustics}) \]
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 $\delta^-$ is denoted by $d^-$
Basic equations

- Solution

\[ f(t) = -w(t) \ast \eta(t) \exp(-At)M^{-1}q \]

- \( \eta(t) \) 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
  \[ \langle x, y \rangle = y^H WM x \quad \| x \| = \langle x, x \rangle^{1/2} \]
- 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
Introduce
\[ d^p = \frac{1}{2}(I + d^-) \quad \text{and} \quad d^m = \frac{1}{2}(I - d^-) \]

Write \( f = f(q) \) to indicate that the field is generated by a source \( q \)

Reciprocity

Source vector: \( q = d^p q \), receiver vector \( r = d^p r \)
\[ \langle f(q), r \rangle = \langle q, f(r) \rangle \]

Source vector: \( q = d^p q \), receiver vector \( r = d^m r \)
\[ \langle f(q), r \rangle = -\langle q, f(r) \rangle \]
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: $\beta_i$
- Comparison with FDTD: $1/\beta_i = \text{time step of Lanczos}$
- 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)

\[ \partial_k \leftrightarrow \chi_k^{-1} \partial_k \quad k = x, y, z \]

- Stretching function

\[ \chi_k(k, s) = \alpha_k(k) + \frac{\beta_k(k)}{s} \]
PML

- Stretched first-order system
  \[
  \left[ \mathcal{D}(s) + S + sM \right] \hat{F} = -\hat{w}(s)Q
  \]

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

- Leads to nonlinear eigenproblems for spatial dimensions $> 1$
Linearization of the PML

Spatial finite-difference discretization using complex PML step sizes

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

System matrix

\[A_{cs} = M^{-1}(D_{cs} + S)\]


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

\[ f(t) = -w(t) \ast 2\eta(t)\Re[\eta(A_{cs})\exp(-A_{cs}t)q] \]

- Complex Heaviside unit step function

\[ \eta(z) = \begin{cases} 
1 & \text{Re}(z) > 0 \\
0 & \text{Re}(z) < 0 
\end{cases} \]
PML

- Frequency-domain stability-corrected wave function

\[ \hat{f}(s) = -\hat{\nu}(s)[r(A_{cs}, s) + r(\bar{A}_{cs}, s)]q \]

with

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

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

\[ f_m(t) = -w(t) \star 2\|M^{-1}q\| \eta(t) \text{Re} [V_m \eta(H_m) \exp(-H_m t)e_1] \]
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

\[ \mathbb{K}_{m_1,m_2} = \text{span}\{A^{-m_1+1}q, ..., A^{-1}q, q, Aq, ..., A^{m_2-1}q\} \]

- 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 ≈ 93 million
Extended Krylov reduction

- SEG Salt model - generalized EKS implementation

![Graph showing frequency range 2.5Hz to 7.5Hz with L2 Error vs Iteration number. The graph includes markers for different frequency ranges: +/-3, +/-5, +/-7, and +/-Inf.]

Frequency range 2.5Hz to 7.5Hz
Extended Krylov reduction

- SEG Salt model - generalized EKS implementation

![Graph showing L2 Error vs Iteration number with frequency range 1Hz to 7.5Hz and various error bounds.](image)
Extended Krylov reduction

- SEG Salt model - generalized EKS implementation

Frequency range 0.5Hz to 7.5Hz

L2 Error vs. Iteration number
**Extended Krylov reduction**

- SEG Salt model - generalized EKS implementation

![Graph showing frequency range 0.1Hz to 7.5Hz and L2 Error against iteration number.](image)
Rational Krylov reduction

- In a rational Krylov method, we approximate the field by the span of snapshots
  
  \[ \hat{f}(s_1), \hat{f}(s_2), \ldots, \hat{f}(s_m) \]

  for different frequencies \( s_i, \ i = 1, 2, \ldots, m \)

- 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
  \[ \mathcal{K}_m = \text{span}\{\hat{f}(s_1), \hat{f}(s_2), ..., \hat{f}(s_m)\} \]
  
  and take
  \[ \mathcal{K}_m^R = \text{span}\{\text{Re}\mathcal{K}_m, \text{Im}\mathcal{K}_m\} \]
  
  as an expansion and projection space
- Note that
  \[ \hat{f}(s_i) \in \mathcal{K}_m^R \quad \text{and} \quad \hat{f}(s_i^*) \in \mathcal{K}_m^R \quad i = 1, 2, ..., m \]
Rational Krylov approximations

- Let $V_m$ be a basis matrix of $\mathcal{K}_m^R$
- Field approximation
  
  $$f_m(s) = V_m \hat{a}_m(s)$$

  Expansion coefficients are determined from Galerkin condition

  Structure-preserving reduced-order model

  $$\hat{f}_m(s) = V_m \hat{R}^{-1}_m(s)V_m^T \hat{q} \quad R_m(s) = V_m^T A(s)V_m$$
Rational Krylov approximations

- Interpolation properties

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

- For coinciding source/receiver pairs

\[ \frac{d}{ds} \tilde{q}^T \hat{f}_m(s) \bigg|_{s=s_i,s_i^*} = \frac{d}{ds} \tilde{q}^T \hat{f}(s) \bigg|_{s=s_i,s_i^*} \quad i = 1, 2, \ldots, m \]
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
Complex PML step sizes and stability-correction:

Extended Krylov subspace method:

Phase-preconditioned rational Krylov method