Efficient Wavefield Simulators Based on Krylov Model-Order Reduction Techniques

From Resonators to Open Domains

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Thanks

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and

- Vladimir Druskin, Schlumberger-Doll Research

Happy birthday

- Happy birthday Vladimir!

Introduction

- Back in the day (late 80s, early 90s)
  - SLDM: Spectral Lanczos Decomposition Method
  - Fast convergence for parabolic (diffusion) equations
  - Applicable to lossless (hyperbolic) wave equation as well
  - Not many advantages compared with explicit time-stepping (FDTD)

Main research question

- What happens if we include losses?
- Lossy wavefield systems
- Perfectly Matched Layers (PML, after 1994)

Basic equations

- First-order lossless wavefield system

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

- Plus initial conditions
- Dirichlet boundary conditions (no PML) included

- Lossy wavefield system

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

Maxwell's equations

- Field vector

$$\mathcal{F} = [E_x, E_y, E_z, H_x, H_y, H_z]^T$$

- Source vector

$$\mathcal{Q} = [J_x^{\mathrm{sp}}, J_y^{\mathrm{sp}}, J_z^{\mathrm{sp}}, K_x^{\mathrm{sp}}, K_y^{\mathrm{sp}}, K_z^{\mathrm{sp}}]^T$$

Maxwell's equations

- Medium matrices

$$\mathcal{M} = \begin{pmatrix} \boldsymbol{\varepsilon} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\mu} \end{pmatrix}$$

and

$$\mathcal{S} = \begin{pmatrix} \boldsymbol{\sigma} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$$

Maxwell's equations

- Differentiation matrix

$$\mathcal{D} = \begin{pmatrix} \mathbf{0} & -\boldsymbol{\nabla}\times \\ \boldsymbol{\nabla}\times & \mathbf{0} \end{pmatrix}$$

- Signature matrix

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

Basic equations

- Spatial discretization

$$\left(D + S + M\partial_t\right) f = -w(t)q$$

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

Basic equations

- Medium matrices (isotropic media)
  - S diagonal and semipositive definite
  - M diagonal and positive definite
- Differentiation matrix
  - W step size matrix = diagonal and positive definite
  - Symmetry property

$$D^T W = -WD$$

Basic equations

- System matrix for lossless media: $A = M^{-1}D$
- System matrix for lossy media: $A = M^{-1}(D + S)$
- Evolution operator $= \exp(-At)$

Basic equations

- Lossless media: A is skew-symmetric w.r.t. WM
- Evolution operator is orthogonal w.r.t. WM
- Inner product and norm

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

- Stored field energy in the computational domain

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

- Initial-value problem: norm of f is preserved

Lanczos algorithms

- Lossless media: construct SLDM field approximations via Lanczos algorithm for skew-symmetric matrices
- FDTD can be written in a similar form as Lanczos algorithm

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

Lanczos algorithms

- Lanczos recurrence coefficients: β_i
- Comparison with FDTD: $1/\beta_i =$ time step of Lanczos
- Automatic time step adaptation – no Courant condition

Lanczos algorithms

- Lossy media: system matrix $A = M^{-1}(D + S)$ is no longer skew-symmetric
- Introduce

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

Lanczos algorithms

- Special case: $S = \xi d^{\mathrm{p}}$

$$\sigma(\mathbf{x}) = \xi\varepsilon(\mathbf{x}) \quad \text{for } \textit{all } \mathbf{x} \text{ belonging to computational domain}$$

- Exploit shift invariance of Lanczos decomposition
- Basis for lossless media can be used to describe wave propagation for lossy media (in this special case)

Lanczos algorithms

- Not possible for general lossy media
- Matrix D is symmetric with respect to Wd^{-}

$$D^T Wd^{-} = Wd^{-} D$$

- System matrix A is symmetric w.r.t. WMd^{-}

Lanczos algorithms

- System matrix A is symmetric w.r.t. bilinear form

$$\langle x, y \rangle = y^H W M d^- x$$

- Free-field Lagrangian

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

Lanczos algorithms

- 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 $r = d^{\mathrm{m}} r$

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

Lanczos algorithms

- SLDM field approximations for lossy media can be constructed via modified Lanczos algorithm

Modified Lanczos algorithm

=

Lanczos algorithm for symmetric matrices
with inner product replaced by bilinear form

- Modified Lanczos algorithm can also be obtained from two-sided Lanczos algorithm
- Can the modified Lanczos algorithm breakdown in exact arithmetic?

PML

- No outward wave propagation has been included up to this point
- 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

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

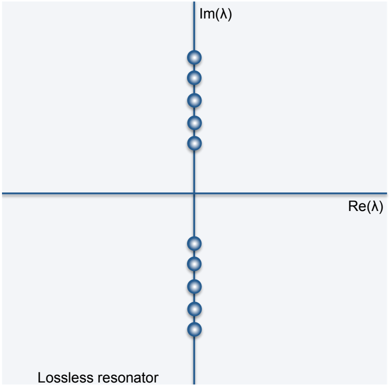
- System matrix

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

- 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.

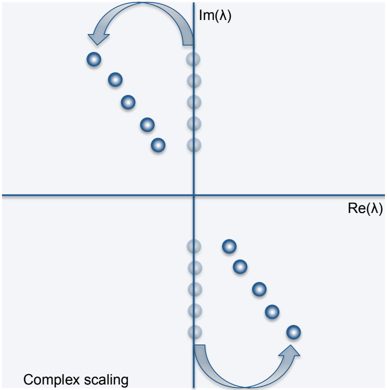
PML

- What about the spectrum of the system matrix?



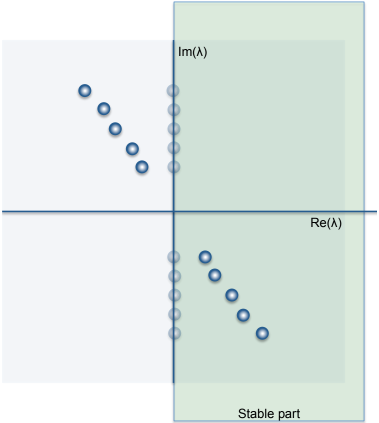
PML

- Eigenvalues move into the complex plane



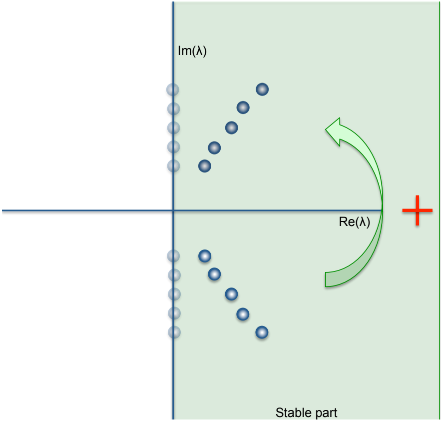
PML

- Stable part of the spectrum



PML

- Stability correction



Stability-Corrected Wave Function

- 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

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

Stability-Corrected Wave Function

- 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}

Stability-Corrected Wave Function

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

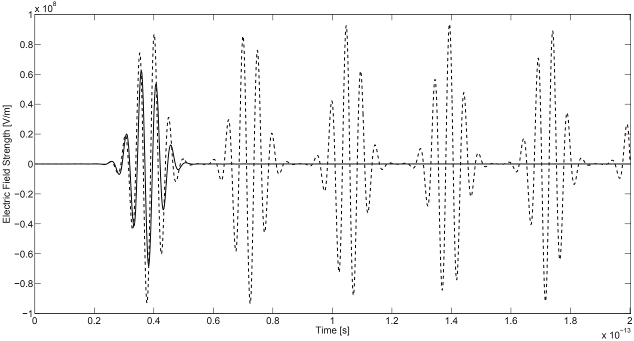
Stability-Corrected Wave Function

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

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

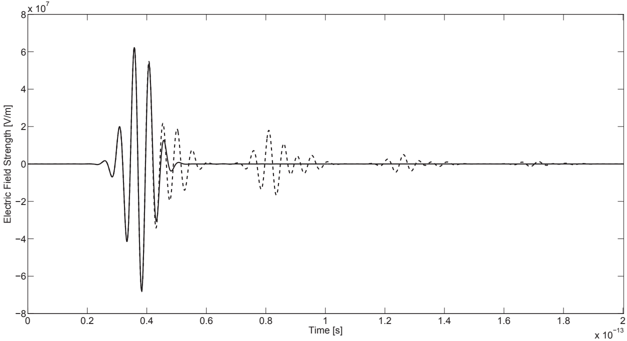
Stability-Corrected Wave Function

- $m = 300$



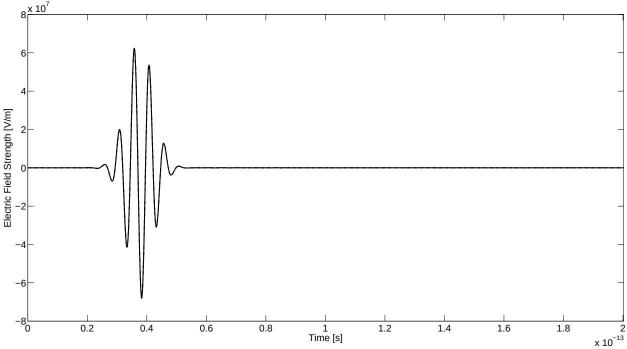
Stability-Corrected Wave Function

- $m = 400$



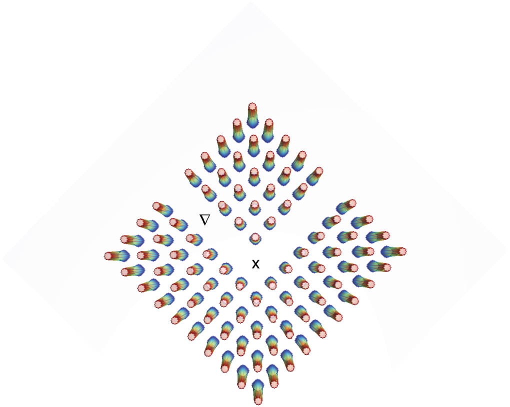
Stability-Corrected Wave Function

- $m = 500$



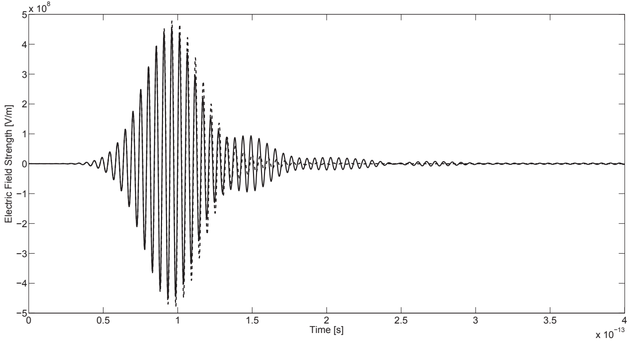
Stability-Corrected Wave Function

- Photonic crystal



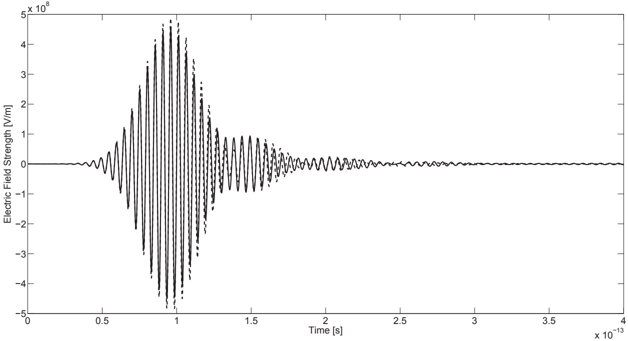
Stability-Corrected Wave Function

- $m = 1000$ vs. 8200 FDTD iterations



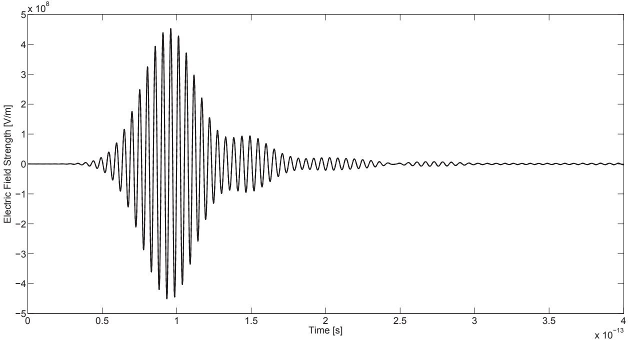
Stability-Corrected Wave Function

- $m = 2000$ vs. 8200 FDTD iterations



Stability-Corrected Wave Function

- $m = 3000$ vs. 8200 FDTD iterations



Extensions

- Approach has been extended for dispersive media in
  - J. Zimmerling, L. Wei, H. Urbach, and R. Remis, A Lanczos model-order reduction technique to efficiently simulate electromagnetic wave propagation in dispersive media, *Journal of Computational Physics*, Vol. 315, pp. 348 – 362, 2016.
- Extended Krylov subspace implementations are discussed in
  - V. Druskin, R. Remis, and M. Zaslavsky, *Journal of Computational Physics*, Vol. 272, pp. 608 – 618, 2014.

Current and future work

- Rational Krylov field approximations
  No stability-correction required
- Phase-preconditioned rational Krylov methods
  Large travel times
- More on this in the coming week!

Thank you for your attention!