Exponentially Convergent Sparse Discretizations and Application to Near Surface Geophysics

Murthy N. Guddati
North Carolina State University

November 9, 2017
Outline

- Part 1: Impedance Preserving Discretization

- Part 2: Absorbing Boundary Conditions (1-sided DtN map)
  - Joint work with Tassoulas, Druksin, Lim, Zahid, Savadatti, Thirunavukkarasu

- Part 3: Complex-length FEM for finite domains (2-sided DtN map)
  - Joint work with Druskin, Vaziri Astaneh

- Part 4: Inversion for Near-surface Geophysics
  - Joint work with Vaziri Astaneh
Part1. Impedance Preserving Discretization
Model Problem

- 3D wave equation in free space
  \[-\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} - \frac{\partial^2 u}{\partial z^2} + \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} = 0\]

- Fourier transform in \(t, y, z\), with \(u = U e^{ik_x y + ik_z z - i\omega t}\)
  \[-\frac{\partial^2 U}{\partial x^2} - k^2 U = 0\]
  \(k = \sqrt{\left(-k^2_y - k^2_z + \frac{\omega^2}{c^2}\right)}\) is complex valued

- Exact solution: \(U = Ae^{ik_x} + Be^{-ik_x}\), where \(k\) is the horizontal wavenumber

- \(U = e^{ik_x} \Rightarrow u = e^{i(kx + k_y y + k_z z - \omega t)}\) is a plane/evanescent wave
Finite Element Solution on a Uniform Grid in $x$

- FE discretization of: $\frac{\partial^2 U}{\partial x^2} - k^2 U = 0$

- Element contribution matrix with uniform element size of $h$:

\[
\mathbf{k}_{\text{elem}} = \frac{1}{h}\begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix} - k^2 h \begin{bmatrix} 1 & 1 \\ 3 & 6 \\ 1 & 1 \\ 6 & 3 \end{bmatrix} = \begin{bmatrix} A & B \\ B & A \end{bmatrix}
\]

\[
A = \frac{1}{h} \left( 1 - \frac{k^2 h^2}{3} \right)
\]

\[
B = \frac{1}{h} \left( -1 - \frac{k^2 h^2}{6} \right)
\]

- Assembly results in the difference equation: $BU_{j-1} + 2AU_j + BU_{j+1} = 0$
Changing Mesh Size: Reflections

- A simple analysis using two uniform meshes with different element sizes \((h, H)\), but the same material

- What happens when a right propagating wave hits the interface?
  - Exact solution – just passes through
  - Finite element solution – reflections due to impedance mismatch

\[ R = \frac{Z_H - Z_h}{Z_H + Z_h} \]

\( Z_h \): discrete impedance of left domain
\( Z_H \): discrete impedance of right domain
Computing Discrete Impedance (Half-space Stiffness)

- Basic idea: discrete half-space + finite element = discrete half-space

\[
\begin{bmatrix}
A & B \\
B & A+Z_h
\end{bmatrix}
\begin{bmatrix}
U_0 \\
U_1
\end{bmatrix} = \begin{bmatrix}
Z_hU_0 \\
0
\end{bmatrix} \Rightarrow \begin{bmatrix}
A-Z_h & B \\
B & A+Z_h
\end{bmatrix}
\begin{bmatrix}
U_0 \\
U_1
\end{bmatrix} = \begin{bmatrix}
0 \\
0
\end{bmatrix} \Rightarrow A^2 - Z_h^2 = B^2
\]

\[
A = \frac{1}{h} \left(1 - \frac{k^2 h^2}{3}\right)
\]

\[
B = \frac{1}{h} \left(-1 - \frac{k^2 h^2}{6}\right)
\]

\[
\Rightarrow Z_h = \sqrt{A^2 - B^2} = ik \sqrt{1 - \frac{(kh)^2}{12}}
\]

- \(Z_h\) depends on element size, resulting in impedance mismatch when the element size changes, resulting in reflections

Error term
Optimal Integration for Minimizing Reflection Error

- Minimize the error in impedance by using generalized integration rules \((-\alpha, +\alpha)\)

\[
A = \frac{1}{h} \left( 1 - \left(\frac{1+\alpha^2}{4}\right) k^2 h^2 \right) \\
B = \frac{1}{h} \left( -1 - \left(\frac{1-\alpha^2}{4}\right) k^2 h^2 \right)
\]

\[
Z_h = \sqrt{A^2 - B^2} = ik \sqrt{1 - \frac{(kh)^2}{4}} - \alpha^2
\]

- Minimize the error term by choosing \(\alpha = 0\)
  - The error in impedance is completely eliminated! No more reflections
  - Formally valid for more general 2\(^{nd}\) order equations (anisotropic, visco-elasticity etc., electromagnetics etc. – G, 2006, CMAME)

**Linear elements + midpoint integration**

= Impedance Preserving Discretization
Part 2. Absorbing Boundary Conditions

Perfectly Matched *Discrete* Layers
Perfectly Matched Discrete Layers

...Impedance Preserving Discretization of PML

- Perfectly Matched Layers (PML) (Berenger, 1994; Chew et al. 1995)
  - Step 1: Bend the domain into complex space
  - Step 2: discretize PMDL domain (in complex space)
    - Impedance is no longer preserved; perfect matching is destroyed
    - Requires a large number of carefully chosen PML layers
  - Impedance preserving discretization comes to the rescue!
    - Impedance is preserved/matched, irrespective of element length, small, large, real, complex – **Perfectly Matching Discrete Layers (PMDL)**
    - Discretize with 3-5 complex-length linear finite elements
    - No discretization error, but truncation causes reflections. The reflection coefficient is derived as

\[ R_{PML} = e^{-2ikL} \]

\[ R_{PMDL} = \prod_{j=1}^{j=nlayer} \left( \frac{1 - ikL_j / 2}{1 + ikL_j / 2} \right)^2 \]
PMDL vs PML: Effectiveness of Midpoint Integration

PMDL with 3 layers  PML with 3 layers
Impedance preservation property is valid for any equation that is linear and second order in space (G, CMAME, 2006)

- Elastic and other complicated wave equations (G, Lim & Zahid, 2007)

- Evanescent waves can be treated effectively
  - Padded PMDL – contains large real lengths with midpoint integration (Zahid & G, CMAME, 2006)
Salient Features of PMDL

- Exponential convergence
  \[ R = \prod_{j=1}^{j=\text{nlayer}} \left( \frac{k - k_j}{k + k_j} \right)^2 \]

- Near optimal discretization
  - Optimal: need staggered grids (with Druskin et al., 2003)

- Links PML to rational ABCs
  - Lindman, Engquist-Majda, Higdon and variants (e.g. CRBC)
  - We started this from E-M/Higdon ABCs (G, Tassoulas, 2000)
  - Extensions to corners is straightforward

- Additional advantage: Provides solutions to some difficult cases
  - Backpropagating waves: anisotropy
  - PML for discrete/periodic media
PMDL for Backpropagating Waves
Opposing signs of phase and group velocities

- Backpropagating waves grow in the PML region
  - PML cannot work! (Bécache, Fauqueux and Joly, 2003)

- A counter-intuitive idea: make the reflections in PML region decay faster than the growth of the incident wave

- Works only with PMDL: needs impedance preserving discretization!

Anisotropic elasticity – Tilted Elliptic Case

Arbitrary parameters

Ideal Slowness

Stable parameters

Anisotropic elasticity – Non-elliptic Case

Two different coordinated materials

Traditional mesh

PMDL for Periodic Media (after discretization)

- Periodic media has internal reflections and transmissions
  - Constructive interference leads to long-range propagation
- PML’s complex stretching spoils this balance and internal reflections and transmissions get mixed up!
- Basic Ideas (Discrete/Periodic PMDL):
  - Periodic media = Discrete vector wave equation (vector size = ndof in a cell)
  - Discrete vector equation = impedance preserving discretization of more complicated wave equation
  - Apply PMDL on the complicated wave equation results in impedance matching for periodic media
- Open problem: stability for complex problems

G & Thirunavukkarasu, JCP (2009), Waves 2011
Part 3. Two-Sided DtN Map

Complex-length Finite Element Method
Facilitating the Approximation of 2-Sided DtN Map

- Consider the equation: $-\frac{\partial^2 u}{\partial z^2} - \omega^2 u = 0, \quad z \in (0, L)$

- Exact 2-sided DtN map: $K_{\text{exact}} = \begin{bmatrix} A & B \\ B & A \end{bmatrix}$

- By definition, exact DtN Map is impedance preserving: $A^2 - B^2 = Z_{\text{exact}}^2$

- Consider impedance preserving discretization of the interval:

  $K_{\text{exact}} = \begin{bmatrix} \bar{A} & \bar{B} \\ \bar{B} & \bar{A} \end{bmatrix}, \quad \bar{A}^2 - \bar{B}^2 = Z_{\text{exact}}^2$

- Error in A and B would be similar since: $\bar{A}^2 - \bar{B}^2 = Z_{\text{exact}}^2 = A^2 - B^2$

- Approximating two-sided map reduces to approximating one-sided map

- Better derivation based on Crank-Nicolson discretization of the propagator
1D Helmholtz Equation

- $-\frac{\partial^2 u}{\partial z^2} - \omega^2 u = 0$

Eigenvalues $\lambda = \pm i \omega$

Downward waves:

$$\begin{bmatrix} u_L \\ \partial u_L / \partial z \end{bmatrix} = \begin{bmatrix} \exp(i \omega L) & 0 \\ 0 & \exp(i \omega L) \end{bmatrix} \begin{bmatrix} u_0 \\ \partial u_0 / \partial z \end{bmatrix}$$
Propagator Approximation

\[ \frac{1}{L_1} \left( \frac{u_1 - u_0}{\overline{v}_1 - \overline{v}_0} \right) = \frac{1}{2} \begin{bmatrix} 0 & i\omega \\ i\omega & 0 \end{bmatrix} \begin{bmatrix} u_1 + u_0 \\ \overline{v}_1 + \overline{v}_0 \end{bmatrix} \]

1st Order Form

\[ \frac{\partial}{\partial z} \begin{bmatrix} u \\ \overline{v} \end{bmatrix} = \begin{bmatrix} 0 & i\omega \\ i\omega & 0 \end{bmatrix} \begin{bmatrix} u \\ \overline{v} \end{bmatrix} \]

Crank-Nicolson

\[ u_L \begin{bmatrix} u_L \\ \partial u_L / \partial z \end{bmatrix} = \begin{bmatrix} \exp(i\omega L) & 0 \\ 0 & \exp(i\omega L) \end{bmatrix} \begin{bmatrix} u_0 \\ \partial u_0 / \partial z \end{bmatrix} \]

Valid for both \( \pm \omega \) Downward AND upward waves!
Padé Approximant

\[ \exp(\alpha L) \approx \prod_{j=1}^{n} \left( \frac{1 + \alpha L_j / 2}{1 - \alpha L_j / 2} \right) \]

\[ \frac{d^j (\exp(\alpha L))}{d\alpha^j} \bigg|_{\alpha=0} = \frac{d^j P_{\text{Padé}}}{d\alpha^j} \bigg|_{\alpha=0} \]

\[ (j = 0, \ldots, 2n) \]

\[ \sum_{j=0}^{n} \frac{(2n-j)!}{j! (n-j)!} (-x)^j = 0 \quad \rightarrow \quad L_j = 2L / x_j \]
Complex-Length FEM: Exponential Convergence

\[ f = 1 \]

\[ L = 1 \]

Laplace Equation

Helmholtz Equation (can’t beat Nyquist limit)
Complex-Length FEM: Some Observations

- Exponentially convergent
- Piecewise linear interpolation – sparse computation
- Edges do not move ($\sum L_j = L$) – can be combined with other types of meshes for other subdomains
- Mesh is not bent outside ($\text{Re}(L_j) > 0$)
- Order of elements do not matter! – more on this later.
- With refinement, and proper ordering, mesh converges to a smooth curve on the complex plane

\[ \exp(\alpha L) \approx \prod_{j=1}^{n} \left( \frac{1 + \alpha L_j/2}{1 - \alpha L_j/2} \right) \]

\[ \frac{d^j \left( \exp(\alpha L) \right)}{d\alpha^j} \bigg|_{\alpha=0} = \frac{d^j P_{\text{Padé}}}{d\alpha^j} \bigg|_{\alpha=0} \]

\[ \sum_{j=0}^{n} \frac{(2n - j)!}{j! (n - j)!} (-x)^j = 0 \quad \rightarrow \quad L_j = \frac{2L}{x_j} \]
Energy Conservation and Eigenvalue Problems

- Do complex lengths lead to energy absorption, like PML?
  - No, due to conjugate pair of lengths – decay grows back!
  - 2-sided DtN Map is Hermitian

- Do complex lengths lead to complex eigenvalues of $K$ with respect to $M$?
  - No. Eigenvalues are real and positive!
  - Eigenvectors are complex (K and M are complex symmetric)

\[ -\frac{\partial^2 u}{\partial z^2} - \omega^2 u = 0 \quad \implies (K - \omega^2 M) \phi = 0 \]
Element Ordering

\[ u = c \exp(\pm i\alpha x) \]
Part 4. Near Surface Geophysical Site Characterization...
...using Guided Wave Inversion
Guided Wave Dispersion

Dispersion Curve
Spectral Analysis

Phase Velocity (m/s) = \frac{Frequency (1/s)}{Wavenumber (1/m)}
Medium Characterization

Inverse Identification

Iteratively Minimize

\[ E = \sum_{i=1}^{N} (c_{i\text{experimental}} - c_{i\text{predicted}})^2 \]

- Optimization Scheme
  - Gradient Based, e.g. Newton-like Methods
  - Global Search, e.g. Genetic Algorithm

Experimental Dispersion Curve

Phase Velocity

Frequency

Forward Problem: Predicted Dispersion Curve

Iteratively Minimize

\[ E = \sum_{i=1}^{N} (c_{i\text{experimental}} - c_{i\text{predicted}})^2 \]
Forward Modeling – State of the Art

\[
\begin{align*}
-\frac{1}{r} \frac{\partial}{\partial r} \left( D_{rr} \frac{\partial u}{\partial r} + D_{rz} \frac{\partial u}{\partial z} + D_{ro} u \right) - \frac{\partial}{\partial z} \left( D_{rz} \frac{\partial u}{\partial r} + D_{zz} \frac{\partial u}{\partial z} + D_{zo} \frac{1}{r} u \right) \\
-\frac{1}{r} \left( -D_{ro} \frac{\partial u}{\partial r} - D_{zo} \frac{\partial u}{\partial z} - \frac{1}{r} D_{oo} u \right) - \left( \rho \omega^2 I \right) u = 0
\end{align*}
\]

Discretize z direction
Hankel Transform r direction

\[
\det(K) = 0
\]

\[
\left( k^2 A + k B + C + \omega^2 D \right) u = 0
\]

\[
k \rightarrow c_p = \frac{\omega}{k}
\]
Reducing the Problem Size: CFEM+PMDL

Complex-Length FEM (Finite Layers)  Perfectly Matched discrete Layers (Halfspace)
Forward Modeling: CFEM vs. FEM

Error in dispersion curve

![Graph showing comparison of FEM and CFEM](image)

- Relative Error vs. Degrees of Freedom
- FEM in green, CFEM in black

33
Inversion: Experimental Dispersion Curve

240 Geophones

36 Geophones

12 Geophones

Experimental Dispersion Curve

Inverse Identification

1st (fundamental) Mode
2nd Mode
3rd Mode
4th Mode
5th Mode
Challenge

- No analytical derivative
- Rough misfit function

Minimize
\[ E = \sum_{i=1}^{N} \left( c_i^{\text{experimental}} - c_i^{\text{predicted}} \right)^2 \]

Existing approach: Finite Difference Method (FDM)

- Expensive: Multiple computations of dispersion curve
- Slow convergence: Oscillatory gradient
Proposed Derivative for Experimental Curve

- **Analytical Derivative**

  \[
  \frac{\partial k_i}{\partial m_j} = -\frac{\phi^\dagger_L \left( \frac{\partial K}{\partial m_j} \right) \phi_R}{\phi^\dagger_L \left( \frac{\partial K}{\partial k_i} \right) \phi_R}
  \]

- **Alternative Approach for Eigenvector**

  \[
  K \left( k^2 A + k B + C + \omega^2 D \right) u = 0 \quad \Rightarrow \quad \phi_R = K^{-1} P
  \]

  \[
  k \neq k_{\text{experimental}} \quad \delta \approx 10^{-6}
  \]
Proposed Derivative

\[
\frac{\partial k_i^{\text{eff.}}}{\partial m_j} \approx -\frac{(P^\dagger K^{-1})(\partial K / \partial m_j)(K^{-1} P)}{(P^\dagger K^{-1})(\partial K / \partial k_i)(K^{-1} P)}
\]

- Analytical vs. FDM Gradient
Inversion Results: Synthetic Examples

- Analytical Gradient

- FDM Gradient
Inversion Results: 14-Layer Soil Profile†

<table>
<thead>
<tr>
<th>Iterations (Existing)</th>
<th>Iterations (Proposed)</th>
<th>CPU Time (Proposed)</th>
<th>CPU Time (Existing)</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>8</td>
<td>11.3 s</td>
<td>2884.6 s</td>
</tr>
</tbody>
</table>

Conclusions

- Discretization that perfectly preserves the impedance is possible
  - Linear FEM with midpoint integration preserves impedance
  - Related to Crank-Nicolson discretization of the propagator
  - Preserves the evanescence in PML region

- Absorbing Boundary Conditions: Perfectly Matched Discrete Layers (PMDL)
  - Exponential convergence
  - Link to other ABCs – we can get the best of both worlds
  - Facilitates stable ABCs for some backward propagating waves
  - Formally extensible to discrete periodic media
  - Open questions: Parameters of discretization for stability and accuracy
Conclusions (Contd.)

- Two-sided DtN Map
  - Exponential convergence on the edges is possible with linear interpolation: **Complex-length Finite Element Method (CFEM)**
  - Impedance preserving discretization is the key!
  - Currently based on Padé approximant; could be further optimized
  - Open questions: further theoretical understanding; extensions to variable coefficients and higher dimensions?

- Guided Wave Inversion
  - Forward modeling: a good application of CFEM
  - Approximate differentiation of the effective dispersion curve facilitates faster convergence and efficient gradient computation
  - Future work: Bayesian and hybrid inversion
Thank you!

Impedance Preserving Discretization
G (2006), Arbitrarily wide angle wave equations for complex media, CMAME

Perfectly Matched Discrete Layers
Asvadurov, Druskin, G, Knizhnerman (2003), On optimal finite-difference approximation of PML, SINUM.
G, Lim (2006), Continued fraction absorbing boundary conditions for convex polygonal domains, IJNME.
Thirunavukkarasu, G (2011), Absorbing boundary conditions for time-harmonic wave propagation in discretized domains, CMAME.
Savadatti, G (2012), Accurate absorbing boundary conditions for anisotropic elastic media. parts 1/2, JCP.

Complex-length FEM
G, Druskin, Vaziri Astaneh (2016), Exponential Convergence through Linear Finite Element Discretization of Stratified Subdomains, JCP.
Vaziri Astaneh, G (2016), Efficient Computation of Dispersion Curves for Multilayered Waveguides and Half-Spaces, CMAME.

Guided Wave Inversion