Exponentially Convergent Sparse Discretizations and Application to Near Surface Geophysics

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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 $u = Ue^{ik_y y + ik_z z - i\omega t}$

$$-\frac{\partial^2 U}{\partial x^2}-k^2 U=0 \qquad k=\sqrt{\left(-k_y^2-k_z^2+\frac{\omega^2}{c^2}\right)} \text{ is complex valued}$$

- Exact solution: $U = Ae^{ikx}+Be^{-ikx}$, where k is the horizontal wavenumber

- $U = e^{ikx} \Rightarrow u = e^{i(kx+k_y y+k_z z-\omega t)}$ 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*:

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

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

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

- 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

$$\begin{bmatrix} A & B \\ B & A+Z_h \end{bmatrix} \begin{Bmatrix} U_0 \\ U_1 \end{Bmatrix} = \begin{Bmatrix} Z_h U_0 \\ 0 \end{Bmatrix} \Rightarrow \begin{bmatrix} A-Z_h & B \\ B & A+Z_h \end{bmatrix} \begin{Bmatrix} U_0 \\ U_1 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \Rightarrow A^2 - Z_h^2 = B^2$$

$$A = \frac{1}{h}\left(1 - \frac{k^2 h^2}{3}\right), \quad B = \frac{1}{h}\left(-1 - \frac{k^2 h^2}{6}\right) \quad \Rightarrow \quad Z_h = \sqrt{A^2 - B^2} = ik\sqrt{1 - \boxed{\frac{(kh)^2}{12}}}$$

Error term

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

Optimal Integration for Minimizing Reflection Error

- Minimize the error in impedance by using generalized integration rules

$$(-\alpha \quad +\alpha)$$

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

$$B = \frac{1}{h}\left(-1 - \left(\frac{1-\alpha^2}{4}\right)k^2h^2\right)$$

$$\Rightarrow \quad Z_h = \sqrt{A^2 - B^2} = ik\sqrt{1 - \boxed{\frac{(kh)^2}{4}\alpha^2}}$$

Error term

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

Linear elements + midpoint integration
= Impedance Preserving Discretization

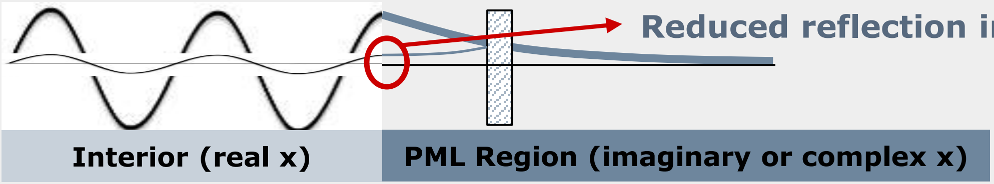
Part 2. Absorbing Boundary Conditions

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

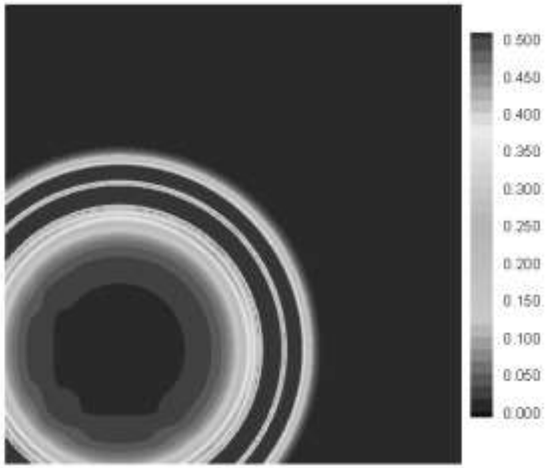


$$R_{PML} = e^{-2ikL}$$

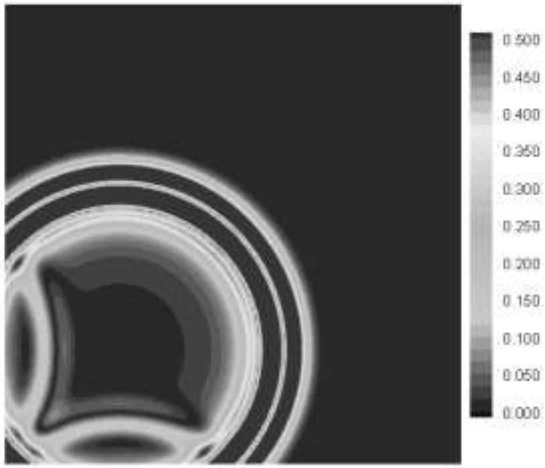
  - Step 2: discretize PMDL domain (in complex space)
    - Impedance is no longer preserved; perfect matching is destroyed
    - Requires a large number of carefully chosen PML layers
- Impedance preserving discretization comes to the rescue!
  - Impedance is preserved/matched, irrespective of element 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

$$R_{PMDL} = \prod_{j=1}^{j=nlayer} \left(\frac{1 - ikL_j/2}{1 + ikL_j/2} \right)^2$$

PMDL vs PML: Effectiveness of Midpoint Integration



PMDL with 3 layers



PML with 3 layers

PMDL: Some More Old Results

- 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)

PMDL with 5 layers

PML with 5 layers

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

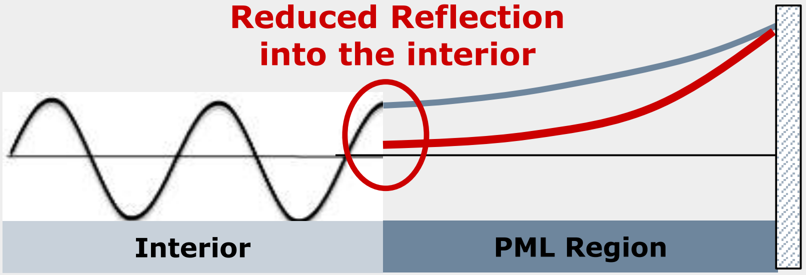
Salient Features of PMDL

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

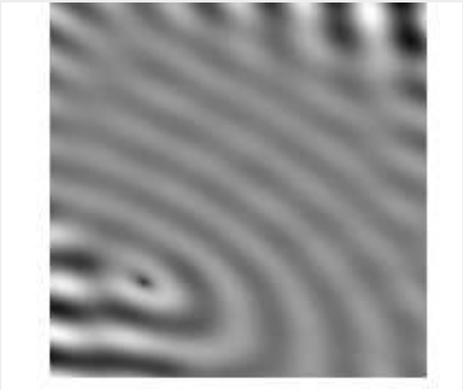
PMDL for Backpropagating Waves

Opposing signs of phase and group velocities

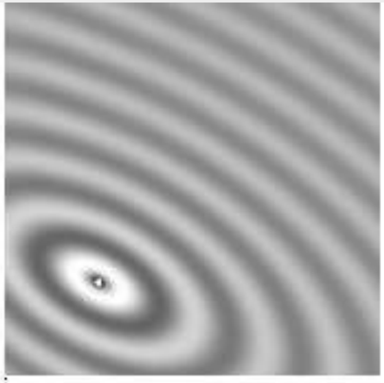
- Backpropagating waves grow in the PML region
  - PML cannot work! (Bécache, Fauqueux and Joly, 2003)



- 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!

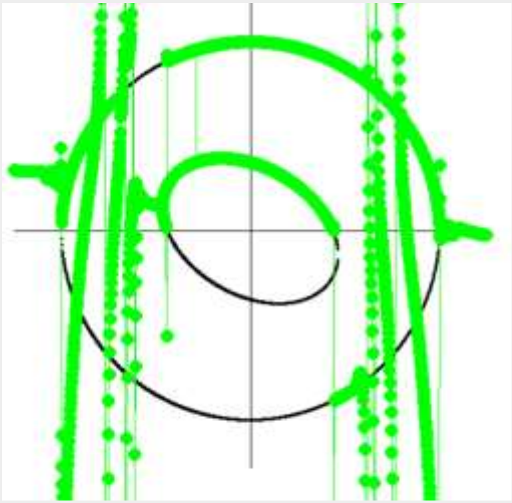


PML result: radiation in anisotropic media

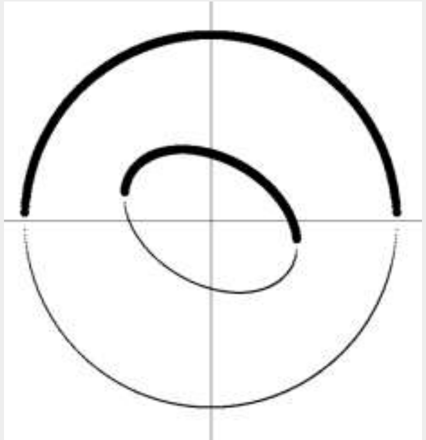


Result from PMDL after the fix

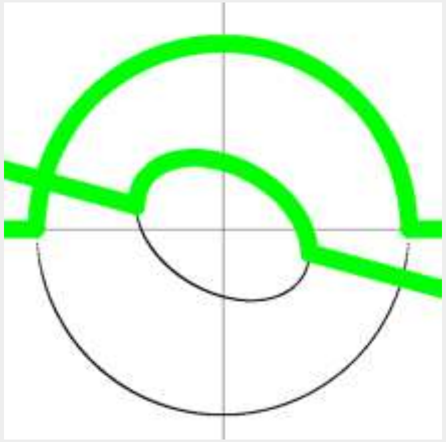
Anisotropic elasticity – Tilted Elliptic Case



Arbitrary parameters

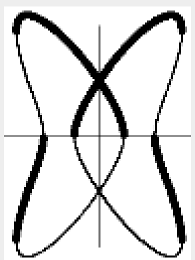


Ideal Slowness

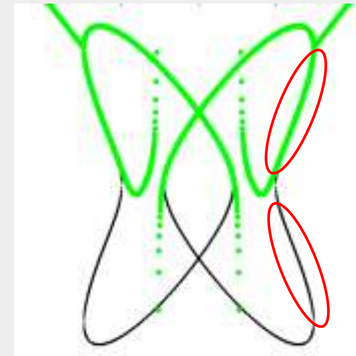


Stable parameters

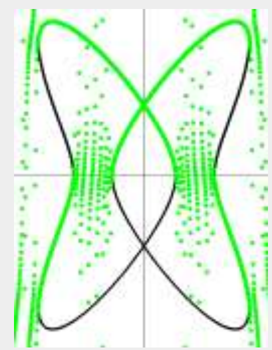
Anisotropic elasticity – Non-elliptic Case



Traditional mesh



Two different
coordinated materials



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

PML for Lattice Waves: 7% reflections w/20 PML layers

Discrete PMDL: less than 1% error w/ 4 PMDL layers

Part 3. Two-Sided DtN Map

Complex-length Finite Element Method

Facilitating the Approximation of 2-Sided DtN Map

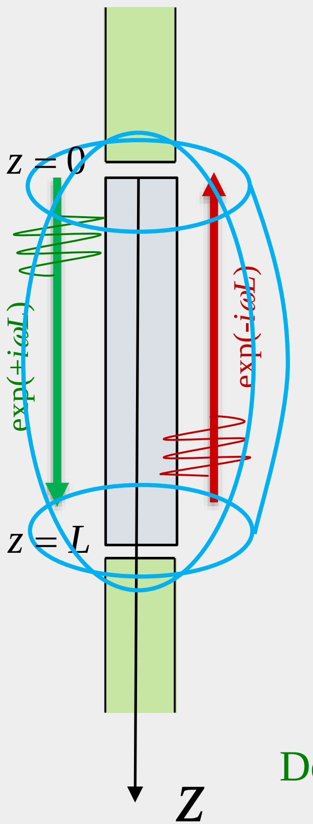
- Consider the equation: $-\dfrac{\partial^2 u}{\partial z^2} - \omega^2 u = 0, \quad z \in (0, L)$
- Exact 2-sided DtN map: $K_{exact} = \begin{bmatrix} A & B \\ B & A \end{bmatrix}$
- By definition, exact DtN Map is impedance preserving: $A^2 - B^2 = Z_{exact}^2$
- Consider impedance preserving discretization of the interval:

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

- Error in A and B would be similar since: $\bar{A}^2 - \bar{B}^2 = Z_{exact}^2 = A^2 - B^2$
- Approximating two-sided map reduces to approximating one-sided map

- Better derivation based on Crank-Nicolson discretization of the propagator

1D Helmholtz Equation



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

$$\begin{Bmatrix} -\partial u_0 / \partial z \\ \partial u_L / \partial z \end{Bmatrix} = \overbrace{i\omega \begin{bmatrix} \coth(i\omega L) & -\operatorname{csch}(i\omega L) \\ -\operatorname{csch}(i\omega L) & \coth(i\omega L) \end{bmatrix}}^{\mathbf{K}^{\text{exact}}} \begin{Bmatrix} u_0 \\ u_L \end{Bmatrix}$$

$\Downarrow$

1st Order Form

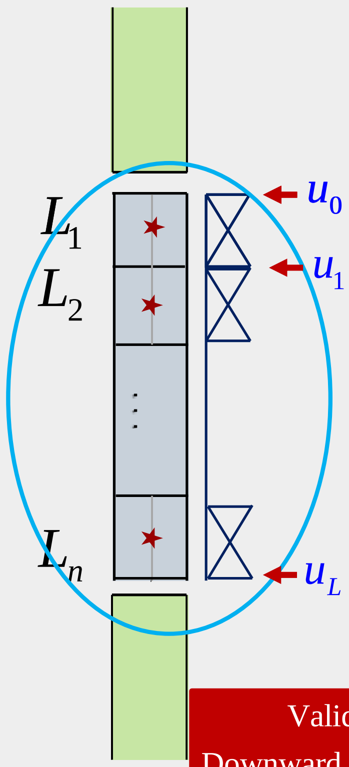
$$v = \partial u / \partial z$$

$$\frac{\partial}{\partial z}\begin{Bmatrix} u \\ v / i\omega \end{Bmatrix} = \begin{bmatrix} 0 & i\omega \\ i\omega & 0 \end{bmatrix} \begin{Bmatrix} i\omega u \\ v / i\omega \end{Bmatrix} \Rightarrow Eigenvalues = \pm i\omega$$

Downward waves: $\begin{Bmatrix} u_L \\ \partial u_L / \partial z \end{Bmatrix} = \overbrace{\begin{bmatrix} \exp(i\omega L) & 0 \\ 0 & \exp(i\omega L) \end{bmatrix}}^{\mathbf{P}^{\text{exact}}} \begin{Bmatrix} u_0 \\ \partial u_0 / \partial z \end{Bmatrix}$

Propagator Approximation

$$\begin{Bmatrix} u_L \\ \partial u_L/\partial z \end{Bmatrix} = \overbrace{\begin{bmatrix} \prod_{j=1}^{n}\left(\frac{1+i\omega L_j/2}{1-i\omega L_j/2}\right) & 0 \\ 0 & \prod_{j=1}^{n}\left(\frac{1-i\omega L_j/2}{1+i\omega L_j/2}\right) \end{bmatrix}}^{\mathbf{P}_n^{\text{approximate}}} \begin{Bmatrix} u_0 \\ \partial u_0/\partial z \end{Bmatrix}$$



$$\frac{1}{L_1}\begin{Bmatrix} u_1 - u_0 \\ \bar{v}_1 - \bar{v}_0 \end{Bmatrix} = \frac{1}{2}\begin{bmatrix} 0 & i\omega \\ i\omega & 0 \end{bmatrix}\begin{Bmatrix} u_1 + u_0 \\ \bar{v}_1 + \bar{v}_0 \end{Bmatrix}$$

1st Order Form $v = \partial u/\partial z, \quad \bar{v} = v/i\omega$

Crank-Nicolson

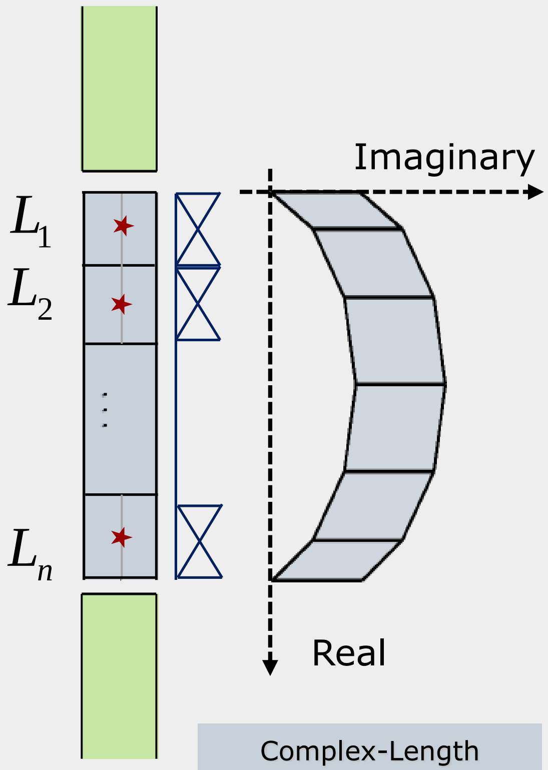
$$\frac{\partial}{\partial z}\begin{Bmatrix} u \\ \bar{v} \end{Bmatrix} = \begin{bmatrix} 0 & i\omega \\ i\omega & 0 \end{bmatrix}\begin{Bmatrix} u \\ \bar{v} \end{Bmatrix}$$

Crank-Nicolson

$$\begin{Bmatrix} u_L \\ \partial u_L/\partial z \end{Bmatrix} = \overbrace{\begin{bmatrix} \exp(i\omega L) & 0 \\ 0 & \exp(i\omega L) \end{bmatrix}}^{\mathbf{P}^{\text{exact}}} \begin{Bmatrix} u_0 \\ \partial u_0/\partial z \end{Bmatrix}$$

Valid for both $\pm\omega$
Downward AND upward waves!

Padé Approximant



Complex-Length Finite Element Method

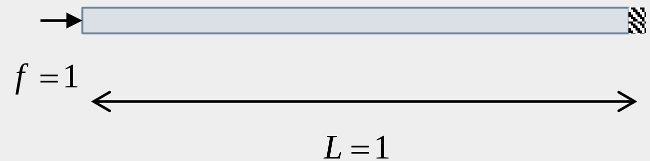
$$\exp(\alpha L) \approx \overbrace{\prod_{j=1}^{n}\left(\frac{1+\alpha L_j/2}{1-\alpha L_j/2}\right)}^{P_{\text{Padé}}}$$

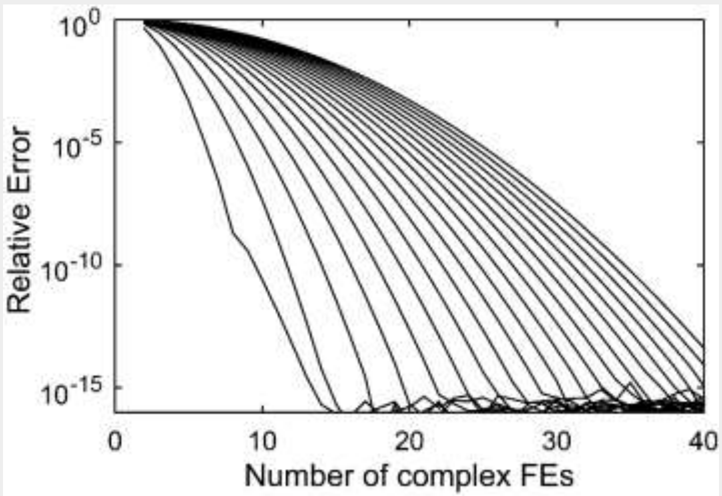
$$\left.\frac{d^j\left(\exp(\alpha L)\right)}{d\alpha^j}\right|_{\alpha=0} = \left.\frac{d^j P_{\text{Padé}}}{d\alpha^j}\right|_{\alpha=0}$$

$$(j = 0,\cdots,2n)$$

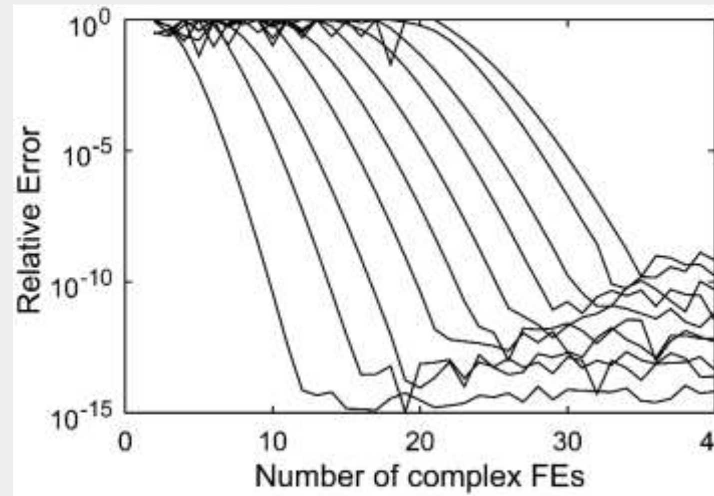
$$\sum_{j=0}^{n}\frac{(2n-j)!}{j!\,(n-j)!}(-x)^j = 0 \quad \rightarrow \quad L_j = 2L/x_j$$

Complex-Length FEM: Exponential Convergence





Laplace Equation



Helmholtz Equation
(can’t beat Nyquist limit)

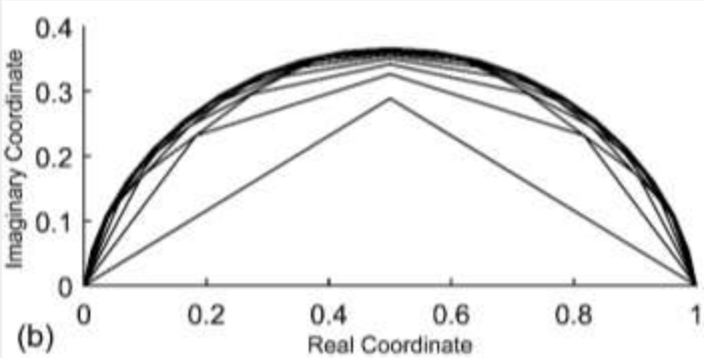
Complex-Length FEM: Some Observations

- 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 ($\mathrm{Re}(L_j) > 0$)
- 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

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

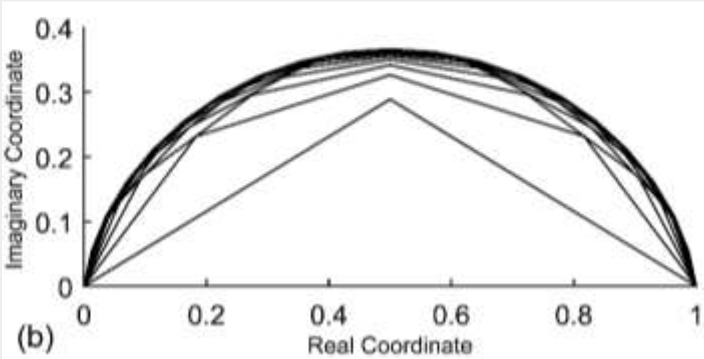
$$\left. \frac{d^j\left(\exp(\alpha L)\right)}{d\alpha^j} \right|_{\alpha=0} = \left. \frac{d^j P_{\text{Padé}}}{d\alpha^j} \right|_{\alpha=0}$$

$$\sum_{j=0}^{n} \frac{(2n-j)!}{j!\,(n-j)!}(-x)^j = 0 \quad \rightarrow \quad L_j = 2L/x_j$$



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

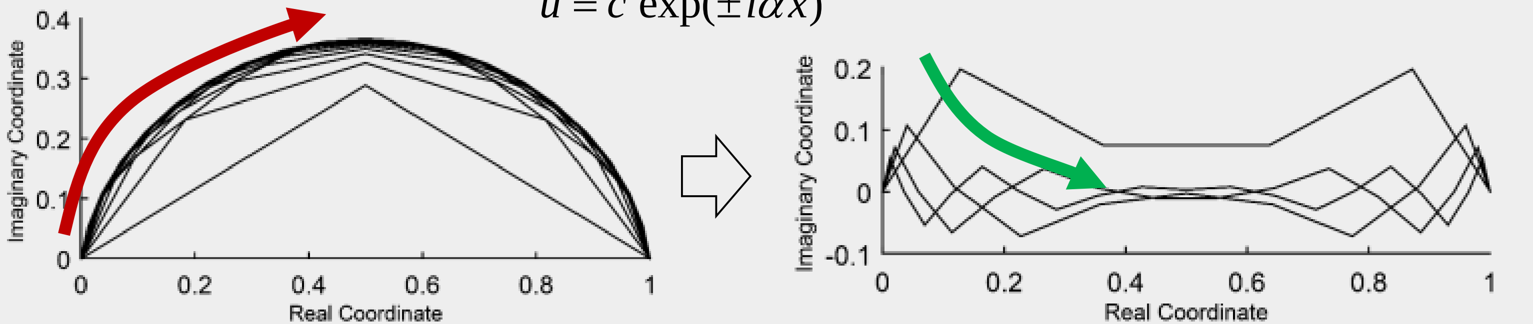


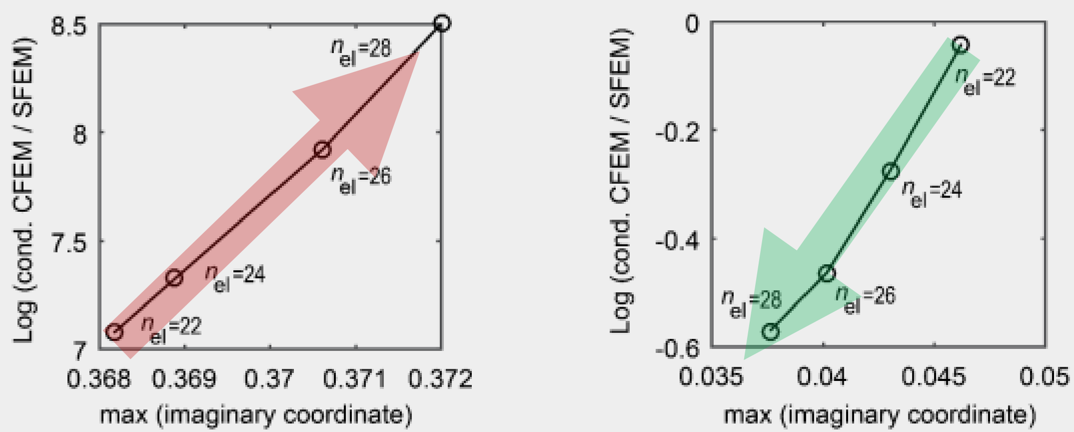
- Do complex lengths lead to complex eigenvalues of K with respect to M?
  - No. Eigenvalues are real and positive!
  - Eigenvectors are complex (K and M are complex symmetric)

$$-\frac{\partial^2 u}{\partial z^2} - \omega^2 u = 0 \;\Rightarrow\; (\mathbf{K} - \omega^2 \mathbf{M})\phi = \mathbf{0}$$

Element Ordering

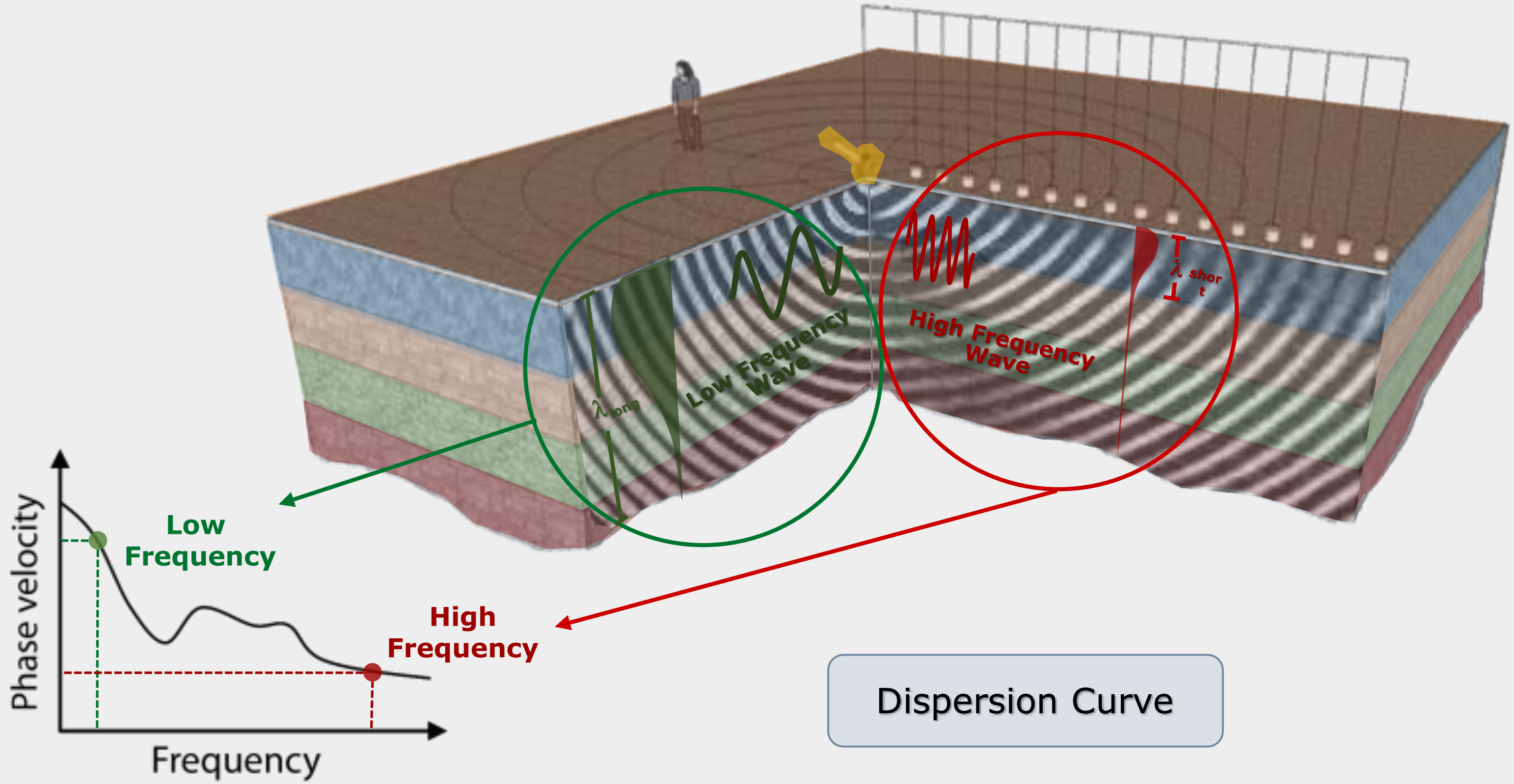
$$u = c\ \exp(\pm i\alpha x)$$





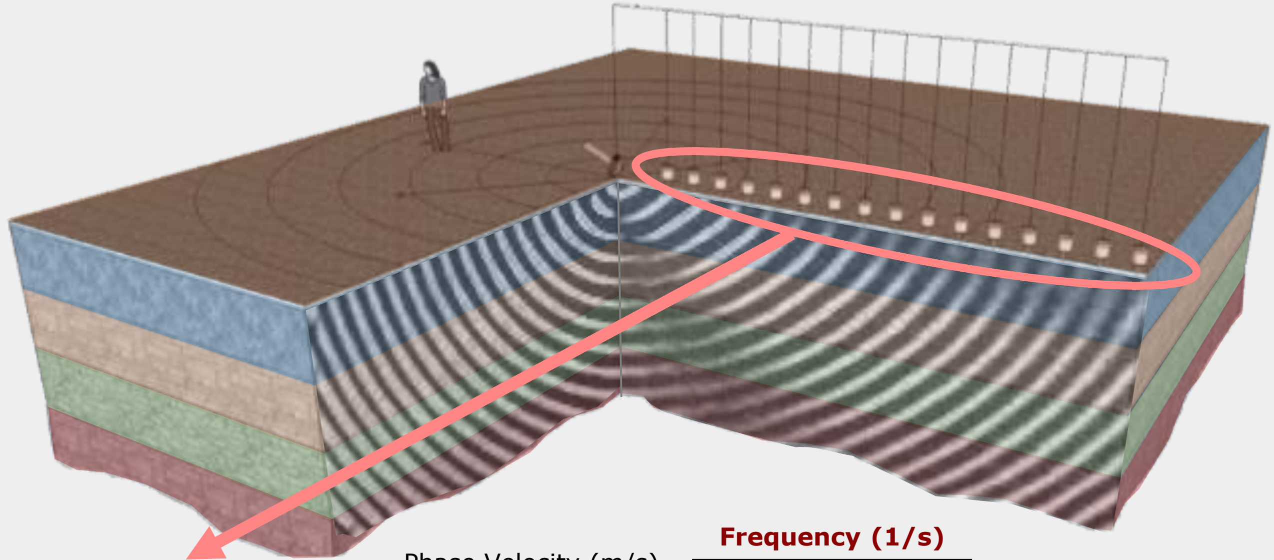
Part 4. Near Surface Geophysical Site Characterization…
…using Guided Wave Inversion

Guided Wave Dispersion

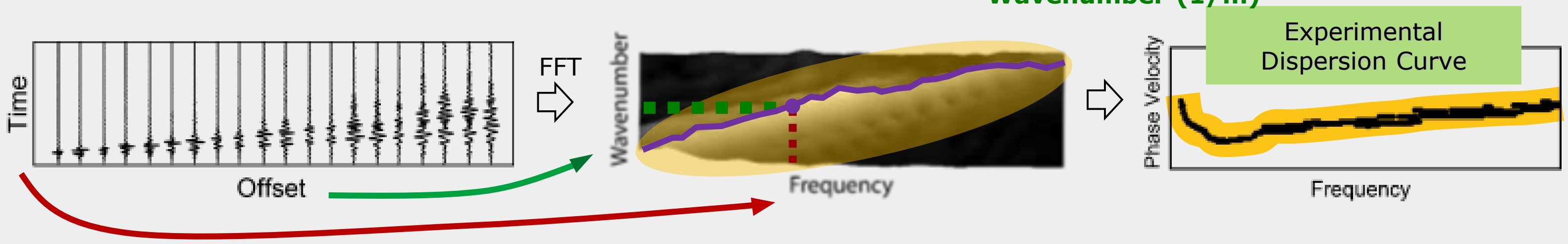


Dispersion Curve

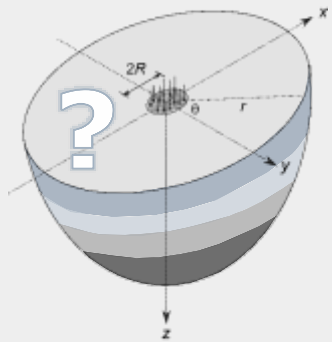
Spectral Analysis



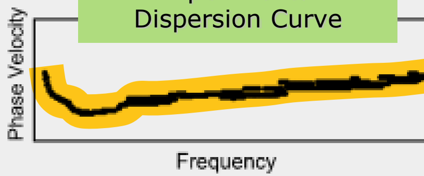
$$\text{Phase Velocity (m/s)} = \frac{\textbf{Frequency (1/s)}}{\textbf{Wavenumber (1/m)}}$$



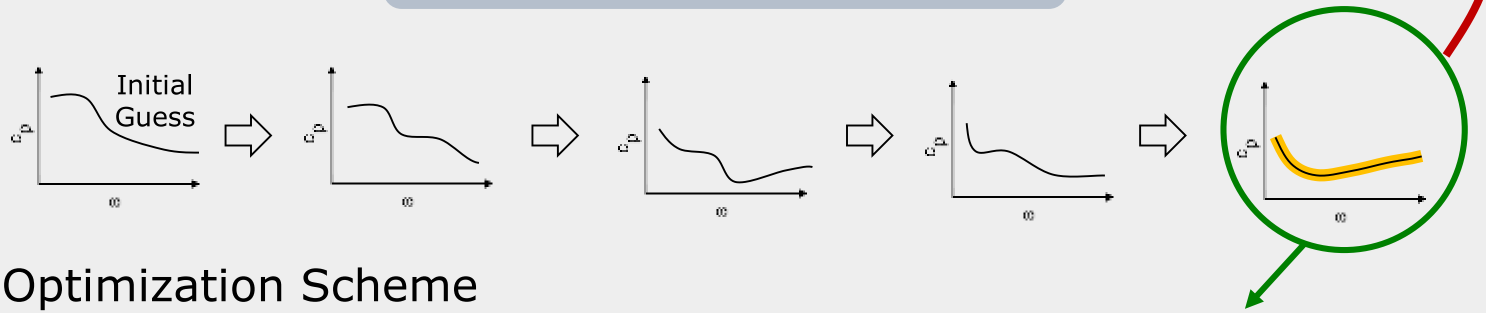
Medium Characterization



Inverse Identification



Iteratively Minimize $$E = \sum_{i=1}^{N} \left(c_i^{\text{experimantal}} - c_i^{\text{predicted}} \right)^2$$



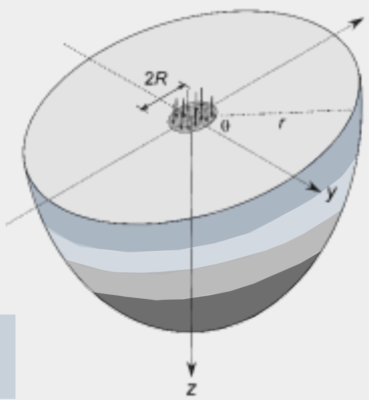
Forward Problem:
Predicted Dispersion Curve

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

Forward Modeling – State of the Art

$$-\frac{1}{r}\frac{\partial}{\partial r}\left(\mathbf{D}_{rr}\, r\frac{\partial \mathbf{u}}{\partial r}+\mathbf{D}_{rz}\, r\frac{\partial \mathbf{u}}{\partial z}+\mathbf{D}_{ro}\mathbf{u}\right)-\frac{\partial}{\partial z}\left(\mathbf{D}_{rz}^{T}\frac{\partial \mathbf{u}}{\partial r}+\mathbf{D}_{zz}\frac{\partial \mathbf{u}}{\partial z}+\mathbf{D}_{zo}\frac{1}{r}\mathbf{u}\right)$$

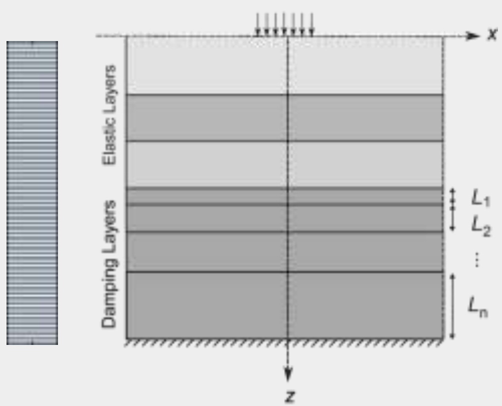
$$-\frac{1}{r}\left(-\mathbf{D}_{ro}^{T}\frac{\partial \mathbf{u}}{\partial r}-\mathbf{D}_{zo}^{T}\frac{\partial \mathbf{u}}{\partial z}-\frac{1}{r}\mathbf{D}_{oo}\mathbf{u}\right)-\left(\rho\omega^{2}\mathbf{I}\right)\mathbf{u}=\mathbf{0}$$



Discretize
z direction

Hankel Transform
r direction

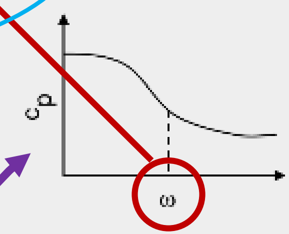
Quadratic
Eigenvalue Problem



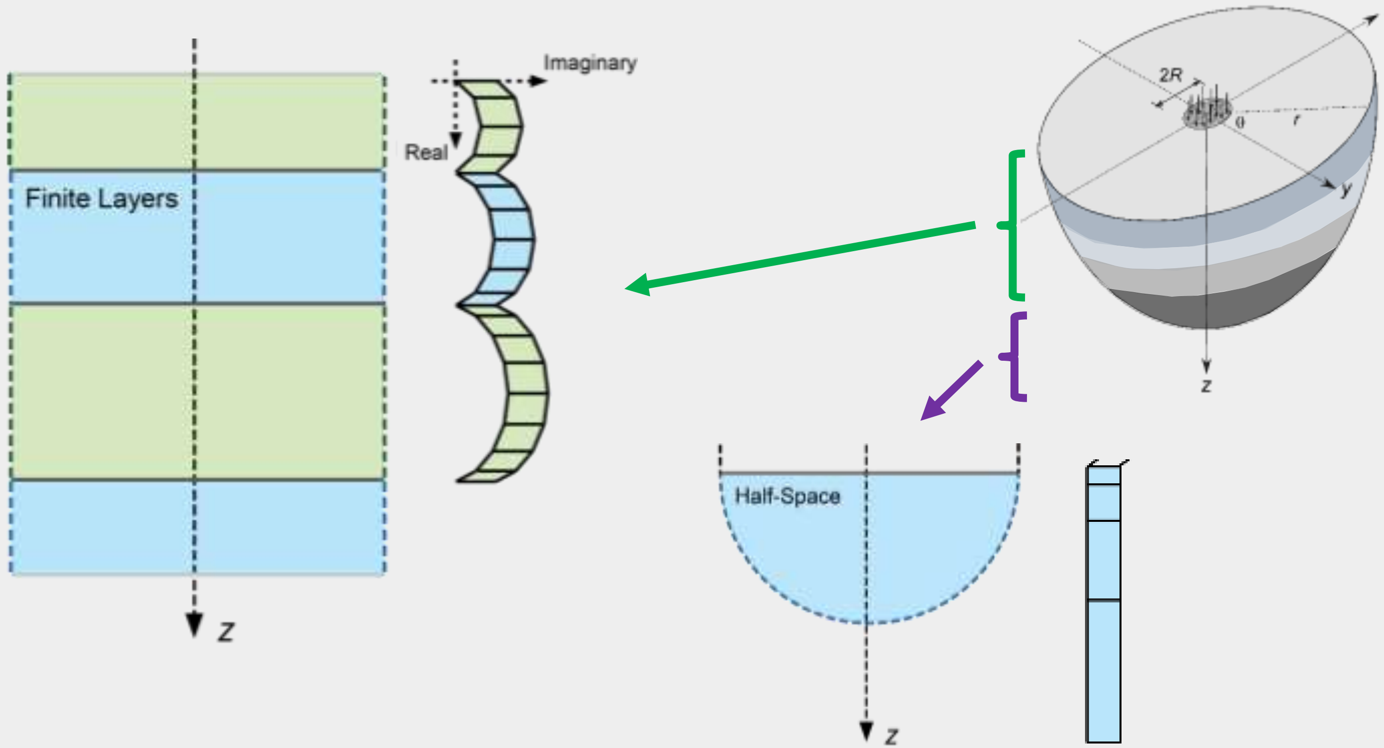
$$\det(\mathbf{K})=0$$

$$\overbrace{\left(k^{2}\,\mathbf{A}+k\,\mathbf{B}+\mathbf{C}+\omega^{2}\,\mathbf{D}\right)}^{\mathbf{K}}\mathbf{u}=\mathbf{0}$$

$$k \longrightarrow c_p=\frac{\omega}{k}$$



Reducing the Problem Size: CFEM+PMDL

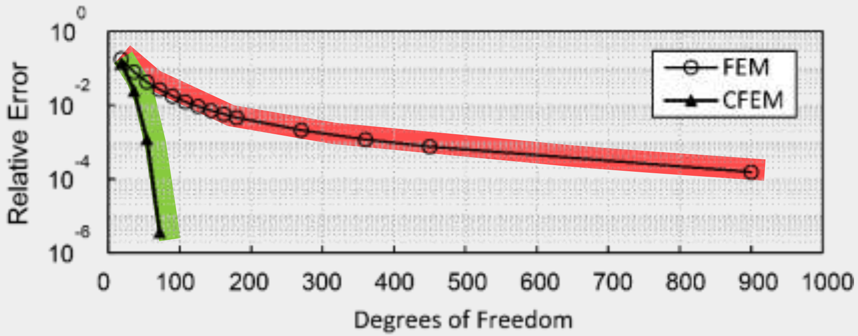


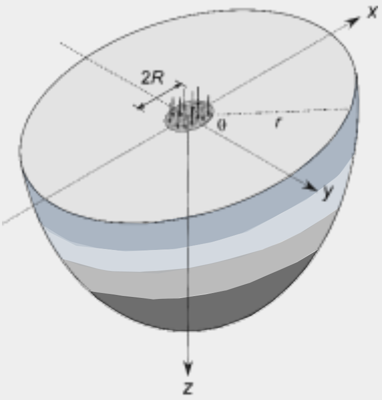
Complex-Length FEM
(Finite Layers)

Perfectly Matched *discrete* Layers
(Halfspace)

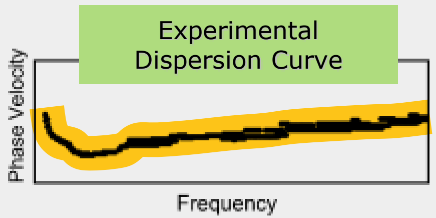
Forward Modeling: CFEM vs. FEM

Error in dispersion curve

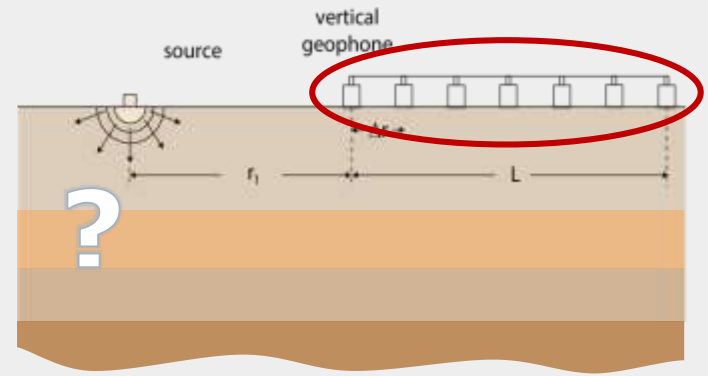


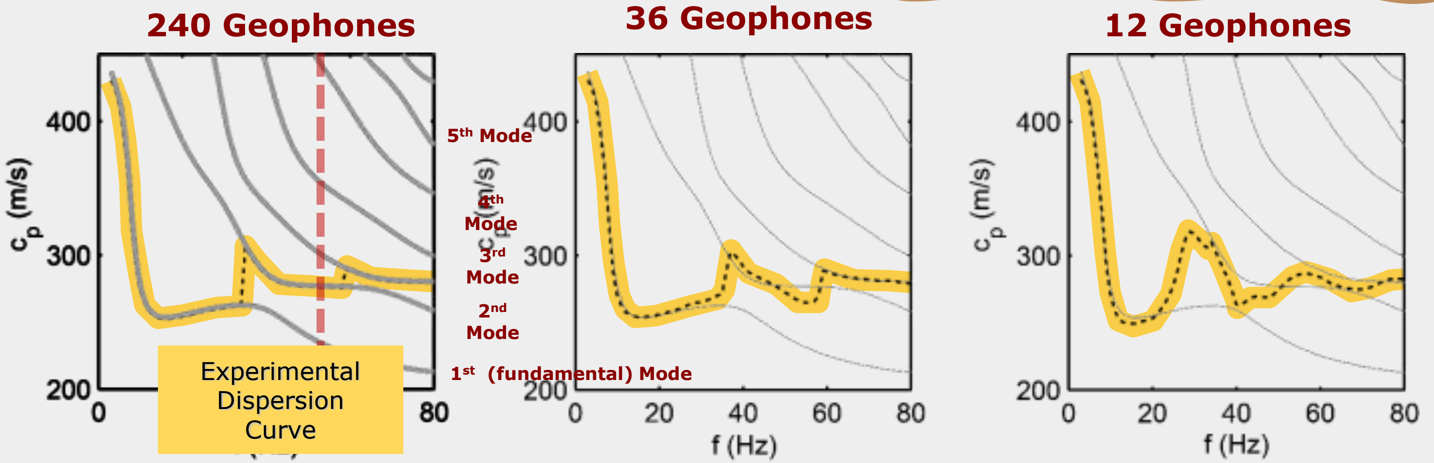


Inversion: Experimental Dispersion Curve



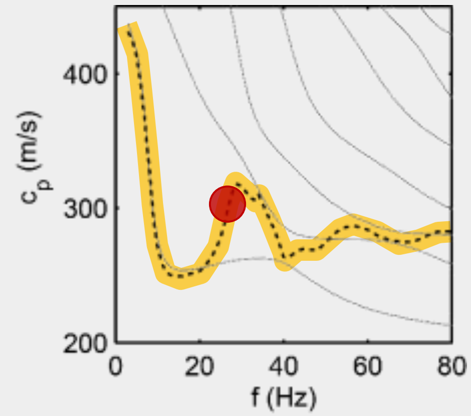
Inverse
Identification





Challenge

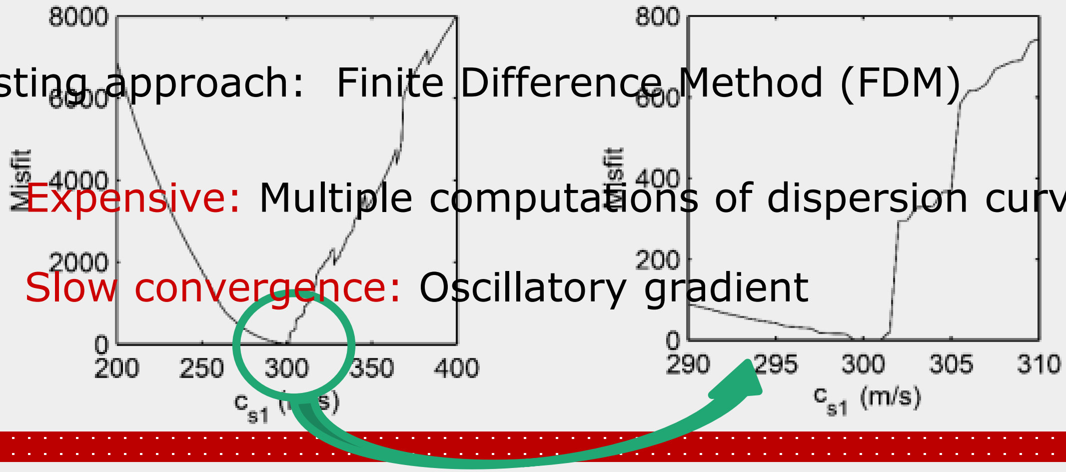
- No analytical derivative



- Rough misfit function

$$\text{Minimize} \quad E = \sum_{i=1}^{N} \left(c_i^{\text{experimantal}} - c_i^{\text{predicted}} \right)^2$$

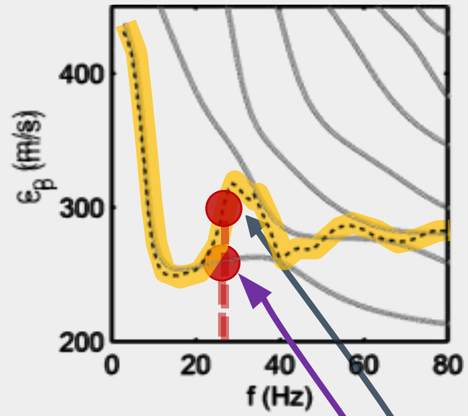
- Existing approach: Finite Difference Method (FDM)
  - Expensive: Multiple computations of dispersion curve
  - Slow convergence: Oscillatory gradient



Proposed Derivative for Experimental Curve

- Analytical Derivative

$$\frac{\partial k_i}{\partial m_j} = -\frac{\boldsymbol{\phi}_L^{\dagger}(\partial \mathbf{K}/\partial m_j)\boldsymbol{\phi}_R}{\boldsymbol{\phi}_L^{\dagger}(\partial \mathbf{K}/\partial k_i)\boldsymbol{\phi}_R}$$



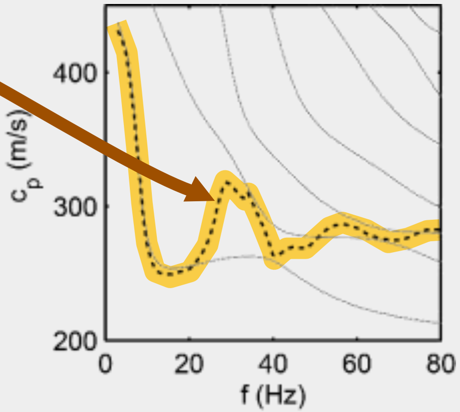
- Alternative Approach for Eigenvector

$$\overbrace{\left(k^2\mathbf{A} + k\mathbf{B} + \mathbf{C} + \omega^2\mathbf{D}\right)}^{\mathbf{K}}\mathbf{u} = \mathbf{0} \quad \Rightarrow \quad \boldsymbol{\phi}_R = \mathbf{K}^{-1}\mathbf{P}$$

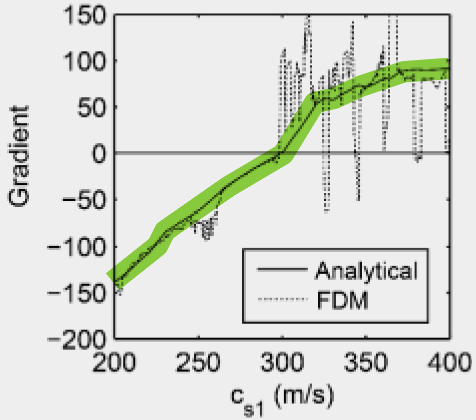
$$k = k_i^{\text{experimental}} + \delta \quad (\delta \approx 10^{-6})$$

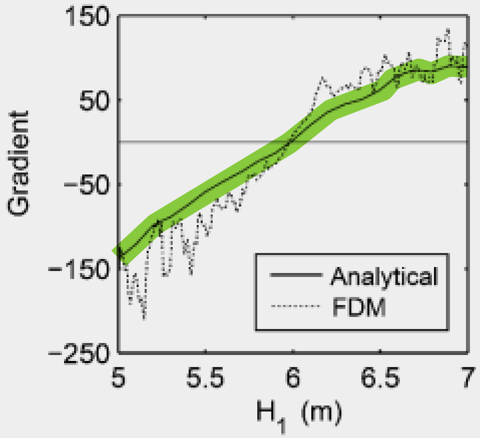
Proposed Derivative

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



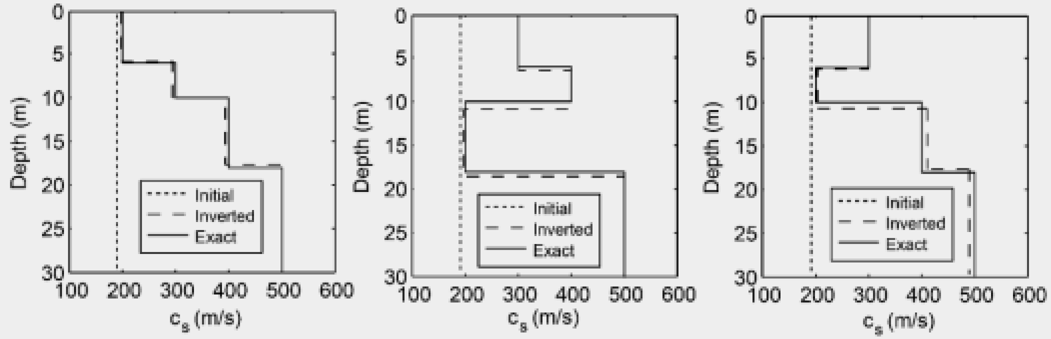
- Analytical vs. FDM Gradient



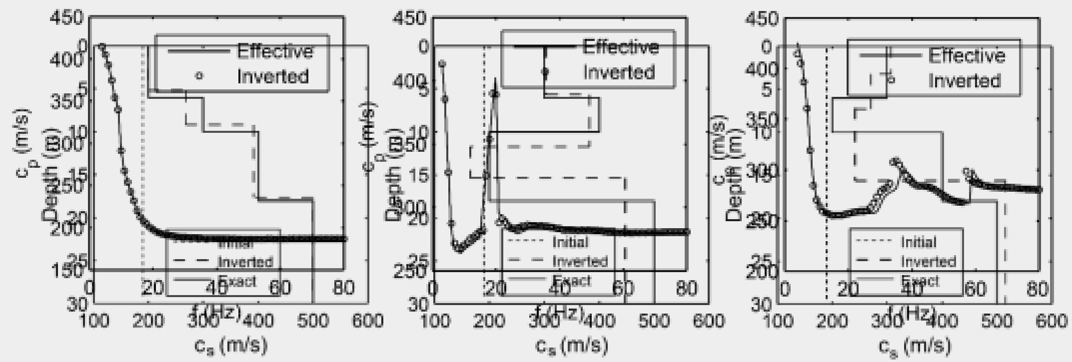


Inversion Results: Synthetic Examples

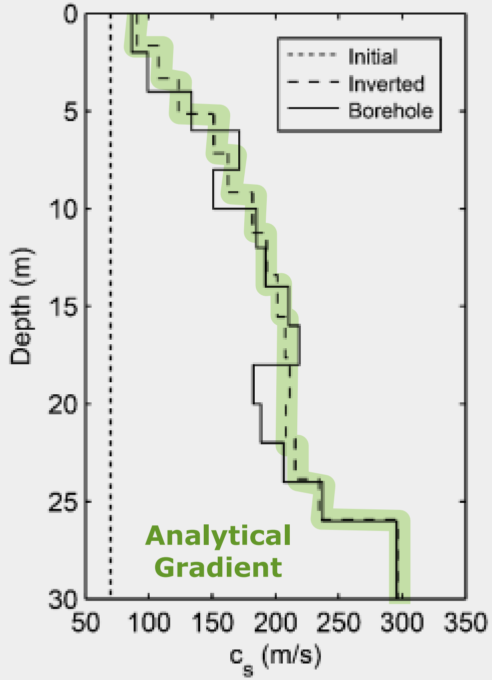
- Analytical Gradient

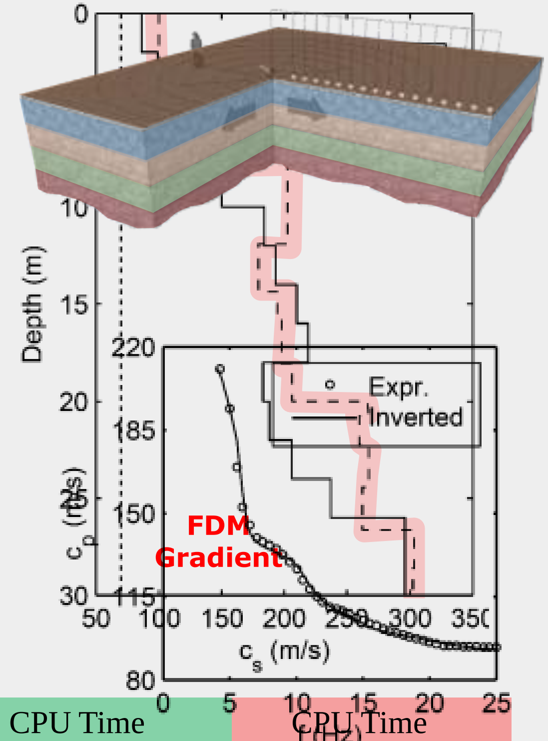


- FDM Gradient



Inversion Results: 14-Layer Soil Profile†





Iterations (Existing)	Iterations (Proposed)	CPU Time (Proposed)	CPU Time (Existing)
14	**8**	**11.3 s**	**2884.6 s**

† Experimental data from: J Xia et al., *J. Environ. Eng. Geophys.*, 5.3, 1-13 (2000)

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 Conds.: 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

G, Tassoulas (2000), Continued fraction absorbing boundary conditions for the wave equation, J Comp. Acoustics.

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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

Vaziri Astaneh, G (2016), Improved Algorithms for Inversion of Surface Waves Using Multistation Analysis, *Geoph. J. Intl.*

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