Recent advances in 3D full-waveform inversion (FWI) for site characterization

Challenges and open issues

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Outline

1. Background

2. 3D forward wave simulation problem
   - PML formulations for elastodynamics

3. 3D inverse medium problem
   - Inversion in PML-truncated elastic media
   - 3D characterization using synthetic data
   - 3D characterization using field data: the NEES@UCSB site

4. Conclusions
   - Summary
   - Challenges
Site characterization (SC) by full-waveform inversion (FWI)

Overarching goal: to reconstruct the material profile of probed, semi-infinite, near-surface, geologic formations using elastic waves for interrogation, and surface records of the complete waveforms of the formation’s response in the time-domain.
SC by FWI - The framework and its challenges

- An imaging problem: infer properties from sensor data
- Sensor deployment is limited - setting inferior to medical imaging
- Properties are spatially distributed
- No *a priori* simplifying assumptions (geometry; layering; etc)
- Physics drives discretization → millions of unknown properties; for a 100m × 100m × 20m domain: 2 million elastic properties
- SC focuses on near-surface deposits: domain truncation needed
- Exploration geophysics drives advances
- Scale issues, complex physics, algorithmic challenges, open problem even for the acoustic case
SC by FWI - Recent advances in our work

Key problem ingredients:

- The forward problem
  - Resolve wave motion in unbounded, arbitrarily heterogeneous, domains

- FWI: an inverse medium problem
  - To address the imaging/inversion: PDE-constrained optimization framework
  - To address the scale: parallel computing
  - To address robustness: physics-based algorithmic tweaks
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Perfectly-Matched-Layer (PML) truncated domains

Forward wave simulation problem - key characteristics
- Probed domain is arbitrarily heterogeneous
- Probed domain is semi-infinite in extent
- The ROI is rather limited in extent...need for domain truncation

Quality domain truncation is paramount → PMLs

The PML is a buffer zone that surrounds a truncated finite computational domain. Within the buffer, the propagating waves are forced to decay exponentially, without generating reflections from the interface (perfectly matched).

Advantages
- absorbs waves without reflection for all non-zero angles-of-incidence and frequencies
- can handle arbitrary heterogeneity
- has tunable parameters
Hybrid formulation (optimal)

Standard displacement-based elastodynamics for $\Omega^{RD}$
Mixed-field (stress-displacement) formulation for $\Omega^{PML}$
The IBVP (3rd-order in time)

Find \( u(x, t) \in \Omega^{RD} \cup \Omega^{PML} \), \( S(x, t) \in \Omega^{PML} \), such that:

\[
\text{div} \left\{ \mu \left[ \nabla \dot{u} + (\nabla \dot{u})^T \right] + \lambda (\text{div} \, \dot{u}) \right\} + b = \rho \ddot{u} \quad \text{in} \ \Omega^{RD} \times J
\]
\[
\text{div} \left( \dot{S}^T \Lambda_e + \dot{S}^T \Lambda_p + S^T \Lambda_w \right) = \rho \left( a \ddot{u} + b \dddot{u} + c \dot{u} + d u \right) \quad \text{in} \ \Omega^{PML} \times J
\]
\[
a \dddot{S} + b \dot{S} + c \dot{S} + d S = \mu \left[ (\nabla \dddot{u}) \Lambda_e + \Lambda_e (\nabla \dddot{u})^T + (\nabla \dot{u}) \Lambda_p + \Lambda_p (\nabla \dot{u})^T \right] + \mu \left[ (\nabla u) \Lambda_w + \Lambda_w (\nabla u)^T \right] + \lambda \left[ \text{div} (\Lambda_e \dddot{u}) + \text{div} (\Lambda_p \dot{u}) + \text{div} (\Lambda_w u) \right] \quad \text{in} \ \Omega^{PML} \times J
\]

BCs:
\[
\left\{ \mu \left[ \nabla \dddot{u} + (\nabla \dddot{u})^T \right] + \lambda (\text{div} \, \dddot{u}) \right\} \mathbf{n}^+ = \dot{g}_n \quad \text{on} \ \Gamma_N^{RD} \times J
\]
\[
(\dot{S}^T \Lambda_e + \dot{S}^T \Lambda_p + S^T \Lambda_w) \mathbf{n}^- = 0 \quad \text{on} \ \Gamma_N^{PML} \times J
\]
\[
u = 0 \quad \text{on} \ \Gamma_D^{PML} \times J
\]
\[
u^+ = \nu^- \quad \text{on} \ \Gamma^I \times J
\]
\[
\left\{ \mu \left[ \nabla \dddot{u} + (\nabla \dddot{u})^T \right] + \lambda (\text{div} \, \dddot{u}) \right\} \mathbf{n}^+ + (\dot{S}^T \Lambda_e + \dot{S}^T \Lambda_p + S^T \Lambda_w) \mathbf{n}^- = 0 \quad \text{on} \ \Gamma^I \times J
\]
Semi-discrete form

\[ M \ddot{d} + C \dot{d} + K d + G d = \dot{f} \]

or \[ M \dot{d} + C \dot{d} + K d + G \dot{d} = f, \quad \dot{d} = \int_0^t d(\tau)|_{PML} \, d\tau \quad \Rightarrow \quad \dot{d} = d|_{PML} \]

\[
M = \begin{bmatrix}
\bar{M}_{RD} + \bar{M}_a & 0 \\
0 & N_a
\end{bmatrix} \\
G = \begin{bmatrix}
\bar{M}_d & A_{wu} \\
-A_{wl}^T & N_d
\end{bmatrix}
\]

\[
C = \begin{bmatrix}
\bar{M}_b & A_{eu} \\
-A_{el}^T & N_b
\end{bmatrix} \\
K = \begin{bmatrix}
\bar{K}_{RD} + \bar{M}_c & A_{pu} \\
-A_{pl}^T & N_c
\end{bmatrix}
\]

\[
d = \begin{bmatrix}
u_h \\
S_h
\end{bmatrix}^T \\
f = \begin{bmatrix}
f_{RD} \\
0
\end{bmatrix}^T
\]
Temporal discretization

Temporal integration:

\[ M \ddot{\mathbf{d}} + C \dot{\mathbf{d}} + K \mathbf{d} + G \mathbf{d} = \mathbf{f}, \quad \ddot{\mathbf{d}} = \int_0^t \mathbf{d}(\tau)|_{\text{PML}} \, d\tau \quad \Rightarrow \quad \dot{\mathbf{d}} = \mathbf{d}|_{\text{PML}} \]

A couple of choices → implicit Newmark Method

\[
\begin{bmatrix}
M & 0 \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
\ddot{\mathbf{d}} \\
\dot{\mathbf{d}}
\end{bmatrix} +
\begin{bmatrix}
C & 0 \\
0 & I
\end{bmatrix}
\begin{bmatrix}
\dot{\mathbf{d}} \\
\mathbf{d}
\end{bmatrix} +
\begin{bmatrix}
K & G \\
-I & 0
\end{bmatrix}
\begin{bmatrix}
\mathbf{d}
\end{bmatrix} =
\begin{bmatrix}
\mathbf{f}
\end{bmatrix}
\quad \text{Un-Symmetric 1}
\]

\[
\begin{bmatrix}
M & 0 \\
0 & I
\end{bmatrix}
\begin{bmatrix}
\ddot{\mathbf{d}} \\
\dot{\mathbf{d}}
\end{bmatrix} +
\begin{bmatrix}
C & 0 \\
-I & 0
\end{bmatrix}
\begin{bmatrix}
\dot{\mathbf{d}} \\
\mathbf{d}
\end{bmatrix} +
\begin{bmatrix}
K & G \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
\mathbf{d}
\end{bmatrix} =
\begin{bmatrix}
\mathbf{f}
\end{bmatrix}
\quad \text{Un-Symmetric 2}
\]

A better choice using spectral elements → explicit Runge-Kutta method

\[
\frac{d}{dt} \begin{bmatrix}
x_0 \\
x_1 \\
x_2
\end{bmatrix} =
\begin{bmatrix}
0 & I & 0 \\
0 & 0 & I \\
-G & -K & -C
\end{bmatrix}
\begin{bmatrix}
x_0 \\
x_1 \\
x_2
\end{bmatrix} +
\begin{bmatrix}
0 \\
0 \\
\mathbf{f}
\end{bmatrix}
\]

where \( x_0 = \ddot{\mathbf{d}}, \ x_1 = \dot{\mathbf{d}}, \ x_2 = \mathbf{d}. \)
Numerical experiment: heterogeneous medium with inclusion

\[ c_s(z) = \begin{cases} 
400 \text{ m/s}, & \text{ if } -20m \leq z \leq 0m \\
500 \text{ m/s}, & \text{ if } -50m \leq z < -20m \\
600 \text{ m/s}, & \text{ ellipsoidal inclusion} 
\end{cases} \]

\( \nu = 0.25 \)
\( \Delta t = 4.8 \times 10^{-4} \text{s} \)

- element size = 1.25\( m \)
- # elements = 500’000
- # unknowns = 24’228’426
- # unknowns ED = 521’884’704

PML parameters:
- \( m = 2 \)
- \( \alpha_o = 5 \)
- \( \beta_o = 500 \)
Displacements time histories

Enlarged domain
PML-truncated domain

$s_{p8}$
Energy decay

![Graphs showing energy decay over time with different decay rates](image)

- Standard scale
- Logarithmic scale

Enld. dom. 
\( \beta_o = 400 \)
\( \beta_o = 500 \)
\( \beta_o = 600 \)
Long-time stability

125'000 time steps ($\beta_o = 500$)
Snapshots of total displacement taken at $t = 0.111, 0.147, 0.183, 0.219, 0.255, 0.291, 0.327, 0.363$ s.
### PML accuracy - relative error

Error at sampling points between hybrid-PML and enlarged domain solutions

<table>
<thead>
<tr>
<th>sample point</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>error (Example 1)</th>
<th>error (Example 2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>sp1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$1.17 \times 10^{-12}$</td>
<td>$4.61 \times 10^{-10}$</td>
</tr>
<tr>
<td>sp2</td>
<td>+50</td>
<td>0</td>
<td>0</td>
<td>$2.52 \times 10^{-8}$</td>
<td>$6.07 \times 10^{-7}$</td>
</tr>
<tr>
<td>sp3</td>
<td>+50</td>
<td>0</td>
<td>-25</td>
<td>$2.89 \times 10^{-9}$</td>
<td>$2.87 \times 10^{-6}$</td>
</tr>
<tr>
<td>sp4</td>
<td>+50</td>
<td>0</td>
<td>-50</td>
<td>$1.46 \times 10^{-7}$</td>
<td>$7.03 \times 10^{-6}$</td>
</tr>
<tr>
<td>sp5</td>
<td>0</td>
<td>0</td>
<td>-50</td>
<td>$9.86 \times 10^{-9}$</td>
<td>$1.41 \times 10^{-5}$</td>
</tr>
<tr>
<td>sp6</td>
<td>+50</td>
<td>+50</td>
<td>0</td>
<td>$3.26 \times 10^{-7}$</td>
<td>$1.86 \times 10^{-6}$</td>
</tr>
<tr>
<td>sp7</td>
<td>+50</td>
<td>+50</td>
<td>-25</td>
<td>$5.50 \times 10^{-8}$</td>
<td>$6.72 \times 10^{-6}$</td>
</tr>
<tr>
<td>sp8</td>
<td>+50</td>
<td>+50</td>
<td>-50</td>
<td>$5.08 \times 10^{-7}$</td>
<td>$6.44 \times 10^{-6}$</td>
</tr>
</tbody>
</table>
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Goal: find the distribution of material properties $\lambda(x), \mu(x)$

PDE-constrained optimization problem:

$$\min_{\lambda, \mu} J(\lambda, \mu) := \frac{1}{2} \sum_{j=1}^{N_r} \int_0^T \int_{\Gamma_m} (u - u_m) \cdot (u - u_m) \delta(x - x_j) \, d\Gamma \, dt + R(\lambda, \mu)$$

subject to the continuous forward problem

Regularization:

$$R^{TN}(\lambda, \mu) = \frac{R_\lambda}{2} \int_{\Omega} \nabla \lambda \cdot \nabla \lambda \, d\Omega + \frac{R_\mu}{2} \int_{\Omega} \nabla \mu \cdot \nabla \mu \, d\Omega$$

$$R^{TV}(\lambda, \mu) = \frac{R_\lambda}{2} \int_{\Omega^{RD}} (\nabla \lambda \cdot \nabla \lambda + \epsilon)^{\frac{1}{2}} \, d\Omega + \frac{R_\mu}{2} \int_{\Omega^{RD}} (\nabla \mu \cdot \nabla \mu + \epsilon)^{\frac{1}{2}} \, d\Omega$$
The Lagrangian functional

\[ L(u, S, w, T, \lambda, \mu) := \frac{1}{2} \sum_{j=1}^{N_r} \int_0^T \int_{\Gamma_m} (u - u_m) \cdot (u - u_m) \delta(x - x_j) \, d\Gamma \, dt + R(\lambda, \mu) \]

\[ - \int_0^T \int_{\Omega_{RD}} \nabla w : \{ \mu [\nabla u + (\nabla u)^T] + \lambda (\text{div } u) I \} \, d\Omega \, dt \]

\[ - \int_0^T \int_{\Omega_{PML}} \nabla w : (\dot{S}^T \Lambda_e + S^T \Lambda_p + \bar{S}^T \Lambda_w) \, d\Omega \, dt - \int_0^T \int_{\Omega_{RD}} w \cdot \rho \ddot{u} \, d\Omega \, dt \]

\[ - \int_0^T \int_{\Omega_{PML}} w \cdot \rho (a \ddot{u} + b \ddot{u} + c \ddot{u} + d \ddot{u}) \, d\Omega \, dt + \int_0^T \int_{\Gamma_{RD}} w \cdot g_n \, d\Gamma \, dt \]

\[ + \int_0^T \int_{\Omega_{RD}} w \cdot b \, d\Omega \, dt - \int_0^T \int_{\Omega_{PML}} T : (a \dot{S} + b \dot{S} + c \bar{S} + d \ddot{S}) \, d\Omega \, dt \]

\[ + \int_0^T \int_{\Omega_{PML}} T : \mu [(\nabla \ddot{u}) \Lambda_e + \Lambda_e (\nabla \ddot{u})^T + (\nabla u) \Lambda_p + \Lambda_p (\nabla u)^T + (\nabla \ddot{u}) \Lambda_w + \Lambda_w (\nabla \ddot{u})^T] \]

\[ + T : \lambda [\text{div} (\Lambda_e \ddot{u}) + \text{div} (\Lambda_p u) + \text{div} (\Lambda_w \ddot{u})] I \, d\Omega \, dt \]
Optimality system

Stationarity enforced by the vanishing of first-order Gâteau derivatives

State (forward) problem: \( \mathcal{L}'(u, S, w, T, \lambda, \mu)(\tilde{w}, \tilde{T}) = 0 \)
an initial value BVP

Adjoint problem: \( \mathcal{L}'(u, S, w, T, \lambda, \mu)(\tilde{u}, \tilde{S}) = 0 \)
a final value BVP

Control problem: \( \mathcal{L}'(u, S, w, T, \lambda, \mu)(\tilde{\lambda}) = 0 \)
\( \mathcal{L}'(u, S, w, T, \lambda, \mu)(\tilde{\mu}) = 0 \)
Algorithmic tweak: regularization factor continuation

\[ \tilde{M}g = R \, g_{\text{reg}} + g_{\text{mis}} \]

Concept: “size” of \( R \, g_{\text{reg}} \) should be proportional to that of \( g_{\text{mis}} \)

\[ n_{\text{reg}} = \frac{g_{\text{reg}}}{\| g_{\text{reg}} \|}, \quad n_{\text{mis}} = \frac{g_{\text{mis}}}{\| g_{\text{mis}} \|} \]

\[ \tilde{M}g = \| g_{\text{mis}} \| \left( \varphi \, n_{\text{reg}} + n_{\text{mis}} \right), \quad \varphi = R \, \frac{\| g_{\text{reg}} \|}{\| g_{\text{mis}} \|} \approx 0.5 \to 0.3 \]

\[ R = \varphi \, \frac{\| g_{\text{mis}} \|}{\| g_{\text{reg}} \|} \]
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Numerical Experiments

Example 1: smoothly-varying heterogeneous medium
Example 2: layered medium
Example 3: layered medium with inclusion
Example 4: layered medium with 3 inclusions
min \( c_s = 200 \text{ m/s} \)
max \( c_p = 433 \text{ m/s} \)
element size = 1.25 \text{ m}
\( \Delta t = 10^{-3} \text{ s} \)
# time steps = 400/450
# elements = 72'324
# state unknowns = 3'578'136
# material unknowns = 616'850

\[
\lambda(z) = \mu(z) = 80 + 0.45 |z| + 35 \exp \left( -\frac{(|z| - 22.5)^2}{150} \right) \text{ (MPa)}
\]
Smoothly varying medium: target $\lambda$ and $\mu$ (MPa); and profile at $(x, y) = (0, 0)$
Single-parameter inversion ($\mu$ only)

$\lambda$ (a priori known)

$\mu$ (inverted)
Single-parameter inversion ($\mu$ only)

$$(x, y) = (0, 0)$$

$$(x, y) = (10, 10)$$

$$(x, y) = (20, 20)$$
Single-parameter inversion ($\lambda$ only)

\(\lambda\) (inverted)  
\(\mu\) (a priori known)
Single-parameter inversion ($\lambda$ only)

$$(x, y) = (0, 0)$$

$$(x, y) = (10, 10)$$

$$(x, y) = (20, 20)$$
Simultaneous inversion for $\lambda$ and $\mu$ - unbiased

$\lambda$ (inverted)

$\mu$ (inverted)
A physics-based algorithmic tweak

Bias search directions of $\lambda$ by the search directions of $\mu$ during the early stages of the inversion process:

$$s^\lambda_k \leftarrow \|s^\lambda_k\| \left(W \frac{s^\mu_k}{\|s^\mu_k\|} + (1 - W) \frac{s^\lambda_k}{\|s^\lambda_k\|}\right)$$

$$W = 1 \rightarrow 0$$
Simultaneous inversion for $\lambda$ and $\mu$ - biased

$\lambda$ (inverted)

$\mu$ (inverted)
Simultaneous inversion: $\lambda$ cross-sections

$(x, y) = (0, 0)$  
$(x, y) = (10, 10)$  
$(x, y) = (20, 20)$
Simultaneous inversion: $\mu$ cross-sections

$(x, y) = (0, 0)$  
$(x, y) = (10, 10)$  
$(x, y) = (20, 20)$
Misfit history; frequency continuation scheme

\[ f_{\text{max}} = 20 \text{ Hz} \quad f_{\text{max}} = 30 \text{ Hz} \quad f_{\text{max}} = 40 \text{ Hz} \]
Example 2: setup

Layered medium: target $\lambda$ and $\mu$ (MPa); and profile at $(x, y) = (0, 0)$
Simultaneous inversion ($f_{max} = 10$ Hz)
Simultaneous inversion ($f_{max} = 40$ Hz)
Example 3: setup

Layered medium: target $\lambda$ and $\mu$ (MPa); and profile at $(x, y) = (7.5, 0)$
Simultaneous inversion \( (f_{max} = 10 \text{ Hz}) \)

\[ \lambda \text{ (inverted)} \]

\[ \mu \text{ (inverted)} \]
Simultaneous inversion \( (f_{max} = 40 \text{ Hz}) \)
20% Gaussian noise, $f_{max} = 40$ Hz

\( \lambda \) (inverted) \\
\( \mu \) (inverted)
Inversion with Gaussian noise: $\lambda, \mu$ cross-sections

$$(x, y) = (7.5, 0)$$
Example 4: setup

Layered medium with three inclusions: target $\lambda$ and $\mu$ (MPa) at two different cross-sections.

# state unknowns = 9,404,184; # material unknowns = 2,429,586

80 m × 80 m × 45 m medium
Example 4: setup

Layered medium with three inclusions: target $\lambda$ and $\mu$ on (left) the $z = -8.75$ m cross-section; and (right) the $z = -35$ m cross-section
Simultaneous inversion ($f_{max} = 40$ Hz)

\(\lambda\) (inverted)  \hspace{2cm} \(\mu\) (inverted)
Simultaneous inversion ($f_{max} = 40$ Hz)

$\lambda$ (inverted)  

$\mu$ (inverted)
Simultaneous inversion ($f_{max} = 40$ Hz)
Simultaneous inversion \((f_{\text{max}} = 40 \, \text{Hz})\)
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Garner Valley field experiment
The experiment layout

computational domain: 126 × 68 × 40 m + 10 m-thick PML
#material parameters: 718,566
#state unknowns: 3,885,648
FWI profiles

$c_p$ (m/s)  
$c_s$ (m/s)
SASW $c_s$ profile
Cross-sectional profiles: $x = 10 \text{ m}$
Time-history comparisons: \( x = +10 \) m

Sensor locations; from top-left to bottom-right: \( y = 60, 40, 20, 0 \) m
Time-history comparisons: $x = +90$ m

Sensor locations; from top-left to bottom-right: $y = 60, 40, 20, 0$ m
Time-history comparisons: \( x = +100 \text{ m} \)

Sensor locations; from top-left to bottom-right: \( y = 60, 40, 20, 0 \text{ m} \)
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A systematic framework for FWI-based site characterization
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Challenges

- Material attenuation - inversion for attenuation parameters a huge challenge

- Real time - experiment steering

- Ground water level

- Beyond elasticity: poroelasticity / permeability

- Algorithmic improvements for speed and robustness

- Multi-physics probing (unlikely)

- Validation (difficult - control setting)
L. F. Kallivokas, A. Fathi, S. Kucukcoban, K. H. Stokoe II, J. Bielak, O. Ghattas

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A. Fathi, L. F. Kallivokas, K. H. Stokoe II, B. Poursartip
Three-dimensional site characterization using full-waveform inversion: theory, computations, and field experiments, in preparation.