Quantitative inverse scattering via reduced order modeling

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Inverse scattering for generic hyperbolic system

• Primary wave $P^{(s)}(t, \boldsymbol{x})$ and dual wave $\widehat{P}^{(s)}(t, \boldsymbol{x})$ satisfy

$$\partial_t \begin{pmatrix} P^{(s)}(t, \boldsymbol{x}) \\ \widehat{P}^{(s)}(t, \boldsymbol{x}) \end{pmatrix} = \begin{pmatrix} 0 & -L_q \\ L_q^T & 0 \end{pmatrix} \begin{pmatrix} P^{(s)}(t, \boldsymbol{x}) \\ \widehat{P}^{(s)}(t, \boldsymbol{x}) \end{pmatrix}, \quad t > 0, \; \boldsymbol{x} \in \Omega \subset \mathbb{R}^d$$

with homogeneous boundary conditions and initial conditions

$$P^{(s)}(0, \boldsymbol{x}) = b^{(s)}(\boldsymbol{x}), \quad \widehat{P}^{(s)}(0, \boldsymbol{x}) = 0.$$

• Ω is half space ($x_d > 0$) and measurements on $\partial\Omega^+$ at $x_d = 0^+$.

• Array of sensors on $\partial\Omega^+$. Source excitation $b^{(s)}(x)$ supported near $\partial\Omega^+$, where (s) counts sensor index and polarization.

• Finite duration of measurements$\rightsquigarrow$ can truncate Ω to compact cube $\Omega_c \subset \Omega$ with accessible boundary $\partial\Omega_c^{\text{ac}} \subset \partial\Omega$ and inaccessible boundary $\partial\Omega_c^{\text{inac}} \subset \Omega$.

Nonlinear reflectivity to data mapping

• Unknown medium modeled by reflectivity q. First order partial differential operator L_q is affine in q.

Kinematics is assumed known!

• **Inverse scattering problem: Find q in Ω_c from array measurements of reflected primary wave**

$$D_k^{(r,s)} := \left\langle b^{(r)}, P^{(s)}(k\tau, \cdot) \right\rangle = \left\langle b^{(r)}, \cos\left(k\tau\sqrt{L_q L_q^T}\right) b^{(s)} \right\rangle$$

for $r, s = 1, \ldots, m$ and time instants $k\tau, \quad k = 0, \ldots, 2n-1$.

• L_q is affine in q but map $q \mapsto \left(\boldsymbol{D}_k\right)_{0 \le k \le 2n-1}$ to invert is nonlinear

Outline of talk

- Most imaging assumes reflectivity to data map is linear (Born approximation).
- Nonlinear methods: Qualitative (linear sampling, factorization,...) mostly at single frequency. Optimization is difficult.

Goal 1: Use reduced order model (ROM) to approximate the Data to Born (DtB) map

$$(\boldsymbol{D}_k)_{0 \leq k \leq 2n-1} \to (\boldsymbol{D}_k^{\mathrm{Born}})_{0 \leq k \leq 2n-1}$$

$\boldsymbol{D}_k^{\mathrm{Born}}$ defined using Fréchet derivative of map $q \mapsto \boldsymbol{D}_k$ at $q = 0$.

Goal 2: Use the ROM to obtain quantitative estimate of q.

ROM for Data to Born (DtB) transformation

Data are $m \times m$ matrices

$$\boldsymbol{D}_k = \left\langle \boldsymbol{b}, \cos\left(k\tau\sqrt{L_q L_q^T}\right)\boldsymbol{b}\right\rangle, \quad \boldsymbol{b} = \left(b^{(1)}, \dots b^{(m)}\right), \quad 0 \le k \le 2n-1$$

ROM of propagator* $\mathscr{P}_q = \cos\left(\tau\sqrt{L_q L_q^T}\right)$

- Wave at time $k\tau$ is Chebyshev polynomial $\mathcal{T}_k$ of 1st kind of $\mathscr{P}_q$

$$P^{(s)}(k\tau, \boldsymbol{x}) = \cos\left(k\tau\sqrt{L_q L_q^T}\right)b^{(s)}(\boldsymbol{x}) = \mathcal{T}_k(\mathscr{P}_q)b^{(s)}(\boldsymbol{x})$$

- ROM propagator $\boldsymbol{\mathscr{P}}_q^{\text{ROM}}$ gives exact data $\boldsymbol{D}_k$, $0 \le k \le 2n-1$. It is constructed from the data and inherits properties of $\mathscr{P}_q$ to allow DtB transformation.

$^*P^{(s)}((k+1)\tau, \boldsymbol{x}) = 2\mathscr{P}_q P^{(s)}(k\tau, \boldsymbol{x}) - P^{(s)}((k-1)\tau, \boldsymbol{x})$

Algebraic setting: from continuum to fine grid discretization

- Operator $L_q \rightsquigarrow$ lower block bidiagonal matrix $\boldsymbol{L}_q \in \mathbb{R}^{N\times N}$
- Propagator $\mathscr{P}_q = \cos\left(\tau\sqrt{\boldsymbol{L}_q \boldsymbol{L}_q^T}\right)$ is $N \times N$ matrix.
- Snapshots $\boldsymbol{P}_k = \left(P^{(s)}(k\tau,\cdot)\right)_{1\le s\le m} = \mathcal{T}_k(\mathscr{P}_q)\boldsymbol{b} \in \mathbb{R}^{N\times m}$

ROM obtained by projection on range of $\boldsymbol{P} := (\boldsymbol{P}_0,\dots,\boldsymbol{P}_{n-1})$

$$\mathscr{P}_q^{\text{ROM}} = \boldsymbol{V}^T \mathscr{P}_q \boldsymbol{V} \in \mathbb{R}^{nm\times nm} \quad \boldsymbol{b}^{\text{ROM}} = \boldsymbol{V}^T \boldsymbol{b} \in \mathbb{R}^{nm\times n}$$

Here $\boldsymbol{V} \in \mathbb{R}^{N\times nm}$ satisfies

$$\boldsymbol{V}^T\boldsymbol{V} = I_{nm}, \quad \boldsymbol{V}\boldsymbol{V}^T = \text{ orthogonal projector on range}(\boldsymbol{P})$$

Theorem: Projection ROM satisfies

$$\boldsymbol{D}_k = \boldsymbol{b}^T \mathcal{T}_k(\mathscr{P}_q)\boldsymbol{b} = (\boldsymbol{b}^{\text{ROM}})^T \mathcal{T}_k(\mathscr{P}_q^{\text{ROM}})\boldsymbol{b}^{\text{ROM}}, \; 0 \le k \le 2n-1.$$

Proof:

Step 1: Prove $\boldsymbol{P}_k = \boldsymbol{V}\mathcal{T}_k(\mathscr{P}_q^{\text{ROM}})\boldsymbol{b}^{\text{ROM}}$ for $k = 0, \ldots, n-1$.

Step 2: This gives

$$\boldsymbol{D}_k = \boldsymbol{b}^T \boldsymbol{P}_k = \boldsymbol{b}^T \boldsymbol{V}\mathcal{T}_k(\mathscr{P}_q^{\text{ROM}})\boldsymbol{b}^{\text{ROM}} = (\boldsymbol{b}^{\text{ROM}})^T \mathcal{T}_k(\mathscr{P}_q^{\text{ROM}})\boldsymbol{b}^{\text{ROM}}, \quad 0 \le k \le n-1$$

Step 3: For $n \le k \le 2n-1$ use the above and the recursion

$$\mathcal{T}_k(x) = 2\mathcal{T}_{n-1}(x)\mathcal{T}_{k-n+1}(x) - \mathcal{T}_{|2n-2-k|}(x)$$

□

Proof that $\boldsymbol{P}_k = \boldsymbol{V}\mathcal{T}_k(\mathscr{P}_q^{\text{ROM}})\boldsymbol{b}^{\text{ROM}}$ for $k = 0, \ldots, n-1$

Using definition $\mathscr{P}_q^{\text{ROM}} = \boldsymbol{V}^T\mathscr{P}_q\boldsymbol{V}$ and $\boldsymbol{b}^{\text{ROM}} = \boldsymbol{V}^T\boldsymbol{b}$

- For $k = 0$ we have $\boldsymbol{P}_0 = \boldsymbol{b} = VV^T\boldsymbol{b} = V\boldsymbol{b}^{\text{ROM}} = V\mathcal{T}_0(\mathscr{P}_q^{\text{ROM}})\boldsymbol{b}^{\text{ROM}}$
- Hypothesis: true for $k < n-1$.
- For $k+1$ use $\mathcal{T}_{k+1}(x) = 2x\mathcal{T}_k(x) - \mathcal{T}_{k-1}(x)$

$$\begin{aligned}
\boldsymbol{V}\mathcal{T}_{k+1}(\mathscr{P}_q^{\text{ROM}})\boldsymbol{b}^{\text{ROM}} &= 2\boldsymbol{V}\mathscr{P}_q^{\text{ROM}}\mathcal{T}_k(\mathscr{P}_q^{\text{ROM}})\boldsymbol{b}^{\text{ROM}} - \boldsymbol{V}\mathcal{T}_{k-1}(\mathscr{P}_q^{\text{ROM}})\boldsymbol{b}^{\text{ROM}} \\
&= 2\boldsymbol{V}\boldsymbol{V}^T\mathscr{P}_q\boldsymbol{V}\mathcal{T}_k(\mathscr{P}_q^{\text{ROM}})\boldsymbol{b}^{\text{ROM}} - \boldsymbol{P}_{k-1} \\
&= \boldsymbol{V}\boldsymbol{V}^T 2\mathscr{P}_q\boldsymbol{P}_k - \boldsymbol{P}_{k-1} \\
&= \boldsymbol{V}\boldsymbol{V}^T(\boldsymbol{P}_{k+1} + \boldsymbol{P}_{k-1}) - \boldsymbol{P}_{k-1} = \boldsymbol{P}_{k+1}
\end{aligned}$$

Our choice of V

Note: Any $\boldsymbol{V}$ satisfies the data interpolation. Which $\boldsymbol{V}$ is best?

- Define $\boldsymbol{V}$ by Gram-Schmidt (QR factorization)

$$\boldsymbol{P} = \boldsymbol{V}\boldsymbol{R}$$

- Causality and finite speed of propagation make $\boldsymbol{P} \approx$ block upper-tridiagonal with coordination of temporal and spatial mesh. This requires knowing kinematics!

Basis that transforms $\boldsymbol{P}$ to block upper-tridiagonal $\boldsymbol{R}$ is almost the canonical one $\rightsquigarrow$ $\boldsymbol{V}$ is approximate identity.

Theorem: Matrix $\boldsymbol{V}$ from QR factorization makes $\mathscr{P}_q^{\text{ROM}} = \boldsymbol{V}^T \mathscr{P}_q \boldsymbol{V}$ **block tridiagonal**.

This result proved using recursion relations of polynomials becomes important in inversion.

Illustration for sound waves in 1-D

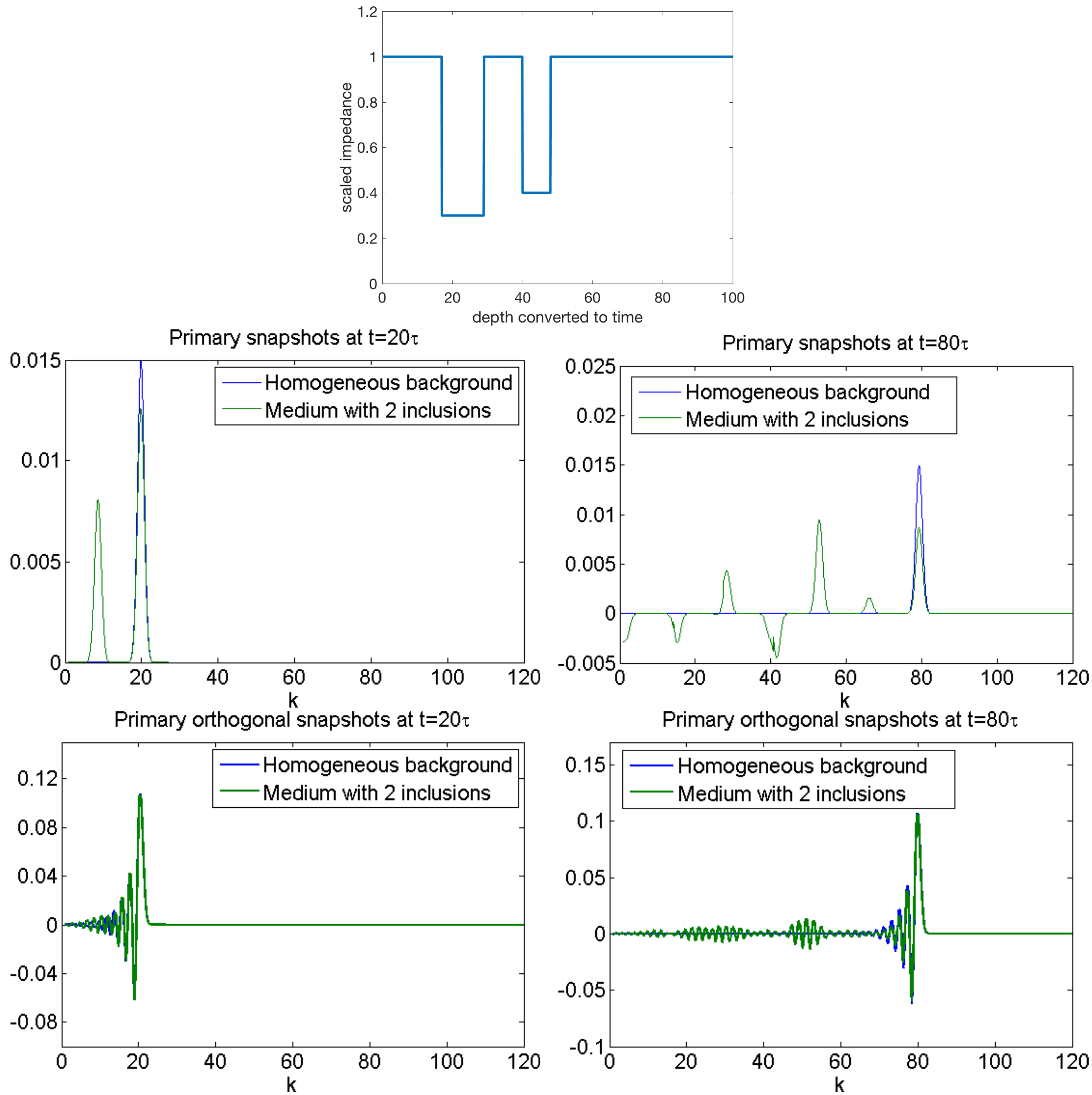
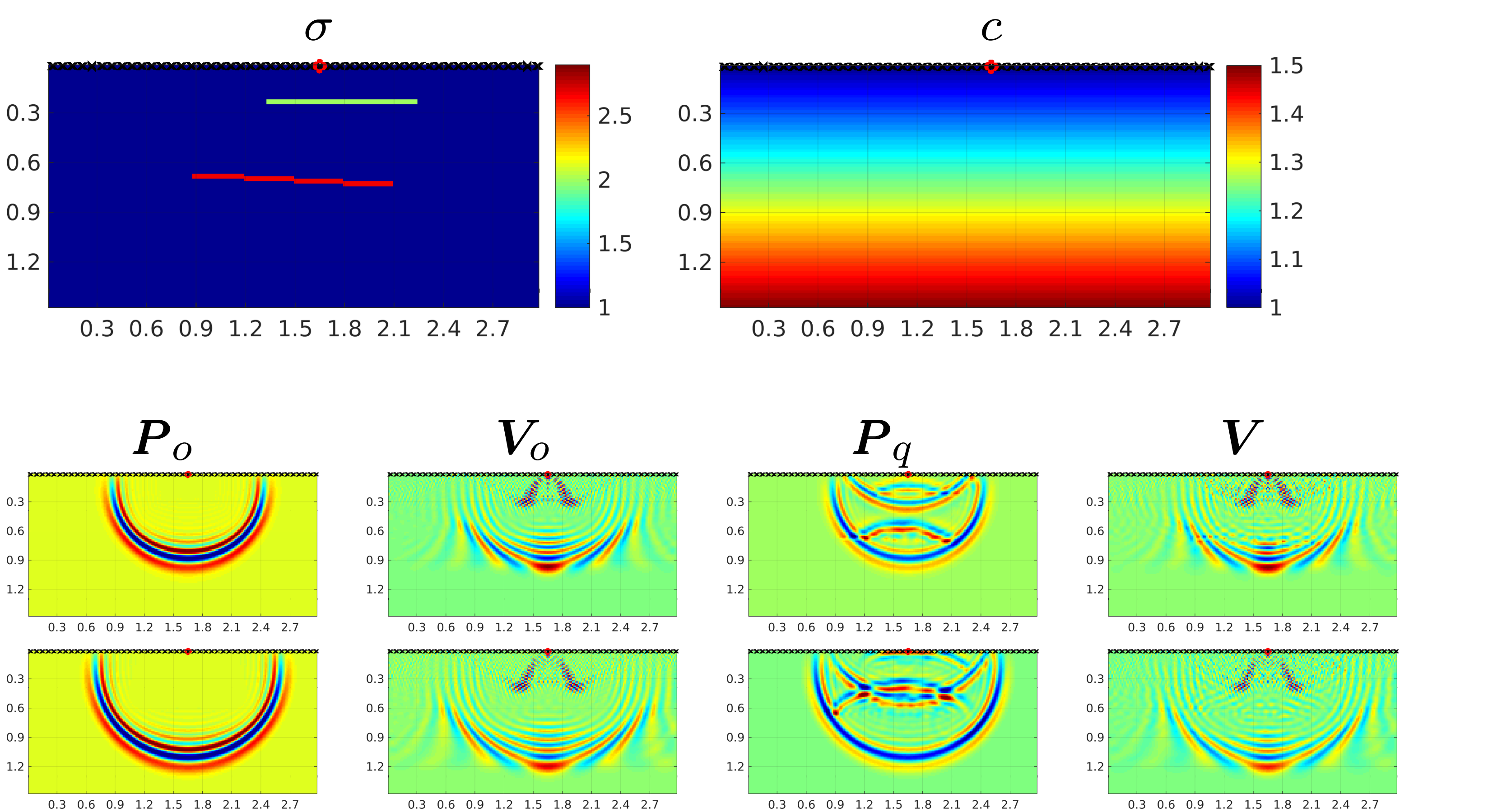


Illustration for sound waves in 2-D



Array with $m = 50$ sensors $\times$

Snapshots plotted for a single source $\circ$

- Start with $\mathrm{P} = (\boldsymbol{P}_0, \dots, \boldsymbol{P}_{n-1}) = \boldsymbol{V}\boldsymbol{R}$ and use $\boldsymbol{P}_j = \mathcal{T}_j(\mathscr{P}_q)\boldsymbol{b}$

$$(\mathrm{P}^T\mathrm{P})_{jk} = \boldsymbol{b}^T\mathcal{T}_j(\mathscr{P}_{\boldsymbol{q}})\mathcal{T}_k(\mathscr{P}_q)\boldsymbol{b} = \frac{1}{2}\boldsymbol{b}^T\Big[\mathcal{T}_{j+k}(\mathscr{P}_q) + \mathcal{T}_{|j-k|}(\mathscr{P}_q)\Big]\boldsymbol{b}$$
$$= \frac{1}{2}\Big(\boldsymbol{D}_{j+k} + \boldsymbol{D}_{|j-k|}\Big) = (\boldsymbol{R}^T\boldsymbol{R})_{jk}, \quad 0 \le j,k \le n-1.$$

Block Cholesky decomposition to get $\boldsymbol{R}$ is ill-conditioned part of computation $\rightsquigarrow$ spectral truncation of Gramian $\boldsymbol{P}^T\boldsymbol{P}$.

- ROM propagator: $\mathscr{P}_q^{\text{ROM}} = \boldsymbol{V}^T\mathscr{P}_q\boldsymbol{V} = \boldsymbol{R}^{-T}\Big(\boldsymbol{P}^T\mathscr{P}_q\boldsymbol{P}\Big)\boldsymbol{R}^{-1}$

$$\Big(\boldsymbol{P}^T\mathscr{P}_q\boldsymbol{P}\Big)_{j,k} = \frac{1}{4}\Big(\boldsymbol{D}_{j+k+1} + \boldsymbol{D}_{|k-j+1|} + \boldsymbol{D}_{|k-j-1|} + \boldsymbol{D}_{|k+j-1|}\Big)$$

- ROM sensor function: $\boldsymbol{b}^{\text{ROM}} = \boldsymbol{V}^T\boldsymbol{b} = \boldsymbol{V}^T\boldsymbol{P}_0 = \boldsymbol{V}^T\boldsymbol{V}\boldsymbol{R}\mathrm{E}_1 = \boldsymbol{R}\mathrm{E}_1$

Properties of ROM propagator

- Propagator factorization

$$\frac{2}{\tau^2}\left(\boldsymbol{I} - \mathscr{P}_q\right) = \frac{2}{\tau^2}\left(\boldsymbol{I} - \cos\left(\tau\sqrt{\boldsymbol{L}_q\boldsymbol{L}_q^T}\right)\right) = \mathcal{L}_q\mathcal{L}_q^T, \qquad \mathcal{L}_q \approx \boldsymbol{L}_q$$

$\boldsymbol{L}_q =$ block lower bidiagonal (discretized 1^{st} order operator L_q).

- By construction ROM propagator is symmetric, block tridiagonal with factorization

$$\frac{2}{\tau^2}\left(\boldsymbol{I}_{nm} - \mathscr{P}_q^{\text{ROM}}\right) = \mathcal{L}_q^{\text{ROM}}(\mathcal{L}_q^{\text{ROM}})^T = \boldsymbol{V}^T\mathcal{L}_q\mathcal{L}_q^T\boldsymbol{V}.$$

- Cholesky factor $\mathcal{L}_q^{\text{ROM}} = \boldsymbol{V}^T\mathcal{L}_q\widehat{\boldsymbol{V}}$ is block lower bidiagonal.

$\rightsquigarrow$ Galerkin approximation on spaces of primary and dual snapshots with orthogonal bases in $\boldsymbol{V}$ and $\widehat{\boldsymbol{V}}$.

Data to Born transformation

- Approximate Fréchet derivative of

$$q \mapsto \boldsymbol{D}_k = (\boldsymbol{b}^{\text{ROM}})^T \mathcal{T}_k(\mathscr{P}_q^{\text{ROM}})\boldsymbol{b}^{\text{ROM}}$$

using

- $\mathcal{L}_q^{\text{ROM}} = \boldsymbol{V}^T \mathcal{L}_q \widehat{\boldsymbol{V}}$ is approximately affine in q.
- $\boldsymbol{b}^{\text{ROM}} = \boldsymbol{V}^T \boldsymbol{b}$ is independent of q.

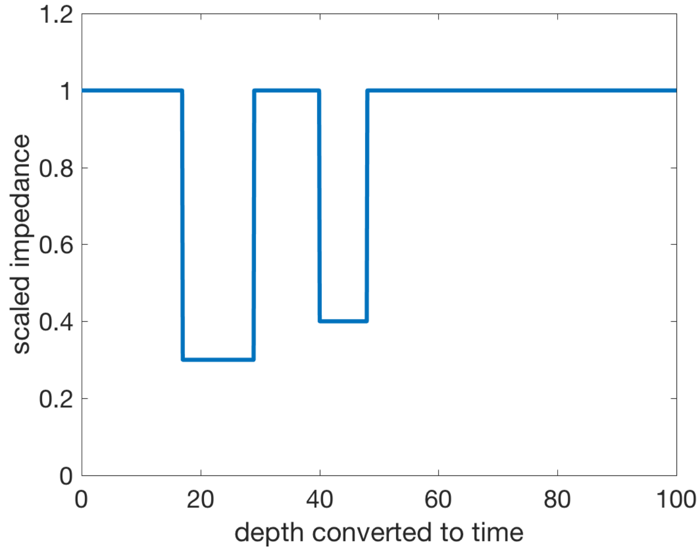
- For a scaled down reflectivity ϵq, with $\varepsilon \ll 1$,

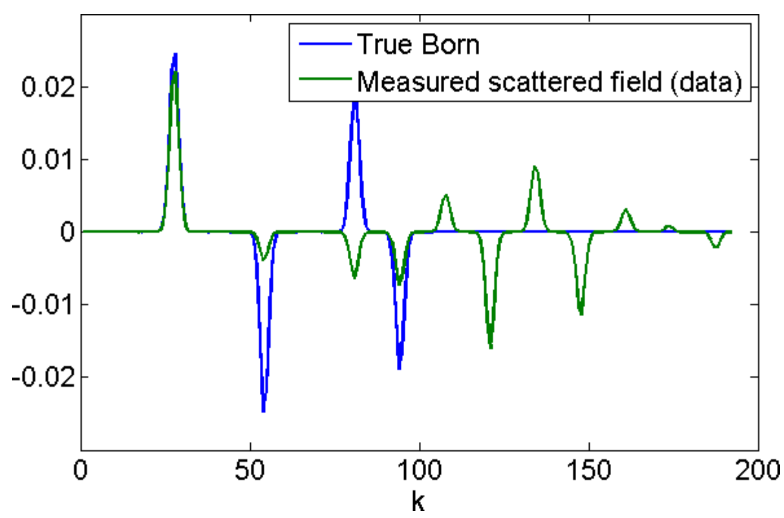
$$\mathcal{L}_{\varepsilon q}^{\text{ROM}} := \mathcal{L}_0^{\text{ROM}} + \varepsilon\Big(\mathcal{L}_q^{\text{ROM}} - \mathcal{L}_0^{\text{ROM}}\Big), \quad \mathscr{P}_{\varepsilon q}^{\text{ROM}} := \boldsymbol{I}_{mn} - \frac{\tau^2}{2}\mathcal{L}_{\varepsilon q}^{\text{ROM}}(\mathcal{L}_{\varepsilon q}^{\text{ROM}})^T$$

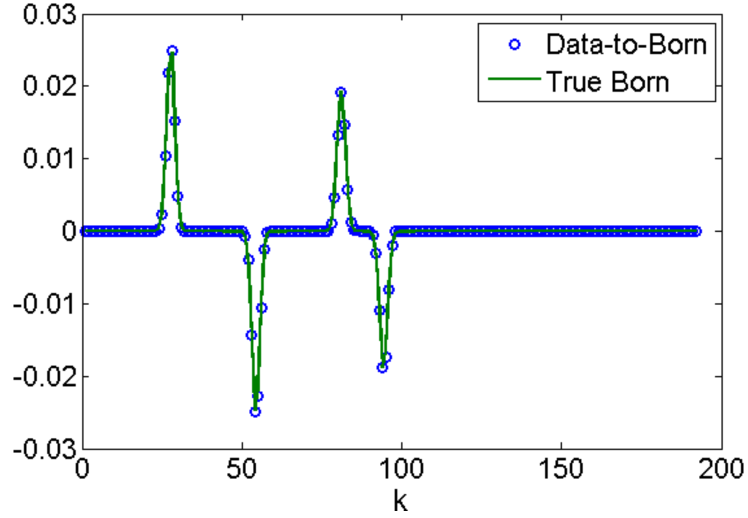
- The transformed (to Born) data:

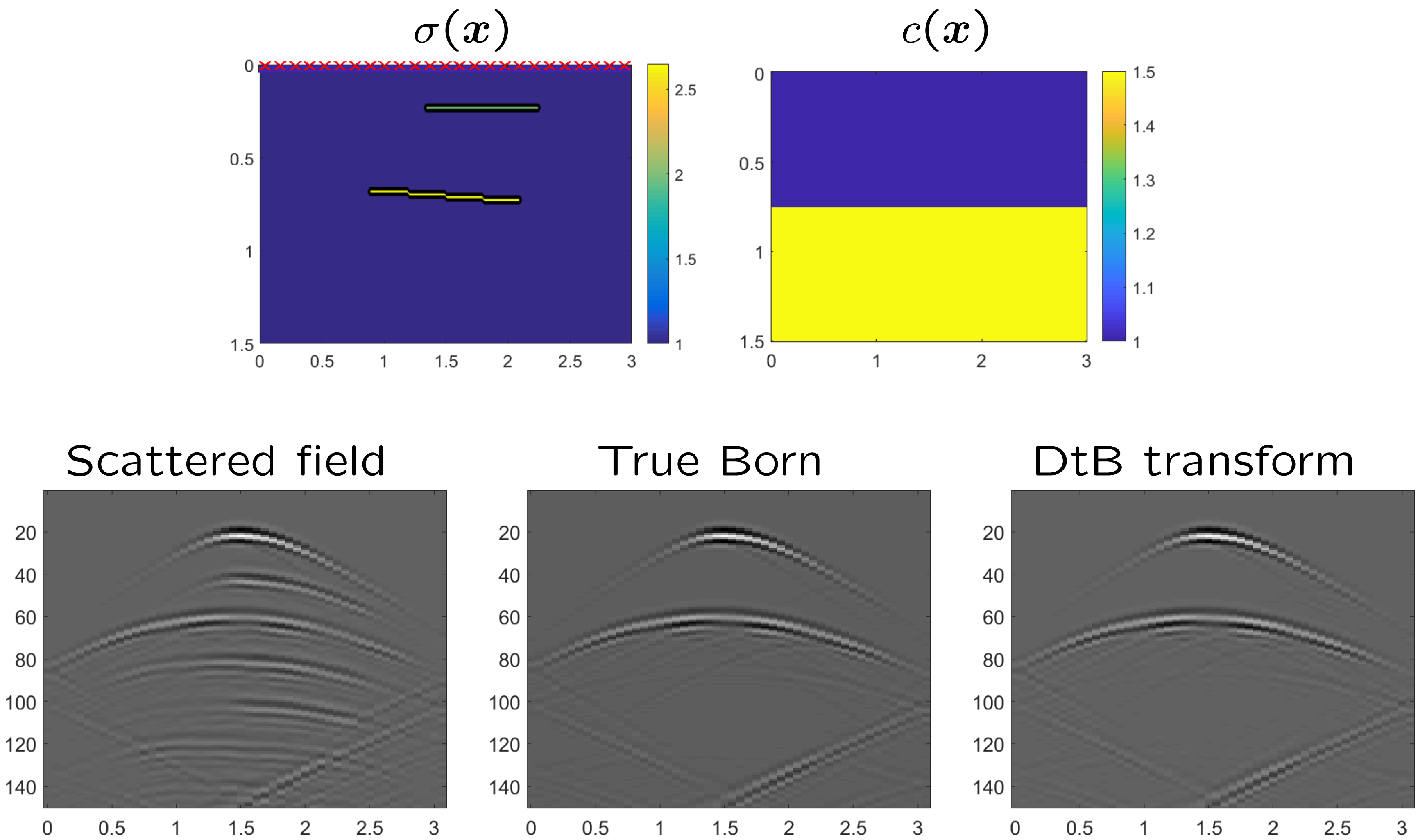
$$\boldsymbol{D}_k^{\text{Born}} := \boldsymbol{D}_{0,k} + (\boldsymbol{b}^{\text{ROM}})^T \frac{d}{d\varepsilon}\mathcal{T}_k(\mathscr{P}_{\varepsilon q}^{\text{ROM}})\Big|_{\varepsilon=0} \boldsymbol{b}^{\text{ROM}}, \quad 0 \le k \le 2n-1$$

DtB transformation: Sound waves 1-D



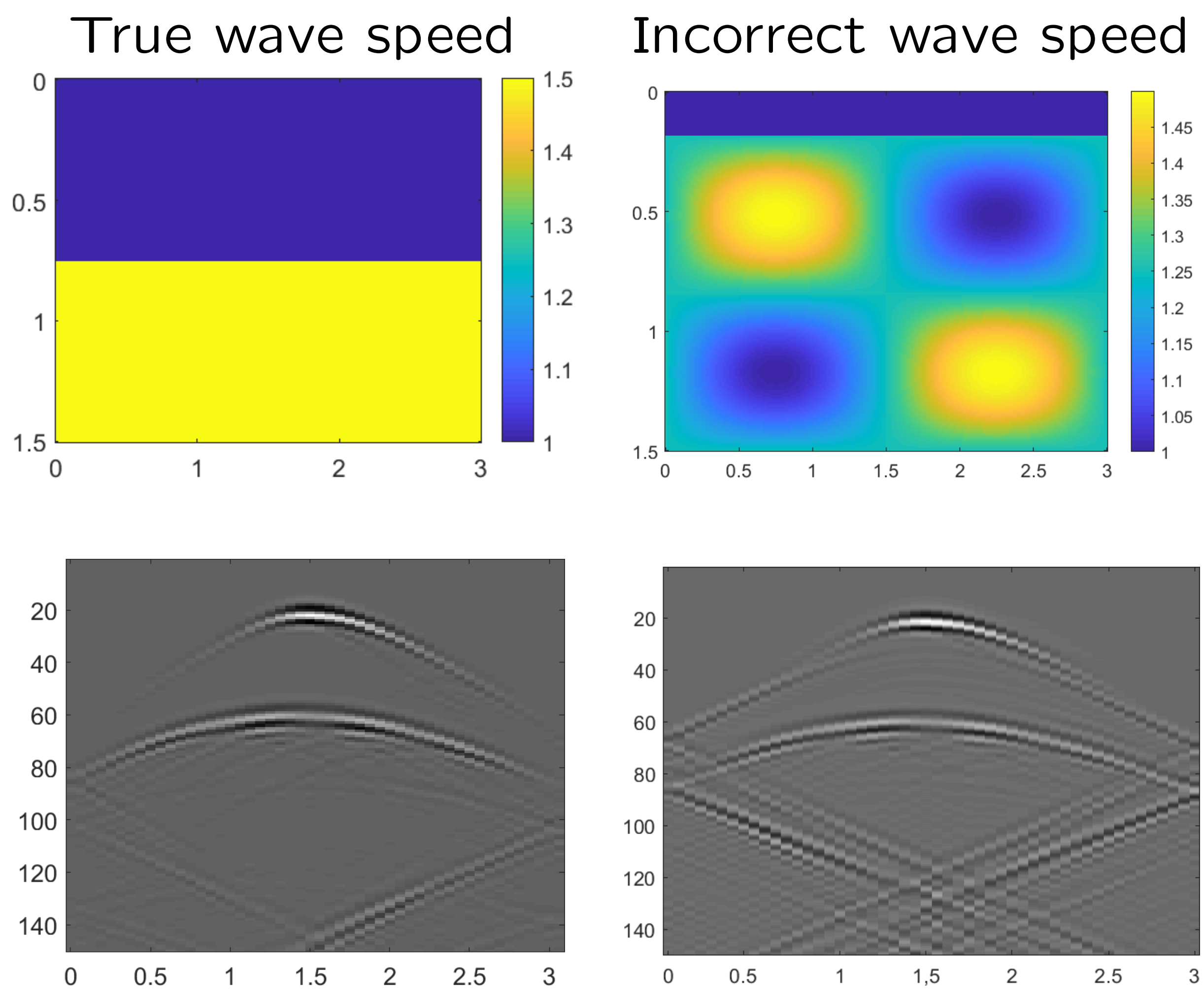






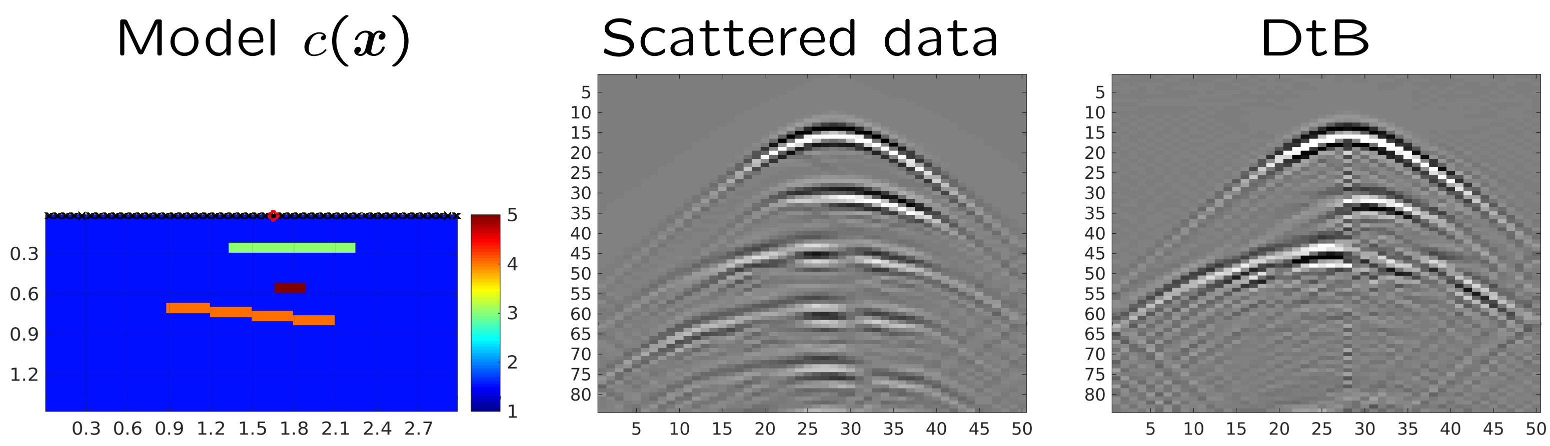
Axes in km. Colorbars show σ, c normalized by values at array.

Robustness of transformation to background velocity



Wrong velocity model induces artifacts due to domain boundary

DtB transformation: Sound waves - 2D



• Here we considered constant ρ and variable velocity. Only the constant background c_o is assumed known.

• Note how the echo from small reflector, masked by a multiple, is revealed by the DtB transformation.

Results for 2-D isotropic elasticity are in our paper.

Quantitative inversion: 2 possibilities

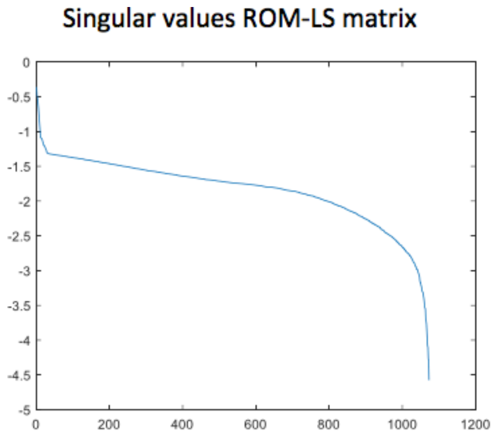
- Use DtB output in linear least-squares Born data fit:

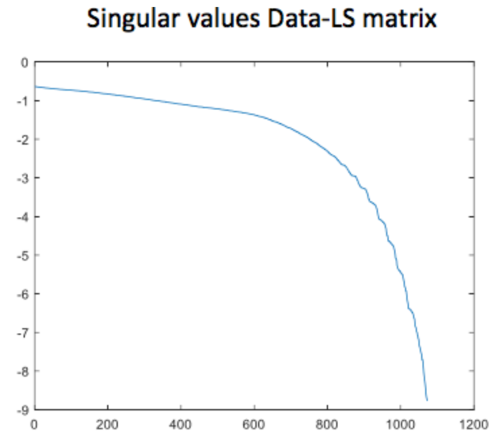
$$q = \text{arg min}_{q^s} \sum_{k=0}^{2n-1} \|\boldsymbol{D}^{\text{Born}} - F^{\text{Born}}(q^s)\|_F^2$$

- Match ROM instead. Since $\mathcal{L}_q^{\text{ROM}} \approx$ affine in $q(x) \approx \sum_j q_j \phi_j(x)$

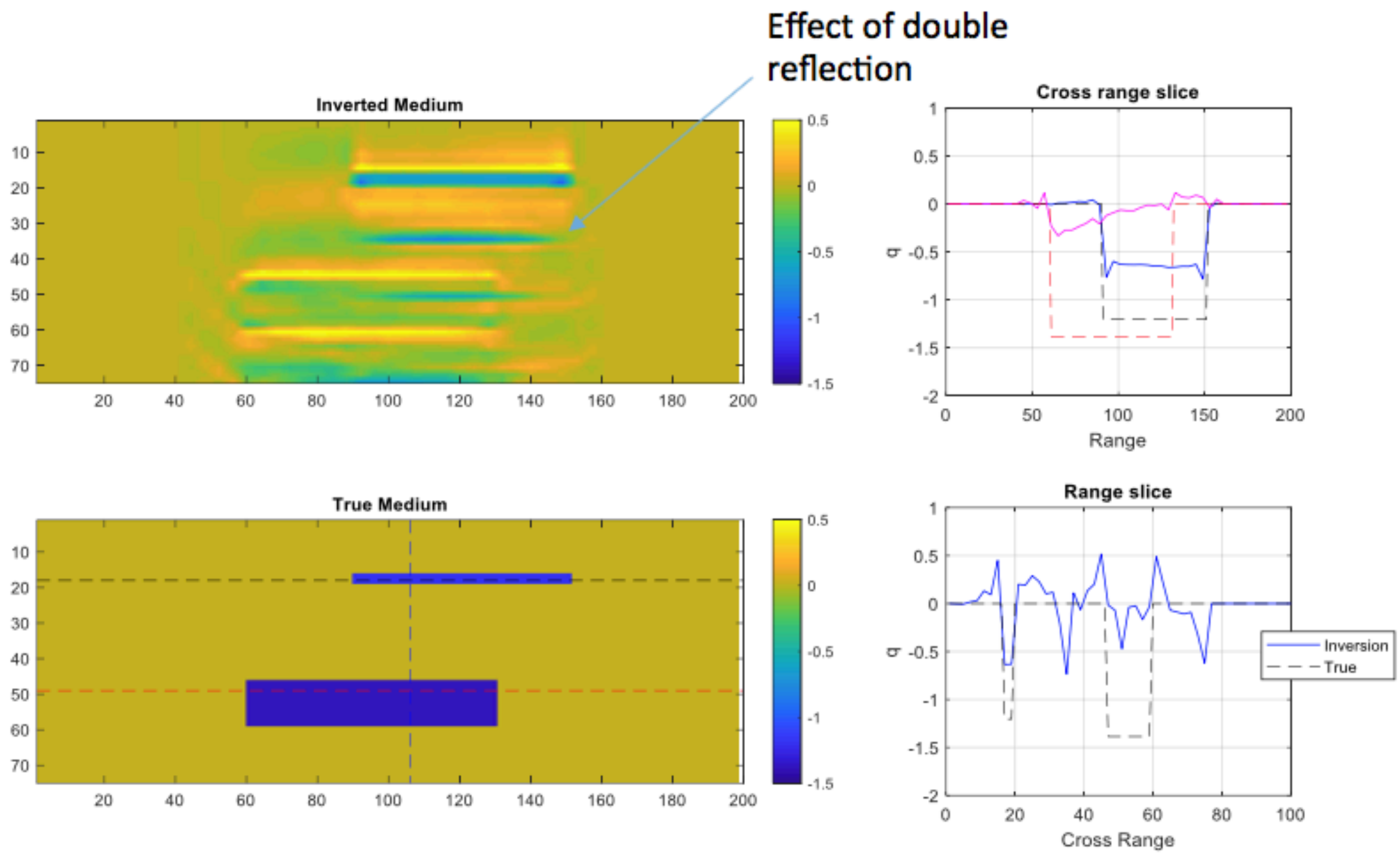
$$q = \text{arg min}_{q^s} \|\mathcal{L}_{q^s}^{\text{ROM}} - \mathcal{L}_q^{\text{ROM}}\|_F^2, \qquad \mathcal{L}_{q^s}^{\text{ROM}} = \mathcal{L}_0^{\text{ROM}} + \sum_j q_j^s \left[\mathcal{L}_{\phi_j}^{\text{ROM}} - \mathcal{L}_0^{\text{ROM}}\right]$$

Grid from $\mathcal{L}_0^{\text{ROM}}(\mathcal{L}_0^{\text{ROM}})^T$ (tridiagonal matrix discretization of Δ)

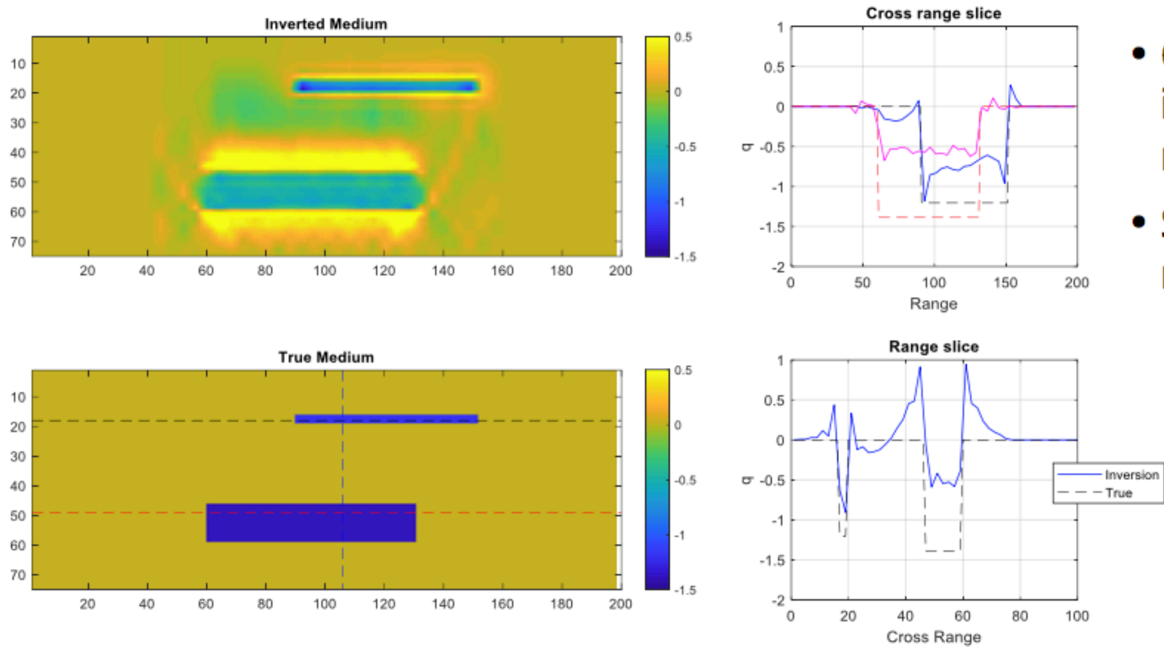




Quantitative inversion

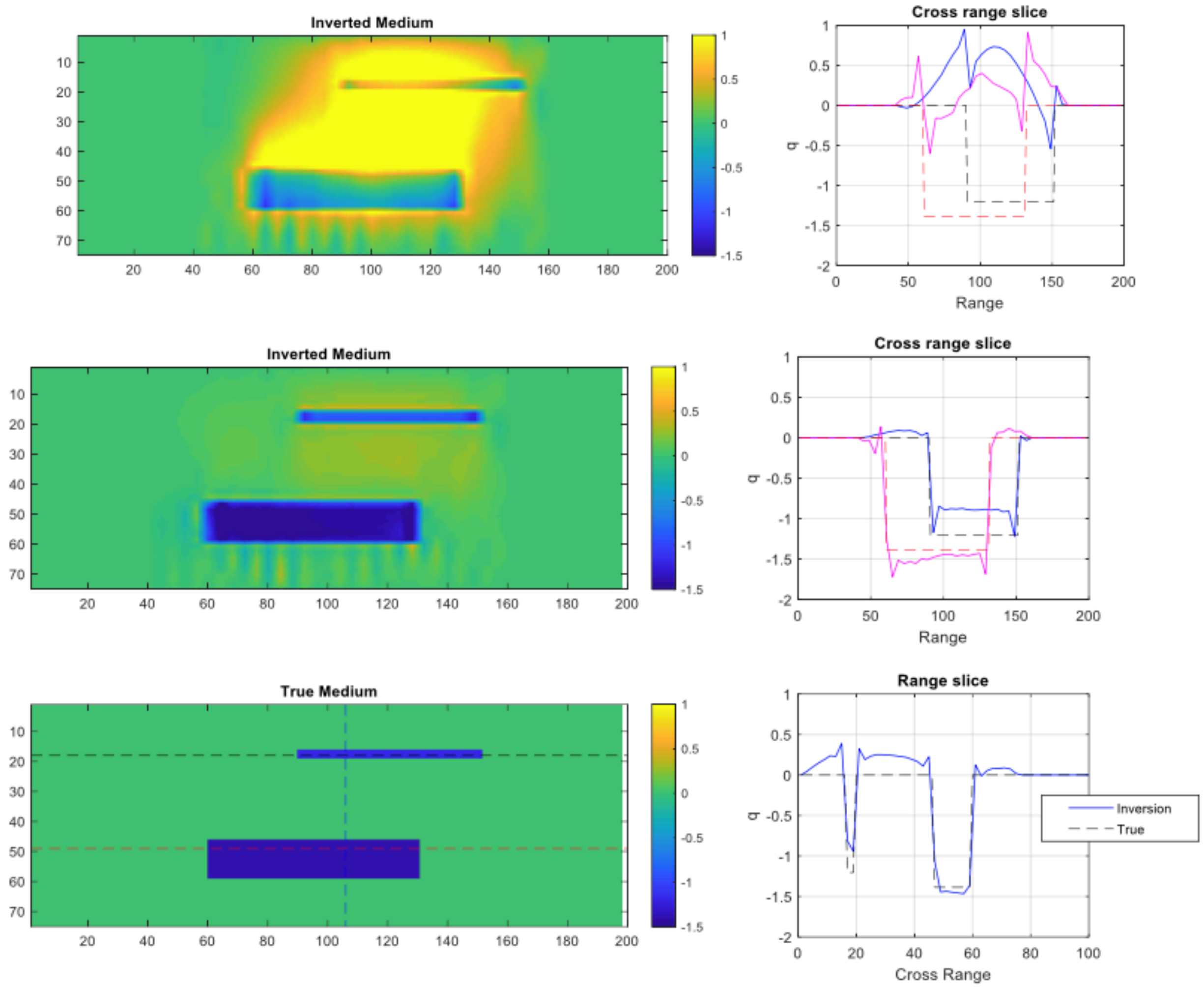


Linear LS data fit without the DtB transformation.



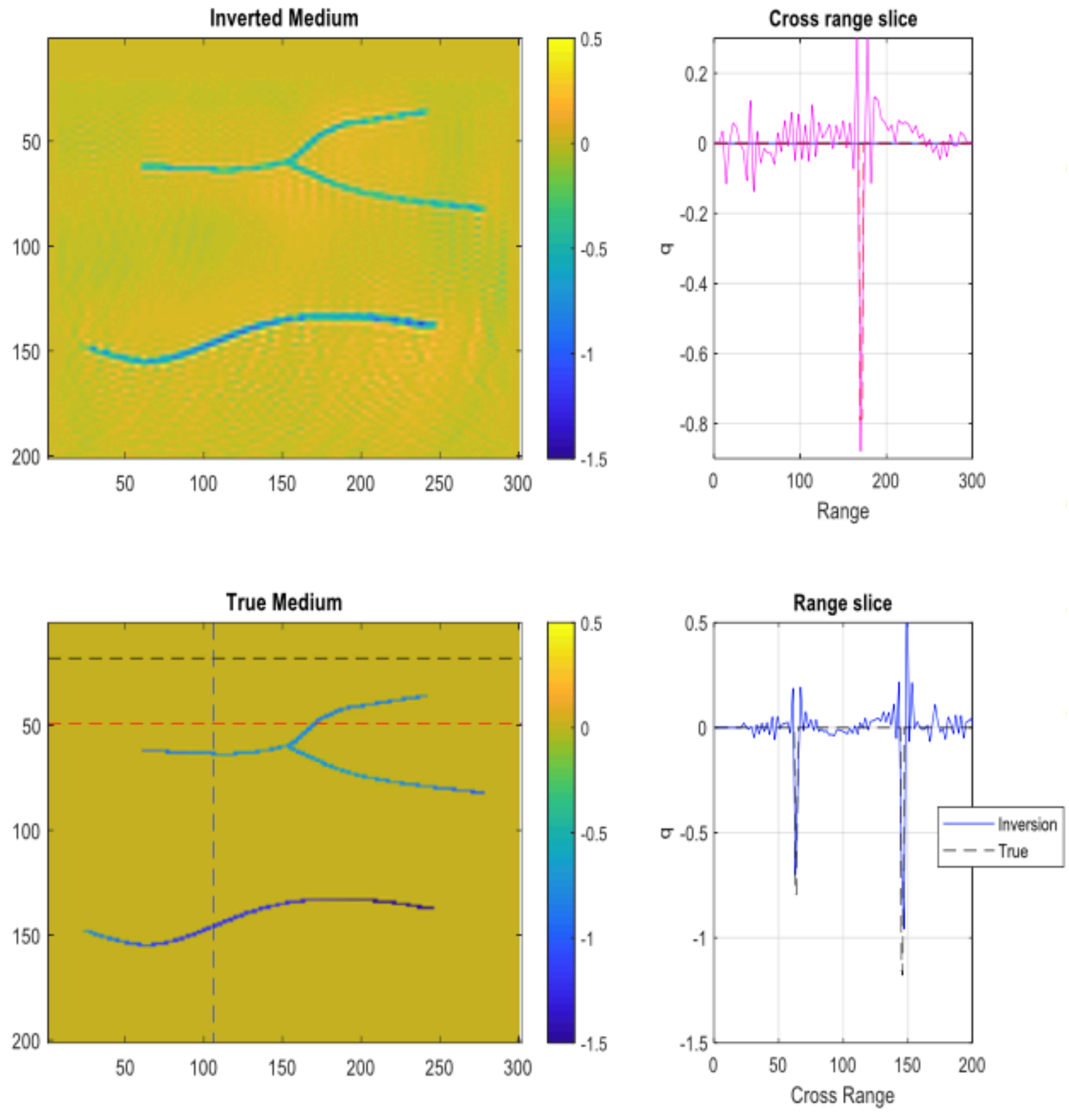
- Can possibly be improved with regularization
- Sensitive to regularization

Linear LS data fit with the DtB transformation.



Iteration 1 and 6 (top and middle) and true medium bottom.

Quantitative inversion: ROM match (iteration 3)



Conclusions

• We introduced a linear algebraic algorithm for transforming the scattered wave measured by an active array of sensors to the single scattering (Born) approximation which is linear in the unknown reflectivity.

• We showed that ROM can be used for quantitative inversion.

Lots left to do:

• Synthetic aperture setup; transmission setup; **time harmonic waves**, **anisotropic and attenuating media**.

• Approach can be extended to select multiple scattering effects.

References

• Borcea, Druskin, Mamonov, Zaslavsky, *Robust nonlinear processing of active array data in inverse scattering via truncated reduced order models*, Journal of Computational Physics 381, 2019, p. 1-26.

• Borcea, Druskin, Mamonov, Zaslavsky, *Untangling the nonlinearity in inverse scattering with data-driven reduced order models*, Inverse Problems 34 (6), 2018, p. 065008.

• Quantitative inversion paper in preparation: Borcea, Druskin, Mamonov, Zimmerling.

Sound waves. Constant density.

•Medium modeled by wave speed $c(\boldsymbol{x})$ and density ρ

$$(\partial_t^2 + A)p(t, \boldsymbol{x}; \boldsymbol{x}_s) = \partial_t f(t)\delta(\boldsymbol{x} - \boldsymbol{x}_s), \quad A = -c^2(\boldsymbol{x})\Delta$$

"Primary wave" defined by pressure and "dual wave" by velocity.

• Even time extension

$$p^{\text{even}}(t, \boldsymbol{x}; \boldsymbol{x}_s) = p(t, \boldsymbol{x}; \boldsymbol{x}_s) + p(-t, \boldsymbol{x}; \boldsymbol{x}_s) = \cos(t\sqrt{A})\widehat{f}(\sqrt{A})\delta(\boldsymbol{x} - \boldsymbol{x}_s)$$

• Data are

$$D_k^{(r,s)} = p^{\text{even}}(t_k, \boldsymbol{x}_r; \boldsymbol{x}_s) = \frac{1}{\rho}\left\langle \sqrt{\rho}\, c\, b^{(r)}, \cos\left(t_k\sqrt{A}\right)\sqrt{\rho}\, c\, b^{(s)}\right\rangle_{\frac{1}{c^2}}$$

"Sensor function" $b^{(s)}(\boldsymbol{x})$ is defined* by $\sqrt{p^{\text{even}}(0, \boldsymbol{x}; \boldsymbol{x}_s)}$ and is localized near $\boldsymbol{x}_s$.

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* $\widehat{f} \geq 0$ can be achieved by convolution of echoes with time reversed pulse.

- Equivalently, $D_k^{(r,s)} = \frac{1}{\rho}\left\langle \sqrt{\rho}\, c\, b^{(r)}, p^{(s)}(t_k, \cdot)\right\rangle_{\frac{1}{c^2}}$ where

$$\partial_t \begin{pmatrix} p^{(s)}(t,\boldsymbol{x}) \\ -\mathbf{u}^{(s)}(t,\boldsymbol{x}) \end{pmatrix} = \begin{pmatrix} 0 & \rho c^2(\boldsymbol{x})\nabla\cdot \\ \frac{1}{\rho}\nabla & 0 \end{pmatrix} \begin{pmatrix} p^{(s)}(t,\boldsymbol{x}) \\ -\mathbf{u}^{(s)}(t,\boldsymbol{x}) \end{pmatrix}$$

with initial conditions

$$p^{(s)}(0,\boldsymbol{x}) = \sqrt{\rho}\, c(\boldsymbol{x})\, b^{(s)}(\boldsymbol{x}), \quad \mathbf{u}^{(s)}(0,\boldsymbol{x}) = \mathbf{0}.$$

- We need first order system with L_q affine in reflectivity $q(\boldsymbol{x})$.

- Let $c(\boldsymbol{x}) = c_o(\boldsymbol{x})\left[1 + q(\boldsymbol{x})\right]$ with unknown $q(\boldsymbol{x}) = \frac{c(\boldsymbol{x}) - c_o(\boldsymbol{x})}{c_o(\boldsymbol{x})}$

- "Primary wave" is $P^{(s)}(t,\boldsymbol{x}) = \frac{p^{(s)}(t,\boldsymbol{x})}{\sqrt{\rho}\, c(\boldsymbol{x})}$

- "Dual wave" is $\widehat{P}^{(s)}(t,\boldsymbol{x}) = -\sqrt{\rho}\,\mathbf{u}^{(s)}(t,\boldsymbol{x})$

- First order system becomes

$$\partial_t \begin{pmatrix} P^{(s)}(t,\boldsymbol{x}) \\ \widehat{P}^{(s)}(t,\boldsymbol{x}) \end{pmatrix} = \begin{pmatrix} 0 & -L_q \\ L_q^T & 0 \end{pmatrix} \begin{pmatrix} P^{(s)}(t,\boldsymbol{x}) \\ \widehat{P}^{(s)}(t,\boldsymbol{x}) \end{pmatrix}$$

with initial conditions $P^{(s)}(0,\boldsymbol{x}) = b^{(s)}(\boldsymbol{x})$, $\widehat{P}^{(s)}(0,\boldsymbol{x}) = 0$.

- The first order operator is

$$L_q \widehat{P}^{(s)}(t,\boldsymbol{x}) = -[1 + q(\boldsymbol{x})] c_o(\boldsymbol{x}) \nabla \cdot \widehat{P}^{(s)}(t,\boldsymbol{x}).$$

- Data are, for $1 \leq r, s \leq m$ and $t_k = k\tau$, with $0 \leq k \leq 2n-1$

$$D_k^{(r,s)} = \left\langle b^{(r)}, P^{(s)}(t_k,\cdot) \right\rangle = \left\langle b^{(r)}, \cos\left(t_k \sqrt{L_q L_q^T}\right) b^{(s)} \right\rangle$$