Reduced Order Models for Quantitative Imaging with Diffusive Fields and Waves

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Motivation and overview

- Develop a **unified framework** for **quantitative imaging (inversion)** of PDE coefficient from boundary data based on **reduced order models (ROM)**
- Under **appropriate parametrization** of PDE, the ROM is **approximately affine** in the unknown coefficient
- ROM computation transforms the **nonlinear** imaging problem to an **approximately linear** one!
- Can be solved either **directly** or in a **very few iterations**
- **Data fit** step is **separated** from imaging step, allows for a separate **flexible regularization** of both
- Admits both **time and frequency domain** formulations

Forward model: diffusion equation

- First, consider an **inverse problem** for coefficient q of diffusion equation in the **frequency domain**

$$-\Delta u_s(\mathbf{x};\omega) + q(\mathbf{x})u_s(\mathbf{x};\omega) + \omega u_s(\mathbf{x};\omega) = b_s(\mathbf{x}), \quad \mathbf{x} \in \Omega$$

  driven by sources $b_s(\mathbf{x})$, $s = 1, \ldots, m$, located near $\partial\Omega$, from measurements at **collocated sensors** of

$$F_{rs}(\omega) = \langle b_r, u_s(\,\cdot\,;\omega)\rangle = \int_\Omega b_r(\mathbf{x})u_s(\mathbf{x};\omega)d\mathbf{x}, \quad \omega \geq 0,$$

  where $r, s = 1, \ldots, m$

- That is, the **response** of the system is $\mathbf{F}(\omega)$, a **symmetric** $m \times m$ matrix function of frequency

Quantitative Imaging Problem (QIP)

- For technical reasons we measure both $\mathbf{F}(\omega)$ and its derivative at n frequencies
$$\mathcal{D}_q = \left\{ \mathbf{F}(\omega_k), \frac{\partial \mathbf{F}}{\partial \omega}(\omega_k) \right\}_{k=1}^{n}$$

- The **Quantitative Imaging Problem (QIP)** is an inverse problem of estimating $q(\mathbf{x})$, $\mathbf{x} \in \Omega$ quantitatively from $\mathcal{D}_q$

- QIP is **severely ill-posed** due to instability of the mapping from $\mathcal{D}_q$ to q

Matrix-vector formulation

- Assemble solutions and sources into **row-vector-valued** functions

$$\begin{aligned} \mathbf{u}(\mathbf{x};\omega) &= [u_1(\mathbf{x};\omega), u_2(\mathbf{x};\omega), \ldots, u_m(\mathbf{x};\omega)], \\ \mathbf{b}(\mathbf{x}) &= [b_1(\mathbf{x}), b_2(\mathbf{x}), \ldots, b_m(\mathbf{x})]. \end{aligned}$$

- Forward problem becomes

$$(\mathbf{A}_q + \omega \mathbf{I})\mathbf{u}(\mathbf{x};\omega) = \mathbf{b}(\mathbf{x}),$$

with $\mathbf{A}_q = -\Delta + q(\mathbf{x})\mathbf{I}$

- Define "matrix product" of row-vector-valued functions

$$\mathbf{v}^T\mathbf{w} = \begin{bmatrix} \langle v_1, w_1 \rangle & \ldots & \langle v_1, w_N \rangle \\ \vdots & \ddots & \vdots \\ \langle v_M, w_1 \rangle & \ldots & \langle v_M, w_N \rangle \end{bmatrix} \in \mathbb{R}^{M \times N},$$

Reduced order model (ROM)

- In matrix form **response** becomes

$$\mathbf{F}(\omega) = \mathbf{b}^T \mathbf{u}(\,\cdot\,;\omega) = \mathbf{b}^T[(\mathbf{A}_q + \omega \mathbf{I})^{-1}\mathbf{b}] \in \mathbb{R}^{m \times m}$$

- We seek a **reduced order model (ROM)** $\widetilde{\mathbf{A}}_q \in \mathbb{R}^{mn \times mn}$, $\widetilde{\mathbf{b}} \in \mathbb{R}^{mn \times m}$ with a **transfer function**

$$\widetilde{\mathbf{F}}(\omega) = \widetilde{\mathbf{b}}^T(\widetilde{\mathbf{A}}_q + \omega \mathbf{I}_{mn})^{-1}\widetilde{\mathbf{b}} \in \mathbb{R}^{m \times m}$$

that **interpolates the data**

$$\widetilde{\mathbf{F}}(\omega_k) = \mathbf{F}(\omega_k), \quad \frac{\partial \widetilde{\mathbf{F}}}{\partial \omega}(\omega_k) = \frac{\partial \mathbf{F}}{\partial \omega}(\omega_k), \quad k = 1, \ldots, n$$

Projection-type ROM

- To satisfy **interpolation conditions** the ROM must be of **projection type**

$$\widetilde{\mathbf{A}}_q = \mathbf{V}^T[\mathbf{A}_q\mathbf{V}] = \mathbf{V}^T[\mathbf{A}_q\mathbf{v}_1, \ldots, \mathbf{A}_q\mathbf{v}_n], \quad \widetilde{\mathbf{b}} = \mathbf{V}^T\mathbf{b}$$

  where "orthogonal matrix" ($\mathbf{V}^T\mathbf{V} = \mathbf{I}_{mn}$) row-vector-valued function

$$\mathbf{V}(\mathbf{x}) = [\mathbf{v}_1(\mathbf{x}), \ldots, \mathbf{v}_n(\mathbf{x})]$$

  spans the **projection subspace**
- Define **solution snapshots**

$$\mathbf{u}_k(\mathbf{x}) = \mathbf{u}(\mathbf{x}; \omega_k), \quad k = 1, \ldots, n$$

  and assemble them into row-vector-valued function

$$\mathbf{U}(\mathbf{x}) = [\mathbf{u}_1(\mathbf{x}), \ldots, \mathbf{u}_n(\mathbf{x})]$$

Projection-type ROM

- To satisfy **interpolation conditions** the **projection subspace** must be the block rational Krylov subspace

$$\text{colspan}(\mathbf{V}) = \mathcal{K}_n(\mathbf{A}_q, \mathbf{b}) = \text{colspan}(\mathbf{U})$$

- If we knew snapshots $\mathbf{u}_k(\mathbf{x})$ and operator $\mathbf{A}_q$ in the **whole domain** Ω, we could **orthogonalize** them to find $\mathbf{V}(\mathbf{x})$ to compute $\widetilde{\mathbf{A}}_q = \mathbf{V}^T[\mathbf{A}_q\mathbf{V}]$. But we know **neither**!

- Can we compute the ROM from the data $\mathcal{D}_q$ only? Can we have a **data-driven ROM**?

Data-driven ROM

- Viewing projection in **Galerkin** framework, define **mass and stiffness matrices**

$$\mathbf{M} = \mathbf{U}^T\mathbf{U} \in \mathbb{R}^{mn\times mn} \quad \text{and} \quad \mathbf{S} = \mathbf{U}^T[\mathbf{A}_q\mathbf{U}] \in \mathbb{R}^{mn\times mn},$$

  with **blocks**

$$\mathbf{M}_{jk} = \mathbf{u}_j^T\mathbf{u}_k \in \mathbb{R}^{m\times m}, \quad \mathbf{S}_{jk} = \mathbf{u}_j^T[\mathbf{A}_q\mathbf{u}_k] \in \mathbb{R}^{m\times m}, \quad j,k = 1,\dots,n$$

- Then, **M** and **S** can be obtained from the data as

$$\begin{aligned}
\mathbf{M}_{jk} &= \frac{1}{\omega_k - \omega_j}(\mathbf{F}(\omega_j) - \mathbf{F}(\omega_k)), \quad j \neq k, \\
\mathbf{M}_{kk} &= -\frac{\partial \mathbf{F}}{\partial \omega}(\omega_k), \\
\mathbf{S}_{jk} &= \frac{1}{\omega_k - \omega_j}(\omega_j\mathbf{F}(\omega_j) - \omega_k\mathbf{F}(\omega_k)), \quad j \neq k, \\
\mathbf{S}_{kk} &= \mathbf{F}(\omega_k) + \omega_k\frac{\partial \mathbf{F}}{\partial \omega}(\omega_k)
\end{aligned}$$

Extracting q from ROM

- If mass matrix is known, snapshots (not known!) can be orthogonalized $\mathbf{V} = \mathbf{U}\mathbf{M}^{-1/2}$

- Then the ROM is

$$\begin{aligned} \widetilde{\mathbf{A}}'_q &= \mathbf{V}^T[\mathbf{A}_q\mathbf{V}] = \mathbf{M}^{-1/2}\mathbf{U}^T[\mathbf{A}_q\mathbf{U}]\mathbf{M}^{-1/2} = \mathbf{M}^{-1/2}\mathbf{S}\mathbf{M}^{-1/2} \\ \widetilde{\mathbf{b}}' &= \mathbf{V}^T\mathbf{b} = \mathbf{M}^{-1/2}\mathbf{U}^T\mathbf{b} = \mathbf{M}^{-1/2}[\mathbf{F}(\omega_1), \ldots, \mathbf{F}(\omega_n)]^T \end{aligned}$$

- How to use ROM to estimate $q(\mathbf{x})$?

- Observation: $\mathbf{A}_q = -\Delta + q(\mathbf{x})\mathbf{I}$ is **affine in** q, thus perturbation $\delta\mathbf{A} = \mathbf{A}_q - \mathbf{A}_{q_0}$ is **linear in** $\delta q = q - q_0$!

- **Conjecture: ROM perturbation is approximately linear in** δq

- For conjecture to work, ROM must be in a **special form**, need one more transformation

Block Lanczos transform

- ROM perturbation is approximately linear in q if ROM corresponds to a **finite-difference discretization** of $\mathbf{A}_q$
- Perform **block Lanczos** process

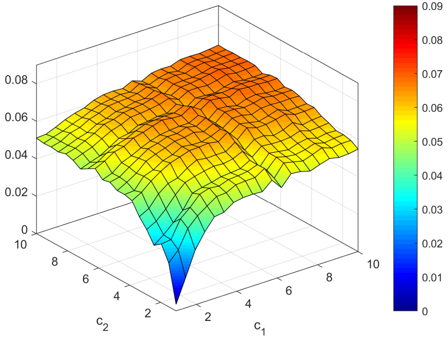
$$\widetilde{\mathbf{A}}_q = \mathbf{Q}^T \widetilde{\mathbf{A}}'_q \mathbf{Q}, \quad \widetilde{\mathbf{b}} = \mathbf{Q}^T \widetilde{\mathbf{b}}'$$

to transform the ROM $(\widetilde{\mathbf{A}}'_q, \widetilde{\mathbf{b}}')$ to **block-tridiagonal form**

$$\widetilde{\mathbf{A}}_q = \begin{bmatrix} \boldsymbol{\alpha}_1 & \boldsymbol{\beta}_2 & \mathbf{0} & \dots & \mathbf{0} \\ \boldsymbol{\beta}_2^T & \boldsymbol{\alpha}_2 & \boldsymbol{\beta}_3 & \ddots & \vdots \\ \mathbf{0} & \boldsymbol{\beta}_3^T & \boldsymbol{\alpha}_3 & \ddots & \mathbf{0} \\ \vdots & \ddots & \ddots & \ddots & \boldsymbol{\beta}_n \\ \mathbf{0} & \dots & \mathbf{0} & \boldsymbol{\beta}_n^T & \boldsymbol{\alpha}_n \end{bmatrix} \in \mathbb{R}^{mn \times mn}, \quad \widetilde{\mathbf{b}} = \begin{bmatrix} \boldsymbol{\beta}_1 \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{bmatrix} \in \mathbb{R}^{mn \times m}$$

- Then, $\delta\widetilde{\mathbf{A}} = \widetilde{\mathbf{A}}_q - \widetilde{\mathbf{A}}_{q_0}$ is **approximately linear** in $\delta q = q - q_0$!

Numerical check: approximate linearity of $\delta\widetilde{\mathbf{A}}$ w.r.t. q

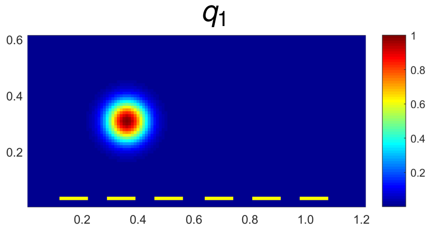


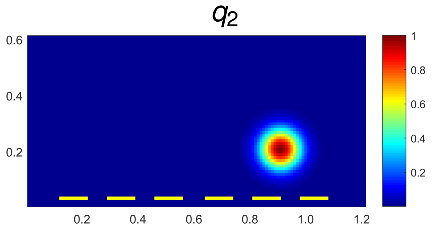
- Left: **approximation error** of

$$\widetilde{\mathbf{A}}_{c_1 q_1 + c_2 q_2} - \widetilde{\mathbf{A}}_{q_0} \approx$$
$$\approx c_1(\widetilde{\mathbf{A}}_{q_1} - \widetilde{\mathbf{A}}_{q_0}) + c_2(\widetilde{\mathbf{A}}_{q_2} - \widetilde{\mathbf{A}}_{q_0})$$

as a function of c_1 and c_2

- Plateaus at around 7%





Quantitative imaging method

1. Choose a **background** $q_0(\mathbf{x})$
2. Choose a **basis** ϕ_i, $i = 1, \ldots, N$ to expand

$$\delta q(\mathbf{x}) = q(\mathbf{x}) - q_0(\mathbf{x}) = \sum_{i=1}^{N} g_i \phi_i(\mathbf{x})$$

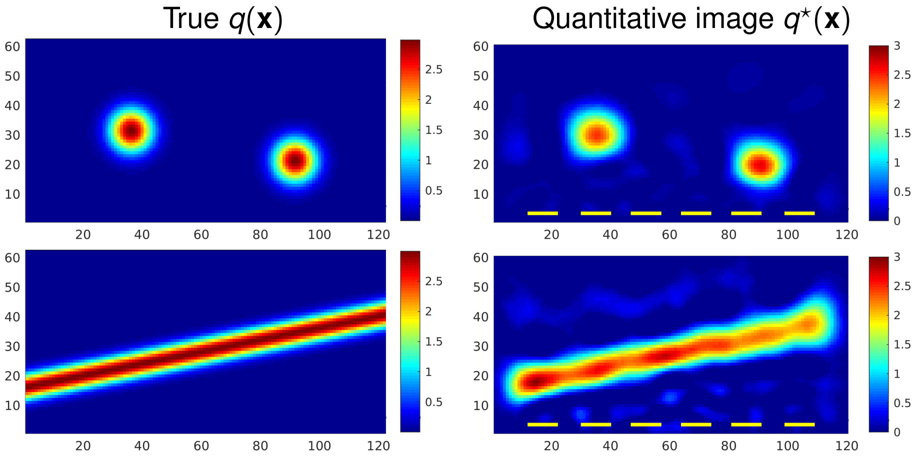
3. Compute the expansion coefficient vector $\mathbf{g} = [g_1, \ldots, g_N]^T$ by solving the **linear least squares** problem

$$[\mathrm{vec}(\widetilde{\mathbf{A}}_{\phi_1} - \widetilde{\mathbf{A}}_{q_0}) \ldots \mathrm{vec}(\widetilde{\mathbf{A}}_{\phi_N} - \widetilde{\mathbf{A}}_{q_0})]\mathbf{g} = \mathrm{vec}(\widetilde{\mathbf{A}}_q - \widetilde{\mathbf{A}}_{q_0}) \qquad (1)$$

4. Form the **quantitative image** $q^\star(\mathbf{x}) = q_0(\mathbf{x}) + \sum_{i=1}^{N} g_i \phi_i(\mathbf{x})$

- Only the right hand side of (1) depends on the data via $\widetilde{\mathbf{A}}_q$
- Left hand side of (1) can be **precomputed** for a fixed Ω and q_0

Numerical results



- Quantitative images from measurements at $m = 6$ extended sensors (yellow) at $n = 4$ frequencies

Imaging with (acoustic) waves

- Similar approach works for **imaging with waves** from **time-domain data**
- Need to separate **kinematics** (wave speed $c(\mathbf{x})$) from **reflective behavior** (acoustic impedance $\sigma(\mathbf{x})$):

$$\partial_t^2 u_s(\mathbf{x}; t) - \sigma(\mathbf{x}) c(\mathbf{x}) \nabla \cdot \left[\frac{c(\mathbf{x})}{\sigma(\mathbf{x})} \nabla u_s(\mathbf{x}; t) \right] = f(t) \delta(\mathbf{x} - \mathbf{x}_s),$$

  as before, $s = 1, \ldots, m$ are source indices
- Time domain data $\mathbf{F}(t) \in \mathbb{R}^{m \times m}$ with entries

$$F_{rs}(t) = \int_\Omega \delta(\mathbf{x} - \mathbf{x}_r) u_s(\mathbf{x}; t) d\mathbf{x} = u_s(\mathbf{x}_r; t), \quad r, s = 1, \ldots, m,$$

  sampled discretely in time $\mathbf{F}(k\tau)$, $k = 0, 1, \ldots, 2n - 1$
- Assume **kinematics** $c(\mathbf{x})$ **is known**, seek **image of** $\sigma(\mathbf{x})$

First order form

- Transform to **first order form** via **Liouville transformation**
$$\begin{bmatrix} 0 & -\mathbf{L}_q \\ \mathbf{L}_q & 0 \end{bmatrix} \begin{bmatrix} u_s(\mathbf{x};t) \\ \widehat{u}_s(\mathbf{x};t) \end{bmatrix} = \frac{\partial}{\partial t} \begin{bmatrix} u_s(\mathbf{x};t) \\ \widehat{u}_s(\mathbf{x};t) \end{bmatrix} - \begin{bmatrix} f(t)\delta(\mathbf{x}-\mathbf{x}_s) \\ 0 \end{bmatrix},$$
where
$$\begin{aligned} \mathbf{L}_q &= -\sqrt{c(\mathbf{x})}\nabla \cdot \sqrt{c(\mathbf{x})} + \frac{c(\mathbf{x})}{2}\nabla q(\mathbf{x}) \cdot, \\ \mathbf{L}_q^T &= \sqrt{c(\mathbf{x})}\nabla \sqrt{c(\mathbf{x})} + \frac{c(\mathbf{x})}{2}\nabla q(\mathbf{x}), \end{aligned}$$
with **reflectivity** $q(\mathbf{x}) = \log \sigma(\mathbf{x})$
- Observe $\mathbf{L}_q$, $\mathbf{L}_q^T$ are **affine in** q, same as $\mathbf{A}_q$ before!
- Data-driven ROM $\widetilde{\mathbf{L}}_q$ of $\mathbf{L}_q$ is **approximately affine** in q
- This approximation is worse than that for diffusion equation, **iteration may be needed**

Quantitative imaging with waves

1. Choose an **initial guess** $q_0^\star(\mathbf{x})$, fix the wave speed $c(\mathbf{x})$
2. Choose a **basis** ϕ_i, $i = 1, \ldots, N$ for expansion

$$\delta q(\mathbf{x}) = \sum_{i=1}^{N} g_i \phi_i(\mathbf{x})$$

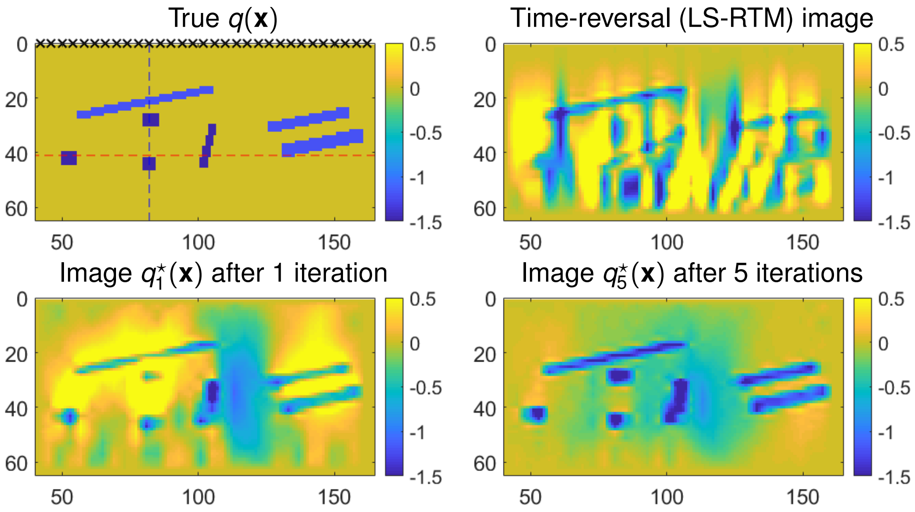
3. For $k = 1, 2, \ldots$ **iterate**
   - Find expansion coefficient vector $\mathbf{g}^k$ by solving the **linear least squares** problem

$$[\text{vec}(\widetilde{\mathbf{L}}_{\phi_1} - \widetilde{\mathbf{L}}_{q^\star_{k-1}}) \ldots \text{vec}(\widetilde{\mathbf{L}}_{\phi_N} - \widetilde{\mathbf{L}}_{q^\star_{k-1}})]\mathbf{g}^k = \text{vec}(\widetilde{\mathbf{L}}_q - \widetilde{\mathbf{L}}_{q^\star_{k-1}})$$

   - **Update** the **quantitative image** $q_k^\star(\mathbf{x}) = q_{k-1}^\star(\mathbf{x}) + \sum_{i=1}^{N} g_i^k \phi_i(\mathbf{x})$

- Above iteration **converges very quickly**, typically $3 - 5$ iterations are sufficient

Numerical results



- Constant wave speed, lots of **multiple reflections**, $m = 50$ sensors (crosses, not all shown)

Conclusions and future work

- Unified **ROM-based** framework for quantitative imaging of PDE coefficients
- Transforms **diffusion** inversion to **essentially a linear problem**: converges in a single iteration
- Greatly improves **imaging with waves** by eliminating the adverse effects of **multiple scattering**
- **Robust** version exists: spectral truncation of the mass matrix

Future work:

- **Vectorial** imaging problems (elasticity, electromagnetics)
- **Partial data** case when not all entries of **F** are measured, including non-collocated sources/receivers, moving sensors, etc.

References

1. *Reduced order models for spectral domain inversion: Embedding into the continuous problem and generation of internal data*, L. Borcea, V. Druskin, A.V. Mamonov, S. Moskow, M. Zaslavsky, **Preprint: arXiv:1909.06460 [math.NA]**.
2. *Reduced Order Model Approach to Inverse Scattering*, L. Borcea, V. Druskin, A.V. Mamonov, M. Zaslavsky, J. Zimmerling, **Preprint: arXiv:1910.13014 [math.NA]**.
3. *Direct, quantitative imaging of absorption coefficient from frequency domain data*, L. Borcea, V. Druskin, A.V. Mamonov, S. Moskow, M. Zaslavsky, **In preparation**.

Related prior work:

1. *Direct, nonlinear inversion algorithm for hyperbolic problems via projection-based model reduction*, V. Druskin, A. Mamonov, A.E. Thaler and M. Zaslavsky, **SIAM Journal on Imaging Sciences 9(2):684–747, 2016**
2. *A nonlinear method for imaging with acoustic waves via reduced order model backprojection*, V. Druskin, A.V. Mamonov, M. Zaslavsky, **SIAM Journal on Imaging Sciences, 11(1):164–196, 2018**
3. *Untangling the nonlinearity in inverse scattering with data-driven reduced order models*, L. Borcea, V. Druskin, A.V. Mamonov, M. Zaslavsky, **Inverse Problems 34(6):065008, 2018**
4. *Robust nonlinear processing of active array data in inverse scattering via truncated reduced order models*, L. Borcea, V. Druskin, A.V. Mamonov, M. Zaslavsky, **Journal of Computational Physics 381:1-26, 2019**