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

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

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

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

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

That is, the **response** of the system is $F(\omega)$, a **symmetric** $m \times m$ matrix function of frequency
For technical reasons we measure both $F(\omega)$ and its derivative at $n$ frequencies

$$\mathcal{D}_q = \left\{ F(\omega_k), \frac{\partial F}{\partial \omega}(\omega_k) \right\}_{k=1}^n$$

The **Quantitative Imaging Problem (QIP)** is an inverse problem of estimating $q(x), x \in \Omega$ 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

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

- Forward problem becomes

\[
(A_q + \omega \mathbf{I})\mathbf{u}(\mathbf{x}; \omega) = \mathbf{b}(\mathbf{x}),
\]

with \( A_q = -\Delta + q(\mathbf{x})\mathbf{I} \)

- Define “matrix product” of row-vector-valued functions

\[
\begin{bmatrix}
\langle v_1, w_1 \rangle & \cdots & \langle v_1, w_N \rangle \\
\vdots & \ddots & \vdots \\
\langle v_M, w_1 \rangle & \cdots & \langle v_M, w_N \rangle
\end{bmatrix} \in \mathbb{R}^{M \times N},
\]
Reduced order model (ROM)

- In matrix form \textbf{response} becomes

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

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

\[
\tilde{F}(\omega) = \tilde{b}^T(\tilde{A}_q + \omega I_{mn})^{-1} \tilde{b} \in \mathbb{R}^{m \times m}
\]

that \textbf{interpolates the data}

\[
\tilde{F}(\omega_k) = F(\omega_k), \quad \frac{\partial \tilde{F}}{\partial \omega}(\omega_k) = \frac{\partial F}{\partial \omega}(\omega_k), \quad k = 1, \ldots, n
\]
Projection-type ROM

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

\[
\tilde{A}_q = V^T[A_qV] = V^T[A_qv_1, \ldots, A_qv_n], \quad \tilde{b} = V^Tb
\]

where “orthogonal matrix” \((V^TV = I_{mn})\) row-vector-valued function

\[
V(x) = [v_1(x), \ldots, v_n(x)]
\]

spans the **projection subspace**

- Define **solution snapshots**

\[
u_k(x) = u(x; \omega_k), \quad k = 1, \ldots, n
\]

and assemble them into row-vector-valued function

\[
U(x) = [u_1(x), \ldots, u_n(x)]
\]
To satisfy **interpolation conditions** the **projection subspace** must be the block rational Krylov subspace

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

If we knew snapshots $u_k(x)$ and operator $A_q$ in the **whole domain** $\Omega$, we could **orthogonalize** them to find $V(x)$ to compute

$$\tilde{A}_q = V^T[A_q V]$$. 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

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

with blocks

\[ M_{jk} = u_j^T u_k \in \mathbb{R}^{m \times m}, \quad S_{jk} = u_j^T [A_q u_k] \in \mathbb{R}^{m \times m}, \quad j, k = 1, \ldots, n \]

- Then, \( M \) and \( S \) can be obtained from the data as

\[ M_{jk} = \frac{1}{\omega_k - \omega_j} (F(\omega_j) - F(\omega_k)), \quad j \neq k, \]

\[ M_{kk} = -\frac{\partial F}{\partial \omega}(\omega_k), \]

\[ S_{jk} = \frac{1}{\omega_k - \omega_j} (\omega_j F(\omega_j) - \omega_k F(\omega_k)), \quad j \neq k, \]

\[ S_{kk} = F(\omega_k) + \omega_k \frac{\partial F}{\partial \omega}(\omega_k) \]
Extracting $q$ from ROM

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

Then the ROM is

$$\begin{align*}
\tilde{A}'_q &= V^T[A_qV] = M^{-1/2}U^T[A_qU]M^{-1/2} = M^{-1/2}SM^{-1/2} \\
\tilde{b}' &= V^Tb = M^{-1/2}U^Tb = M^{-1/2}[F(\omega_1), \ldots, F(\omega_n)]^T
\end{align*}$$

How to use ROM to estimate $q(x)$?

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

Conjecture: ROM perturbation is approximately linear in $\delta q$

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 \( A_q \)
- Perform **block Lanczos** process

\[
\tilde{A}_q = Q^T \tilde{A}_q' Q, \quad \tilde{b} = Q^T \tilde{b}'
\]

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

\[
\tilde{A}_q = \begin{bmatrix}
\alpha_1 & \beta_2 & 0 & \ldots & 0 \\
\beta_2^T & \alpha_2 & \beta_3 & \ddots & \\
0 & \beta_3^T & \alpha_3 & \ddots & 0 \\
\vdots & \ddots & \ddots & \ddots & \beta_n \\
0 & \ldots & 0 & \beta_n^T & \alpha_n
\end{bmatrix} \in \mathbb{R}^{mn \times mn}, \quad \tilde{b} = \begin{bmatrix}
\beta_1 \\
0 \\
\vdots \\
0
\end{bmatrix} \in \mathbb{R}^{mn \times m}
\]

- Then, \( \delta \tilde{A} = \tilde{A}_q - \tilde{A}_{q_0} \) is **approximately linear** in \( \delta q = q - q_0 \)!
Numerical check: approximate linearity of $\delta \tilde{\mathbf{A}}$ w.r.t. $q$

- **Left:** approximation error of
  
  \[
  \tilde{\mathbf{A}} c_1 q_1 + c_2 q_2 - \tilde{\mathbf{A}} q_0 \approx \]
  
  \[
  c_1 (\tilde{\mathbf{A}} q_1 - \tilde{\mathbf{A}} q_0) + c_2 (\tilde{\mathbf{A}} q_2 - \tilde{\mathbf{A}} q_0)
  \]
  
  as a function of $c_1$ and $c_2$

- **Plateaus at around 7%**
Quantitative imaging method

1. Choose a **background** \( q_0(x) \)
2. Choose a **basis** \( \phi_i, i = 1, \ldots, N \) to expand

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

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

\[
[\text{vec}(\tilde{A}_{\phi_1} - \tilde{A}_{q_0}) \ldots \text{vec}(\tilde{A}_{\phi_N} - \tilde{A}_{q_0})]g = \text{vec}(\tilde{A}_q - \tilde{A}_{q_0}) \quad (1)
\]

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

- Only the right hand side of (1) depends on the data via \( \tilde{A}_q \)
- Left hand side of (1) can be **precomputed** for a fixed \( \Omega \) and \( q_0 \)
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 $c(x)$) from reflective behavior (acoustic impedance $\sigma(x)$):

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

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

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

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

- Transform to **first order form** via Liouville transformation

\[
\begin{bmatrix}
0 & -L_q \\
L_q & 0
\end{bmatrix}
\begin{bmatrix}
u_s(x; t) \\
\hat{u}_s(x; t)
\end{bmatrix} = \frac{\partial}{\partial t}
\begin{bmatrix}
u_s(x; t) \\
\hat{u}_s(x; t)
\end{bmatrix} - \begin{bmatrix} f(t)\delta(x - x_s) \\
0
\end{bmatrix},
\]

where

\[
L_q = -\sqrt{c(x)}\nabla \cdot \sqrt{c(x)} + \frac{c(x)}{2} \nabla q(x),
\]

\[
L^T_q = \sqrt{c(x)}\nabla \sqrt{c(x)} + \frac{c(x)}{2} \nabla q(x),
\]

with **reflectivity** \( q(x) = \log \sigma(x) \)

- Observe \( L_q, L^T_q \) are **affine in** \( q \), same as \( A_q \) before!

- Data-driven ROM \( \tilde{L}_q \) of \( L_q \) 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 $q_0^*(x)$, fix the wave speed $c(x)$
2. Choose a basis $\phi_i$, $i = 1, \ldots, N$ for expansion

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

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

\[
[\text{vec}(\tilde{L}_{\phi_1} - \tilde{L}_{q_{k-1}^*}) \ldots \text{vec}(\tilde{L}_{\phi_N} - \tilde{L}_{q_{k-1}^*})] g^k = \text{vec}(\tilde{L}_q - \tilde{L}_{q_{k-1}^*})
\]

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

   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


Related prior work:


