Reduced order models for spectral domain inversion: Embedding into the continuous problem and generation of internal data.

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- Inherent ill-posedness in classical inverse problems
- Difficult to do direct inversion methods on standard discretizations since small errors in forward models lead to large errors in inversion
- Possible fix: spectrally converging reduced order forward models (ROMs).
- Approach: Find reduced order forward model that matches data exactly, extract unknown coefficient from the ROM

Obtaining the ROM from the data - 1d example.

- Consider solving

$$
\begin{aligned}
-u'' + q(x)u + \lambda u &= 0 \quad \text{for} \quad x \quad \text{on} \quad (0,1) \\
-u'(0) &= 1 \\
u(1) &= 0
\end{aligned}
$$

- Define the transfer function $F(\lambda) := u(0)$.
- Read data at m spectral points $\{F(\lambda), F'(\lambda) : \lambda = b_1, \ldots b_m\}$, want to determine q

Obtaining the ROM from the data - 1d example.

- Consider the variational form for above for

$$V = \{\phi \in H^1(0,1) | \phi(1) = 0\},$$

Find $u \in V$ such that

$$\int_0^1 u'\phi' + \int_0^1 qu\phi + \lambda \int_0^1 u\phi = \phi(0)$$

for all $\phi \in V$

Obtaining the ROM from the data - 1d example.

- Pretend we were to have exact solutions to above $u_1, \ldots, u_m$ corresponding to spectral points $\lambda = b_1, \ldots b_m$.
- We could construct the subspace

$$U = \text{span}\{u_1, \ldots, u_m\}$$

and find the Galerkin solution

- $u_G \in U$ such that

$$\int_0^1 u_G' \phi' + \int_0^1 q u_G \phi + \lambda \int_0^1 u_G \phi = \phi(0) \tag{1}$$

for any $\phi \in U$.

Obtaining the ROM from the data - 1d example.

- Searching for the unknown coefficients $\{c_i\}$ for the solution

$$u_G = \Sigma_{i=1}^{m} c_i u_i$$

and by setting $\phi = u_j$ we get

$$M_{ij} = \int_0^1 u_i u_j$$

and

$$S_{ij} = \int_0^1 u_i' u_j' + \int_0^1 q u_i u_j.$$

the mass and stiffness matrices.

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$$S_{ij} = \int_0^1 u_i' u_j' + \int_0^1 q u_i u_j.$$

- For forward solution would solve $(S + \lambda M)\vec{c} = \vec{F}$ where $F_i = F(b_i) = u_i(0)$.

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- Use (1) with $u = u_i$ and $\phi = u_j$ to obtain

$$S_{ij} + b_i M_{ij} = u_j(0) = F(b_j) \quad \text{for all } i, j = 1, \ldots, m. \tag{2}$$

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- By reversing i and j and subtracting, for $i \neq j$ we have

$$(b_i - b_j) M_{ij} = F(b_j) - F(b_i)$$

or

$$M_{ij} = \frac{F(b_j) - F(b_i)}{b_i - b_j} \qquad (3)$$

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- Multiplying (2) by b_j, reversing i and j and subtracting, we get

$$(b_j - b_i)S_{ij} = b_j F(b_j) - b_i F(b_i)$$

or

$$S_{ij} = \frac{b_j F(b_j) - b_i F(b_i)}{b_j - b_i} \tag{5}$$

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- These formulas are well known in the model reduction community.
- The Galerkin model of small size m, S, M is obtained directly from the data.
- This Galerkin discretization of the pde has solutions which match the data exactly.

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- That is, for the above described Galerkin solution u_G, we that have

$$u_G(0) = F_m(\lambda)$$

where $F_m(\lambda)$ is the unique rational Hermite interpolant to the transfer function $F(\lambda)$ at the points $b_1, \ldots, b_m$ of the form

$$F_m(\lambda) = \sum_{i=1}^{m} \frac{y_i}{\lambda - \theta_i}.$$

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- Similar results hold for other forms of spectral data.

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for some positive residues and negative poles.

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  for some positive residues and negative poles.
- Since exact solutions for $\lambda = b_i$ are in the trial space, solution must be exact there, i.e.

$$F_m(b_i) = F(b_i)$$

  for $i = 1, \ldots, m$.

Galerkin solution matches data

- Using that the exact solutions are also in the test space, the variational formulation for λ near b_i and taking limits we get that

$$F'_m(b_i) = F'(b_i).$$

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- The derivatives of F are matched as well as the values. ($2m$ data points)

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- The derivatives of F are matched as well as the values. ($2m$ data points)
- Uniqueness follows from uniqueness of the Hermite Padé interpolant to $F(\lambda)$.

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$$\begin{aligned} -u'' + qu + \lambda u &= 0 \quad \text{on} \quad (0,1) \\ -u'(0) &= 1 \\ u(1) &= 0 \end{aligned} \tag{7}$$

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- Yields special nonuniform grid and spectral convergence at the receiver.

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- There is then a unique three-point staggered difference scheme with tridiagonal matrix L_m for which the approximated data/solution at $x = 0$ is exactly $F_m(\lambda)$.

Original idea of spectrally matched grids

- That is, the rational approximation $F_m(\lambda)$ uniquely determines positive $\gamma_j, \hat{\gamma}_j$, such that solving the finite difference scheme

$$\begin{aligned} -\frac{1}{\hat{\gamma}_j}\left(\frac{U_{j+1}-U_j}{\gamma_j}-\frac{U_j-U_{j-1}}{\gamma_{j-1}}\right)+\lambda U_j &= 0 \quad \text{for } j=1,\ldots N \\ -\frac{U_1-U_0}{\gamma_0} &= 1 \\ U_{N+1}=0 & \end{aligned} \tag{8}$$

yields

$$U_1 = F_m(\lambda)$$

- View γ_j as primary step size and $\hat{\gamma}_j$ as dual grid step size. For example for $q=0$,these are straightforward grid steps.

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- Galerkin solution converges high order everywhere on the domain but system is full
- Spectrally matched grid has high order convergence only at $x = 0$ and system is tridiagonal.

A one-dimensional model: How to use this for inversion ?

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A one-dimensional model: How to use this for inversion ?

- (Borcea, Druskin) For Sturm-Liouville
- Compute above or similar reduced order finite difference model from data.
- Use the spectrally matched grid (or reduced order model) for reference media to extract unknown coefficient
- They proved that the grid depends only very weakly on the medium in the high frequency limit.

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Inversion in higher dimensions.

- (Borcea, Druskin, Guevara-Vasquez, Mamanov, Zaslavsky) Use other new techniques to extend to 2-d
- New methods require better understanding of reduced order model- how to generalize grid?

Equivalence of grids with Galerkin

- Consider again solving

$$\begin{aligned} -u'' + qu + \lambda u &= 0 \quad \text{on} \quad (0,1) \\ -u'(0) = 1 & \qquad u(1) = 0 \end{aligned}$$

with Galerkin subspace $U = \text{span}\{u_1(x), u_2(x), \ldots, u_n(x)\}$, for $\{u_i\}$ the solutions at those same spectral data points $\lambda = b_i$.

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- S and M are full, unlike the finite difference
- Find a new basis in which the Galerkin system is sparse?

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$$B = \{\vec{\delta}, A\vec{\delta}, A^2\vec{\delta}, \ldots, A^{m-1}\vec{\delta}\}.$$

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- Orthogonalize it with Gram-Schmidt with respect to M inner product (yields L^2 orthonormality)

Equivalence of grids with Galerkin

- Get new orthogonalized basis for U:

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- Now redo Galerkin system in this new basis.

A one-dimensional model: Galerkin equivalence

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- Mass $\hat{M}$ matrix will be identity due to orthogonality.
- Stiffness matrix $\hat{S}$ will be tri-diagonal due to Lanczos process
- Right hand side will be nonzero only in first component (an approximate delta)
- The only difference is that the Galerkin stiffness matrix $\hat{S}$ is symmetric while the system (11) is symmetric with respect to the $\hat{\gamma}_i$ diagonal inner product.

A one-dimensional model: Galerkin equivalence

Theorem

If one uses the orthogonalized basis above and forms the Galerkin system

$$(\hat{S} + \lambda \hat{M})\vec{\hat{c}} = \vec{\hat{F}} \tag{10}$$

to solve for $\vec{\hat{c}}$, *this is precisely the symmetrization of the finite difference system (11) for* $\vec{U}$. *More precisely,*

$$u_G = \sum_{i=1}^{m} \sqrt{\hat{\gamma}_i} U_i \hat{u}_i(x).$$

A one-dimensional model: Galerkin equivalence

- That is, the solution components U_j of this difference scheme

$$-\frac{1}{\hat{\gamma}_j}\left(\frac{U_{j+1}-U_j}{\gamma_j}-\frac{U_j-U_{j-1}}{\gamma_{j-1}}\right)+\lambda U_j = 0 \quad \text{for } j=1,\ldots N \quad (1)$$

$$-\frac{U_1-U_0}{\gamma_0} = 1$$

$$U_{N+1}=0$$

can be interpreted as coefficients (with a scaling) of the Galerkin solution in this orthonormal basis.

A one-dimensional model: Galerkin equivalence

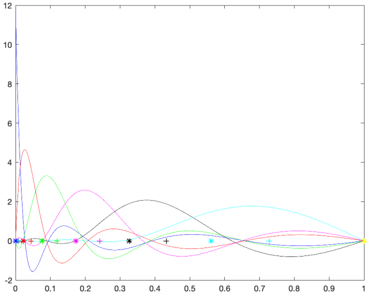

Figure: Spectrally matched finite difference grid with its equivalent Galerkin basis

A one-dimensional model: Inversion

- So the entries of this reduced order model (which can be obtained from the data) are the entries of the stiffness matrix

$$\hat{S}_{ij} = \int \hat{u}_i' \hat{u}_j' + \int_0^1 q \hat{u}_i \hat{u}_j$$

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- The orthogonalized basis functions here actually *depend only very weakly on the coefficient* .

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- The orthogonalized basis functions for the reference medium play the role of the optimal grid for coefficient extraction.

Inversion

- Idea (from time domain papers of Borcea, Druskin, Mamonov, Zaslavsky): Since these appropriately orthogonalized basis functions depend only weakly on q we can use similarly orthogonalized basis functions for some known reference medium.
- The orthogonalized basis functions for the reference medium play the role of the optimal grid for coefficient extraction.
- Unlike the grid, localized basis functions have a natural extension to higher dimensions and other geometries.

A one-dimensional example: Inversion

Consider

$$\begin{aligned} -u'' + q(x)u + \lambda u &= 0 \quad \text{on} \quad (0,1) \\ -u'(0) &= 1 \\ u(1) &= 0 \end{aligned} \tag{12}$$

as a perturbation of the corresponding reference problem $q_0 = 0$

$$\begin{aligned} -u'' + \lambda u &= 0 \quad \text{on} \quad (0,1) \\ -u'(0) &= 1 \\ u(1) &= 0 \end{aligned} \tag{13}$$

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- We read data $F(b_i)$, $F'(b_i)$ for $\lambda = b_1, \ldots b_m$ for the perturbed problem.
- From this generate the $m \times m$ stiffness and mass matrices S, M for Galerkin system for basis of exact solutions.

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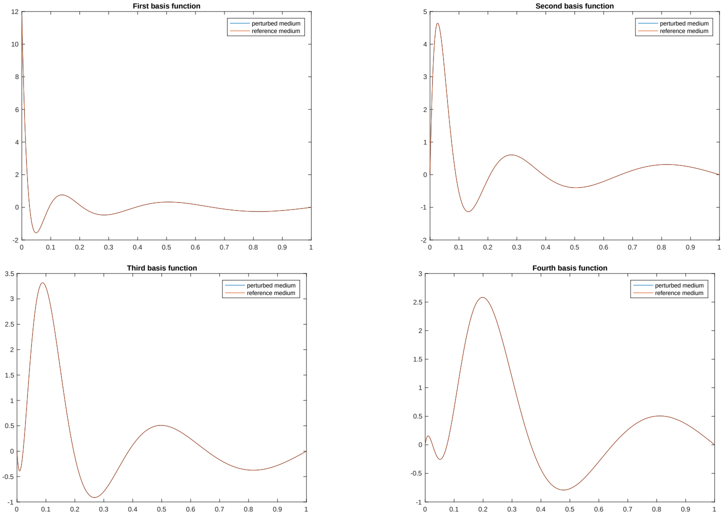
- From this generate the $m \times m$ stiffness and mass matrices S, M for Galerkin system for basis of exact solutions.
- Perform Lanczos orthogonalization to generate Galerkin system $\hat{S}$, $\hat{M}$ for orthogonalized basis

Weak dependence of orthogonalized bases on q



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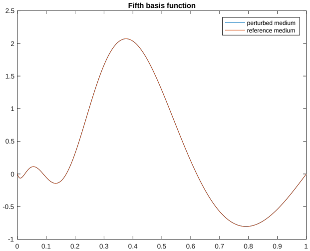

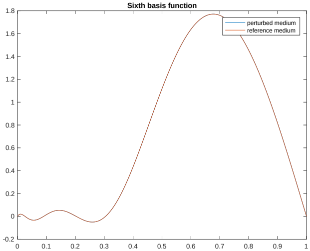

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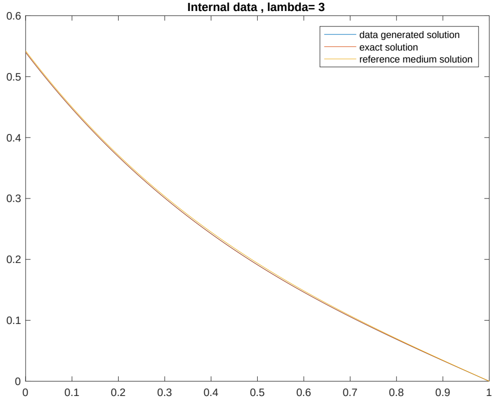
- From the reference medium, we have a highly accurate approximation to the orthogonalized basis.
- By solving the Galerkin system, we get the coefficients
- This yields boundary data generated *internal solutions*

Internal solution

Internal solution for arbitrarily chosen spectral value $\lambda = 3$ generated from data.



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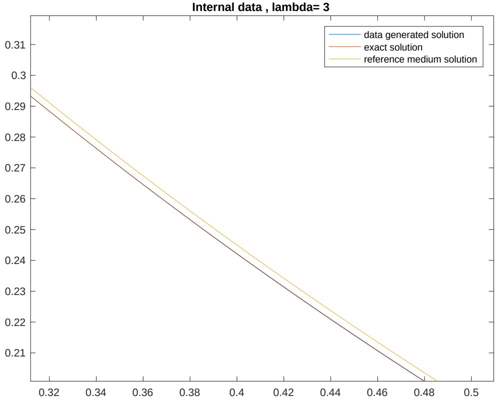

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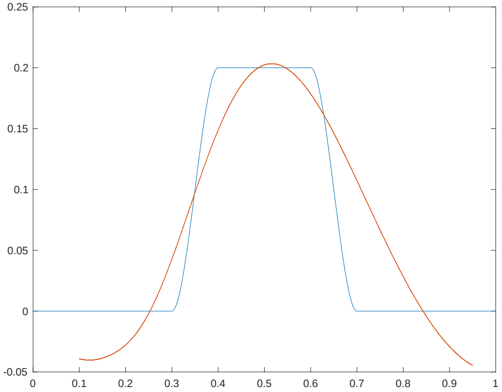
A one-dimensional example: Inversion

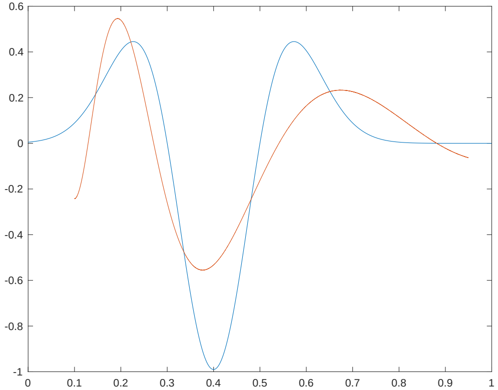
- How to use internal solution to do inversion?
- For example, can compute $(u'' - \lambda u)/u \approx q$
- Can do this for any spectral value.

A one-dimensional example: Inversion



A one-dimensional example: Inversion

A harder example



Inversion possibilities for higher dimensions

- For higher dimensional problems, we can use multiple k sources/receivers:

$$\begin{aligned} -\Delta u_i^r + q(x)u_i^r + b_i u_i^r &= 0 \quad \text{in} \quad \Omega \\ \frac{\partial u_i^r}{\partial \nu} &= g_r \quad \text{on } \partial\Omega \end{aligned} \tag{14}$$

"source" (Neumann data) g_r and spectral value b_i

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"source" (Neumann data) g_r and spectral value b_i

- Now spectral data is in the form of a $k \times k$ block

$$F_{rl}^i := F_{rl}(b_i) = \int_{\partial\Omega} u_i^r g_l$$

and

$$DF_{rl}^i := \frac{dF_{rl}}{d\lambda}(\lambda)|_{\lambda=b_i}$$

Inversion possibilities for higher dimensions

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- is again obtained directly from boundary data :

$$M_{irjl} = \frac{F^j_{lr} - F^i_{lr}}{b_i - b_j}, \tag{15}$$

$$M_{iril} = -DF^i_{lr}, \tag{16}$$

$$S_{irjl} = \frac{b_j F^j_{lr} - b_i F^i_{lr}}{b_j - b_i}, \tag{17}$$

and

$$S_{iril} = (\lambda F_{rl})'(b_i). \tag{18}$$

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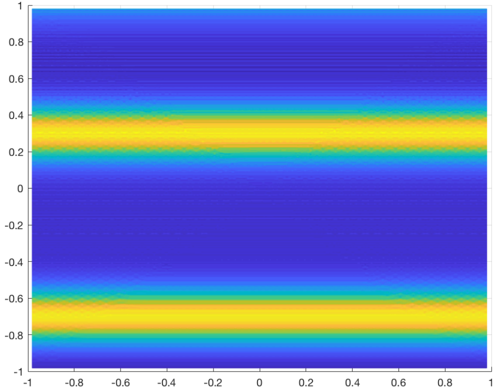
- Try again $(\Delta u - \lambda u)/u \approx q$.

proof of concept 2d, two sources/receivers



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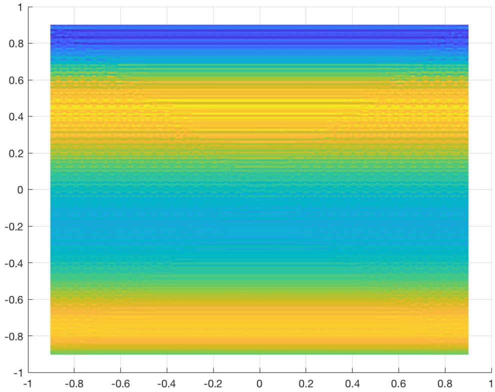
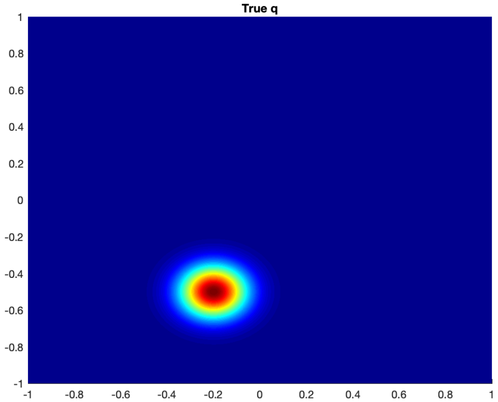
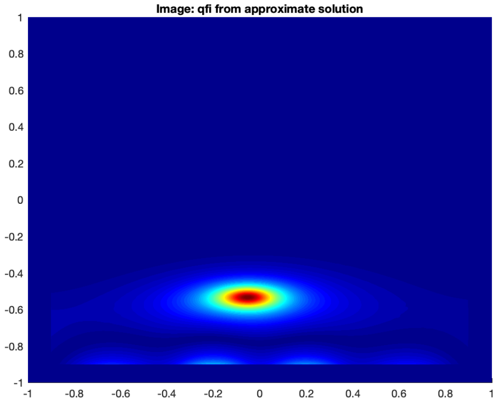


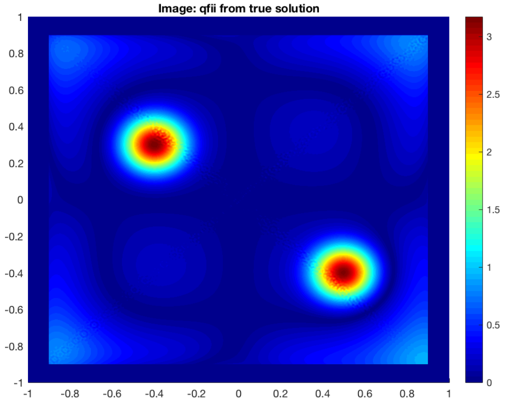
bump profile, four sources on one side



reconstruction using data generated internal solutions , four sources on one side



double bump profile , eight sources around



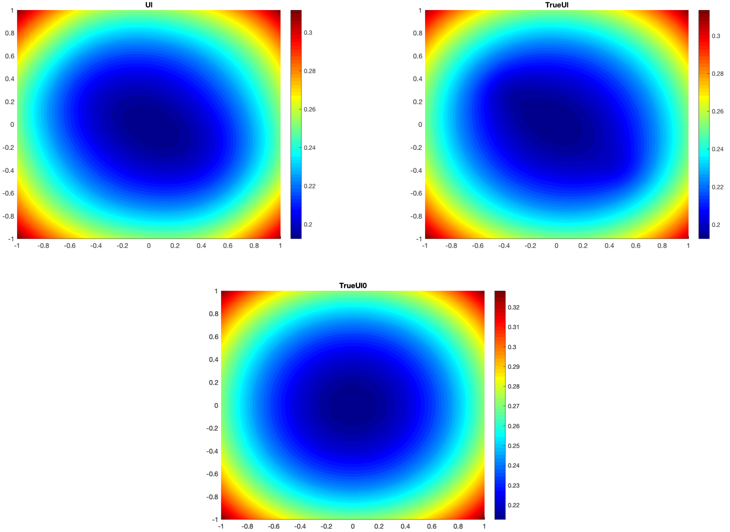


Figure: Relative error between the true and data generated: 0.003930. Relative difference between the true and reference medium: 0.084794.

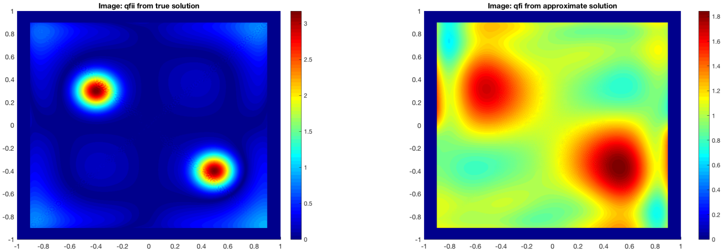


Figure: Reconstruction of two bumps . Eight sources total; two on each side, and six spectral values.

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- Other approaches to use the ROM, reference basis functions, and optimization improve accuracy of reconstructions (current work)