Phase-preconditioned Rational Krylov Subspaces for model reduction of large-scale wave propagation

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Problem Definition

- Solving wave equation for multiple sources and receivers in a *frequency range*

$$\Delta u^{\ell} - \frac{s^2}{v^2} u^{\ell} = \delta(x - x_S^{\ell})$$

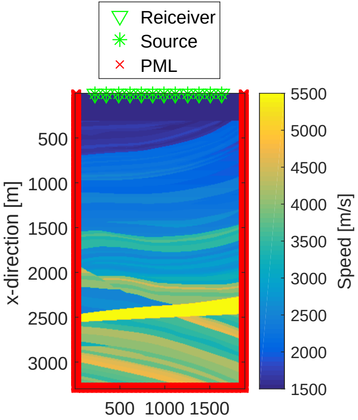
- Transfer function from sources to receivers $f(x_R, x_S, s)$

Scaling of the problem in 3D:

N unknowns in one spatial direction

1. No of Frequency points: $\propto N$
2. Source/Receiver scaling: $\propto N^2$
3. Spatial scaling: $\propto N^3$

- Explorational Geophysics



Problem Formulation

- After finite difference discretization with PML

$$\mathrm{A}(s)\mathrm{u}^{\ell} - s^2\mathrm{u}^{\ell} = \mathrm{b}^{\ell}$$

- (Laplace) frequency dependent $\mathrm{A}(s)$ caused by PML
- Stepsizes in PML: $h_j = \alpha_j + \frac{\beta_j}{s}$
- Transfer function from sources to receivers

$$\mathrm{F}(\mathrm{R}, \mathrm{B}, s) = \mathrm{R}^T\mathrm{W}(s)(\mathrm{A}(s) - s^2\mathrm{I})^{-1}\mathrm{B}$$

- $\mathrm{W}(s)$ a is diagonal weight matrix with FD-voxel weight
- Reduced order modeling of transfer function over frequency range
- Rational Krylov subspaces for ROM

Problem Formulation

- $\mathsf{A}(s)$ passive and causal

$$\mathcal{W}\left\{\mathsf{A}(s)\right\} = \left\{s \in \mathbb{C} : \mathsf{x}^H \mathsf{A}(s)\mathsf{x} = 0\,\forall \mathsf{x} \in \mathbb{C}^k \backslash 0\right\}$$

$$\Re\mathcal{W}\left\{\mathsf{A}(s) - s^2\mathsf{I}\right\} < 0$$

- A is self-adjoint in W-bilinear form due to reciprocity

$$\mathsf{F}(\mathsf{R},\mathsf{B},s) = \mathsf{F}(\mathsf{B},\mathsf{R},s) \Rightarrow \mathsf{W}(s)\mathsf{A}(s) = \mathsf{A}^T(s)\mathsf{W}(s)$$

- Schwartz reflection principle $\mathsf{A}(\bar{s}) = \bar{\mathsf{A}}(s)$ (conjugation symmetry of spectrum)
- Preserve this structure during RKS

Motivation

- FD grid over discretized w.r.t. Nyquist
- approximation $\mathsf{F}(\mathsf{R},\mathsf{B},s)$ to noise level
- PML introduces losses
- limited I/O map

Reduced Order Modeling

- Projection based ROM $\mathsf{u} = \mathsf{u}_m + \epsilon_m$, with $\mathsf{u}_m \in \mathsf{V}_m$,
- Coefficients from the Galerkin condition $(\mathsf{A}(s) - s^2\mathsf{I})\epsilon_m \perp_{\mathsf{W}(s)} \mathsf{V}_m$
- Reduced order solution after projection

$$\begin{aligned} \mathsf{u}^\ell &= (\mathsf{A}(s) - s^2\mathsf{I})^{-1}\mathsf{b}^\ell \\ \Rightarrow \mathsf{u}_m^\ell &= \mathsf{V}_m(\mathsf{V}_m^H\mathsf{A}(s)\mathsf{V}_m - s^2\mathsf{I})^{-1}\mathsf{V}_m^H\mathsf{b}^\ell \\ \Rightarrow \mathsf{F}_m &= \mathsf{R}^T\mathsf{V}_m(\mathsf{V}_m^H\mathsf{A}(s)\mathsf{V}_m - s^2\mathsf{I})^{-1}\mathsf{V}_m^H\mathsf{B} \end{aligned}$$

- Define Rational Krylov subspace with shifts $\kappa = [\kappa_1, \ldots, \kappa_m]$

$$\mathcal{K}^m(\kappa) = \mathrm{span}\{(\mathsf{A}(\kappa_1) - \kappa_1^2\mathsf{I})^{-1}\mathsf{b}^\ell, \ldots, (\mathsf{A}(\kappa_m) - \kappa_m^2\mathsf{I})^{-1}\mathsf{b}^\ell\}$$

Structure preserving rational Krylov subspace approach

- To preserve Schwarz-reflection principle we project onto the real space

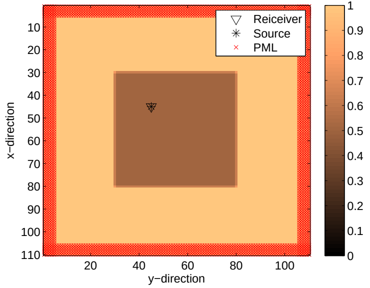
$$\mathcal{K}_R^m(\kappa) = \operatorname{span}\{\Re\mathcal{K}^m(\kappa), \Im\mathcal{K}^m(\kappa)\}$$

- Reduced order model $\mathsf{H}_m(s)$ obtained by projection onto basis V_m in symmetry preserving from

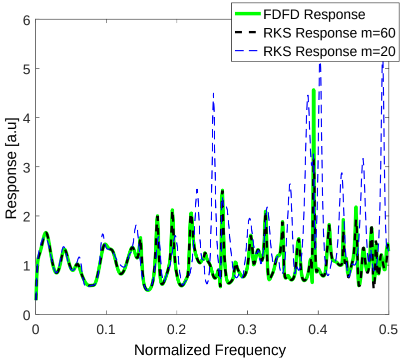
$$\mathsf{H}_m(s) = \mathsf{V}_m^H \mathsf{W}(s)\mathsf{A}(s)\mathsf{V}_m$$

- Reduced order model $\mathsf{H}_m(s)$
  - ROM tranferfunction interpolates on $\bar{\kappa} \cup \kappa$, (if $\mathsf{R} = \mathsf{B}$ tangentially)
  - symmetric
  - passive
  - follows Schwarz-reflection principle
- (Nonlinear) numerical range of reduced operator lies in convex hull of the numerical range of full operator

RKS example: 100 x 100 dielectric box



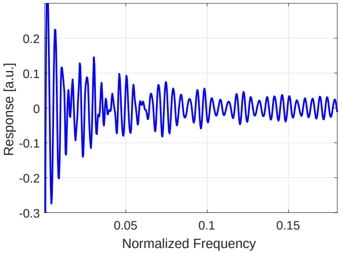
(a) Wavespeed in the box configuration.



(b) Imaginary part transfer function.

Problem of RKS

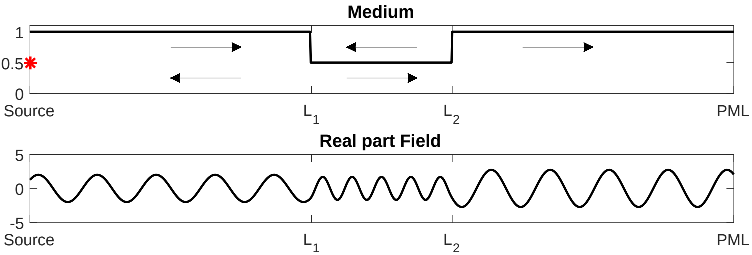
- In geophysical structures we typically have late arrivals
- Late arrival means oscillatory Frequency domain $(*\delta(t-T) \xrightarrow{\mathcal{L}} \cdot \exp(-sT))$
- FD frequency domain sampling at Nyquist rate $\Delta s = i\pi / T^{\mathrm{arr}}_{\mathrm{max}}$



Idea of phase-preconditioning

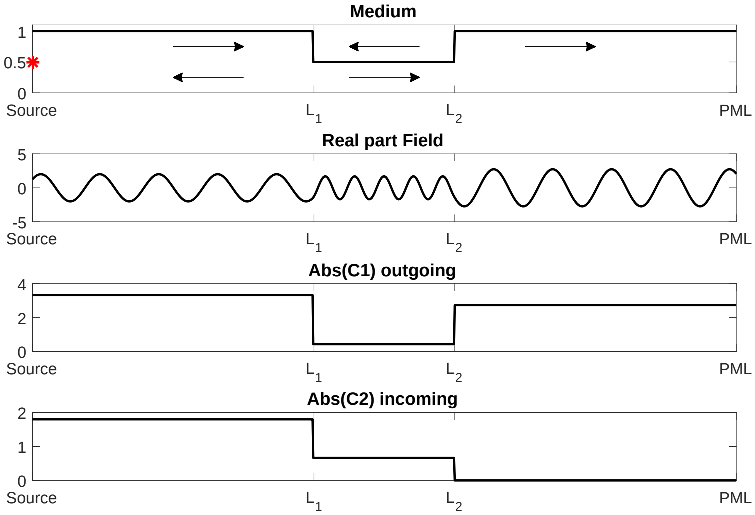
- Precondition the RKS by incorporating travel time information
- Eikonal Solution: $|\nabla T|^2 = \frac{1}{v^2}$
- Can we factor out main oscillations?

Decomposition in 1D

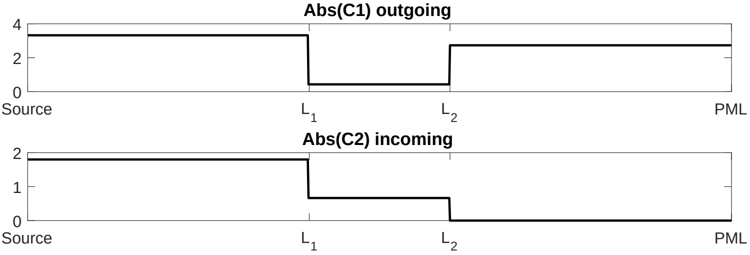


- Consider a layered medium of 3 Layers
- Outgoing and incoming waves
- Decompose into $c_{out}(\kappa_j)\exp(-\kappa_j T_{eik})$, and $c_{in}(\kappa_j)\exp(\kappa_j T_{eik})$
- $c_{out/in}$ obtainable form one way wave equations

Decomposition in 1D



Decomposition in 1D



- After 3 iterations $c_{out}(\kappa_j)\exp(-sT_{eik})$, and $c_{in}(\kappa_j)\exp(sT_{eik})$ form a basis for *ALL* solutions (iff linear independent)

$$u(s) \in \mathrm{span}\{c_{out}(\kappa_1)\exp(-sT_{eik}), \ldots, c_{in}(\kappa_1)\exp(sT_{eik}), \ldots\}$$

- Required iterations are dependent on complexity of medium (layers) not on arrival time

Summary of Phase preconditioning

Theorem - (analytical)

For a one-dimensional problem, with k homogenous layers and an arbitrarily located source, there exist $m \leq k+1$ non-coinciding interpolation points, such that the solution $\mathrm{u}(s) \in \mathcal{K}^{2m}_{\mathrm{EIK;R}}(\kappa, s) \forall s$

$$\mathcal{K}^{2m}_{\mathrm{EIK}}(\kappa, s) = \mathrm{span}\{ \exp(-s\mathrm{T}_{\mathrm{eik}})\mathrm{c}_{\mathrm{out}}(\kappa_1), \ldots, \exp(-s\mathrm{T}_{\mathrm{eik}})\mathrm{c}_{\mathrm{out}}(\kappa_m), \\ \exp(\quad s\mathrm{T}_{\mathrm{eik}})\mathrm{c}_{\mathrm{in}}\quad(\kappa_1), \ldots, \exp(\quad s\mathrm{T}_{\mathrm{eik}})\mathrm{c}_{\mathrm{in}}\quad(\kappa_m)\}$$

- General: Correct amplitudes $c_{out/in}$ with asymptotic solution $s \to i\infty$ $\mathrm{g}_{\mathrm{asym}}$ and project problem

$$\mathrm{u}_m(s) = \mathrm{g}_{\mathrm{asym}}(s\mathrm{T}_{\mathrm{eik}}) \sum_{j=1}^{m} a_j \mathrm{c}_{\mathrm{out}}(\kappa_j) + \bar{\mathrm{g}}_{\mathrm{asym}}(s\mathrm{T}_{\mathrm{eik}}) \sum_{j=1}^{m} d_j \mathrm{c}_{\mathrm{in}}(\kappa_j)$$

Summary of Phase preconditioning

- Can't precondition spectral problem unless you have exact pole zero cancelation
$$A(s)u^{\ell} - s^2 u^{\ell} = b^{\ell}$$
- But if RKS-ROM is dominated by solving systems and not by evaluating projections $\Rightarrow$ increase basis
- Enhance convergence by adding (asymptotically) meaningful vectors
- Frequency dependent basis can be seen as spectral weighting, deweight residues far from s (allows extrapolation)

FD grid requirements

- ROM can extrapolate to high frequencies
- Spatially c_{out} and c_{in} are much smoother then u
- $\Rightarrow$ We can compute a basis for $c_{\text{in/out}}$ on a much coarser grid then required for FDFD/FDTD method (Projection accurate Operator)
- Correct numerical dispersion by matching

$$\frac{\exp(2s\mathrm{T}^{\ell}_{\text{eik}})}{s^2}|\nabla_h \cdot \exp(-s\mathrm{T}^{\ell}_{\text{eik}})|^2 = \frac{1}{v^2}$$

Scaling of the problem in 3D: Reduced order modeling

N unknowns in one spatial direction

1. No of Frequency points: $\propto N$: preconditioned ROM
2. Source/Receiver scaling: $\propto N^2$
3. Spatial scaling: $\propto N^3$: Coarse grid $c_{\text{in/out}}$ computation

MIMO extension of algorithm

- Generalization to higher dimensions by decomposing into dimension specific asymptotic functions
- MIMO extension to block algorithm
- Compute $c^{\ell}_{\text{out/in}}$ for every source location ℓ from block solution

$$(\mathrm{A}(\sigma_j) + \sigma_j^2 \mathrm{I})^{-1}\mathrm{B}, \ \text{with } \mathrm{B} = [\mathrm{b}^1, \ldots, \mathrm{b}^{N}_{\text{src}}]$$

- Compress $c^{\ell}_{\text{out/in}}$ basis with truncated SVD to reduce basis

$$\mathrm{u}^{\ell}_m(s) = \sum_{l=1}^{N_{\text{src}}} \left(\mathrm{g}_{\text{asym}}(s\mathrm{T}^{l}_{\text{eik}}) \sum_{j=1}^{N_{\text{SVD}}} a_{j;l}\mathrm{c}^{\text{SVD}}_{\text{out}} + \bar{\mathrm{g}}_{\text{asym}}(s\mathrm{T}^{l}_{\text{eik}}) \sum_{j=1}^{N_{\text{SVD}}} d_{j;l}\mathrm{c}^{\text{SVD}}_{\text{in}} \right)$$

MIMO extension of algorithm

- Important singular vectors $\mathrm{c}_{\mathrm{out/in}}^{\mathrm{SVD}}$ weakly dependent on source location
- We don't have to solve $(\mathrm{A}(\kappa_j) - \kappa_j^2 \mathrm{I})^{-1}\mathrm{b}^\ell$ for every ℓ
- $\Rightarrow$ source compression/Compressions of right hand sides

Scaling of the problem in 3D: Reduced order modeling

N unknowns in one spatial direction

1. No of Frequency points: $\propto N$: preconditioned ROM
2. Source/Receiver scaling: $\propto N^2$: Source compression
3. Spatial scaling: $\propto N^3$: Coarse grid $\mathrm{c}_{\mathrm{in/out}}$ computation

Algorithm Overview

1. Compute T^ℓ via fast marching method
2. Solve shifted systems with a coarse operator $(A_{\text{coarse}}(\kappa_j) - \kappa_j^2 I)^{-1} b^\ell$
3. Decompose into amplitudes $c^{SVD}_{out/in}$ and apply SVD
4. Evaluate reduced order solutions real basis $V_m(s)$ spanning

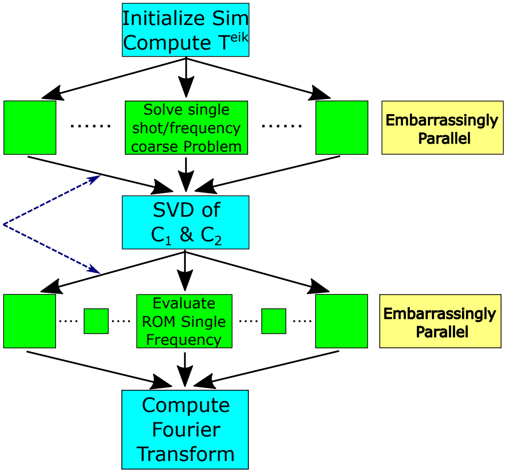
$$\mathcal{K}^{4m}_{\mathrm{EIK;R}}(\kappa, s) = \operatorname{span}\left\{\Re\mathcal{K}^{2m}_{\mathrm{EIK}}(\kappa, s), \Im\mathcal{K}^{2m}_{\mathrm{EIK}}(\kappa, s)\right\}$$

$$\mathcal{K}^{2m}_{\mathrm{EIK}}(\kappa, s) = \operatorname{span}\{g_{asym}(sT^l_{eik})c^{SVD}_{1,out}, \ldots, \bar{g}_{asym}(sT^l_{eik})c^{SVD}_{1,in}, \ldots\}$$

$$F_m(B, B, s) = B^H V_m (V_m^H W(s) A_{\text{fine}}(s) V_m - s^2 I)^{-1} V_m^H B$$

Algorithm Overview

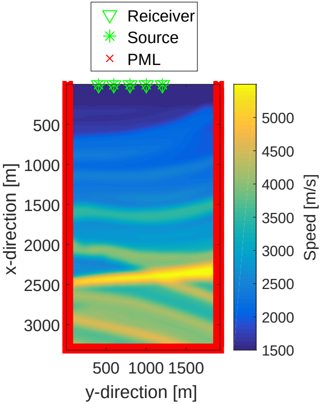
- Main cost: solving coarse wave problem single source & frequency
- Communication cost $n \cdot \log n$ with n processors
- Main part of algorithm embarrassingly parallelizable (frequency and RHS)



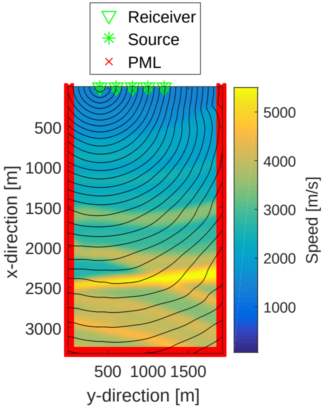
$\#$ Evaluation shots $\cdot$ Frequencies $\gg$ $\#$ interpolation shots $\cdot$ Frequencies

Smooth Layered medium

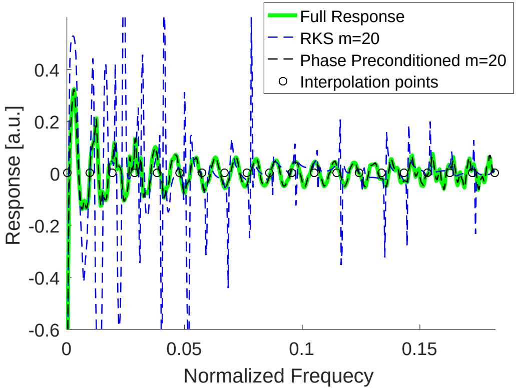
- Smooth layered medium
- Acoustic wave equation
- Travel time dominated
- 5 Sources and 5 Receivers
- No grid coarsening $\Delta x = 4m$



Smooth Layered medium



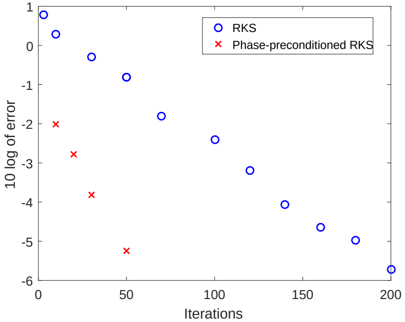
Contour plot of the eikonal solution



Frequency domain transfer function from the left most source to the right most receiver (Real Part)

Convergence Smooth Layered medium

- RKS has double interpolation (2x better then Nyquist)
- Phase preconditioning reduces the iteration count by a factor ≈ 4
- Equidistant shifts on imaginary line



Time Domain Error in dependence of iterations

Convergence Smooth Layered medium

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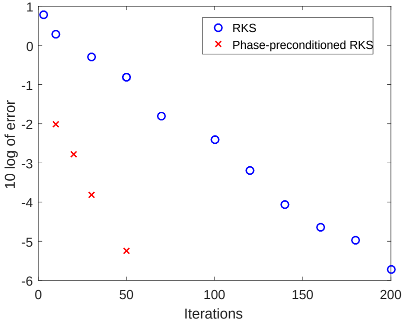
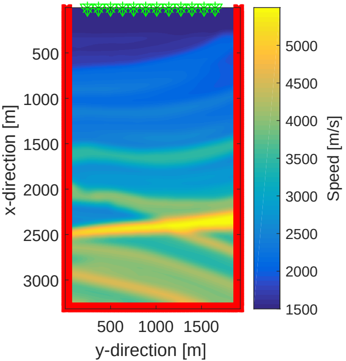


Time Domain Error in dependence of iterations

- $\Rightarrow$ Let us introduce grid coarsening!

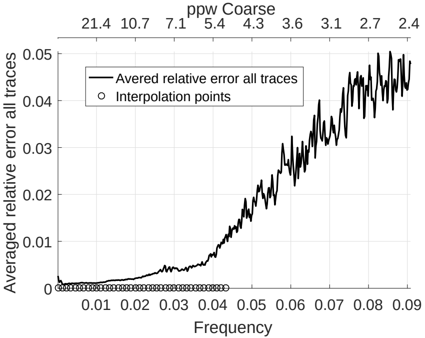
Grid Coarsening

- Asymptotically corrected ROM can extrapolate
- Coarse Grid approach: solve amplitudes $c_{\mathrm{out/in}}$ on coarse grid
- Galerkin and evaluation with finer operator
- Grid coarsening factor 4 (all directions) $\Delta x = 16m$
- Gaussian pulse (center: 5.5 ppw, cutoff 2.7 ppw).



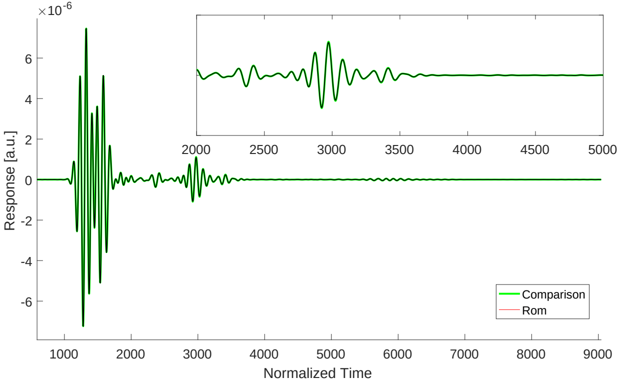
Frequency Domain Error

- From 100ppw-5ppw we use 40 equidistant shifts
- Truncate $c_{in/out}$ SVD after 50 basis functions
- Average error of traces $< 1\%$
- extrapolation error $< 5\%$
- Gaussian pulse supported in interpolation and extrapolation part



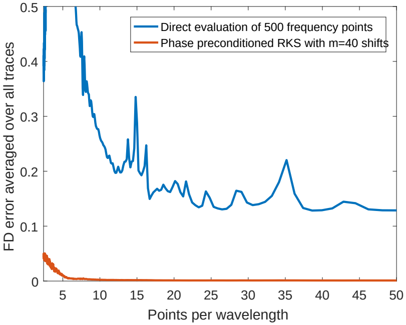
Time Domain Comparison

Most distant source receiver pair well approximated. FDTD with 10000 steps has worth accuracy.



Time Domain Comparison

- Clear advantage of ROM over Direct evaluation of the same grid
- Both cases are second order finite differences
- Comparison solution: 8 times finer Grid



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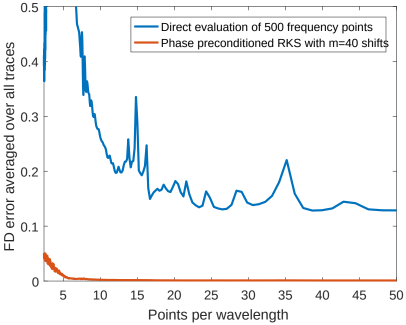
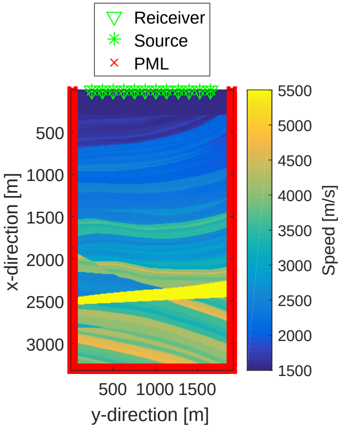


- How about non smooth media?

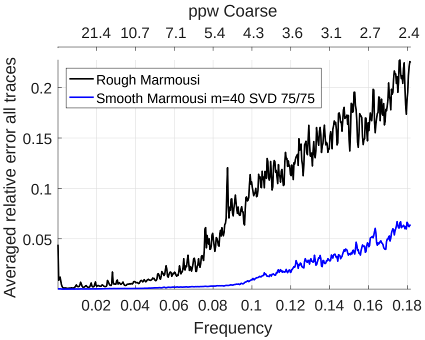
Grid Coarsening: No smoothing

- Same setup without smoothing
- Asymptotic solutions loose validity
- Galerkin approach still valid



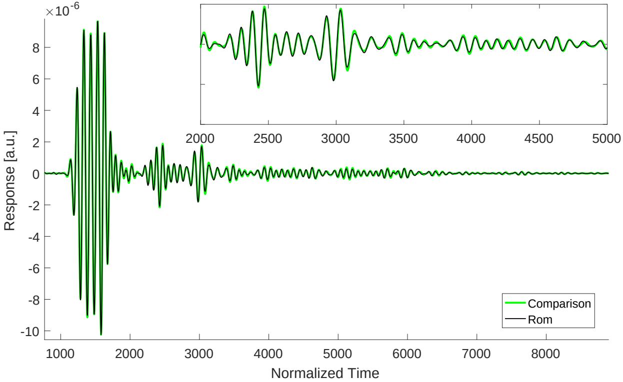
Frequency Domain Error

- From 100ppw-5ppw we use 40 equidistant shifts
- Truncate $c_{in/out}$ SVD after 75 basis functions
- Substantially larger error
- worse extrapolation



Time Domain Comparison

Important features of TD signal still reproduced. Small amplitude shift.



Conclusions

- Main cost is # of coarse frequency domain solves
  $\Rightarrow$ easy to parallelize
- Compression of model can be used in inversion for efficient computation and storage of Jacobian
- Computational cost is dependent on model complexity, but only weakly on time interval (vs linear dependence of FDTD)
- Model order approach can reduce all 3 aspects of 3D problem
  1. No of Frequency points: $\propto N$: preconditioned ROM
  2. Source/Receiver scaling: $\propto N^2$: Source compression
  3. Spatial scaling: $\propto N^3$: Coarse grid $c_{in/out}$ computation
- 2.7 ppw for smooth problem
- generalizable to other PDEs with asymptotic solutions

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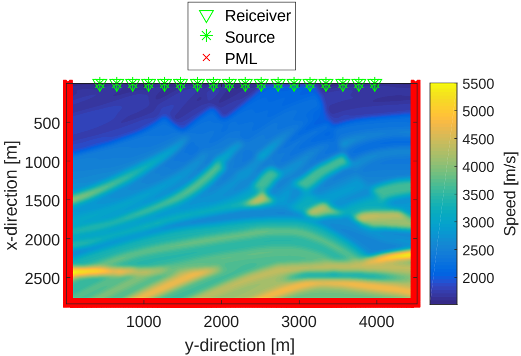
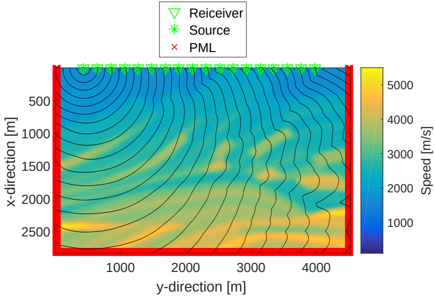
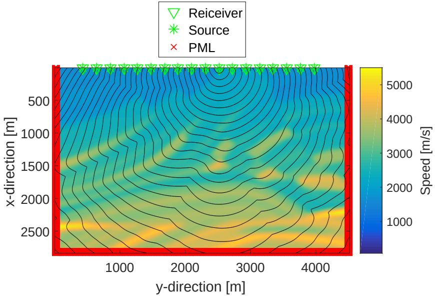
Grid Coarsening: Complex medium

- Complex Marmousi model
- 18 Source Receiver pairs



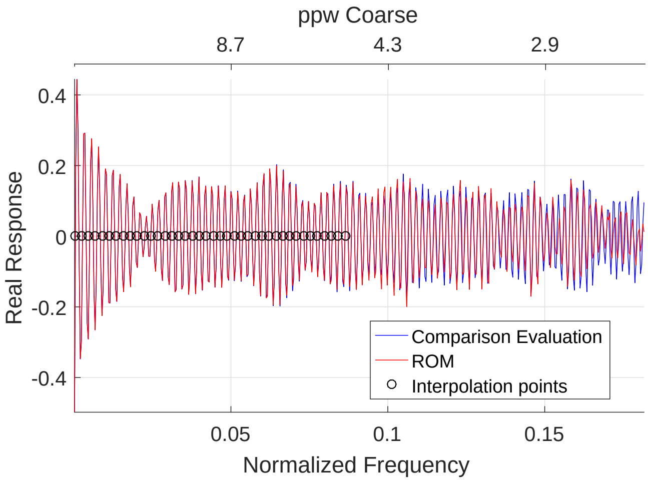
Eikonal Solutions





FD Domain Comparison

Well approximated until 4ppw. Less then 1ppw for first arrival.



TD Domain Comparison

Shifted Gaussian Wavelet applied to FD data with 3.5 ppw cut-off.