

# Model reduction of wave propagation *via phase-preconditioned rational Krylov subspaces*

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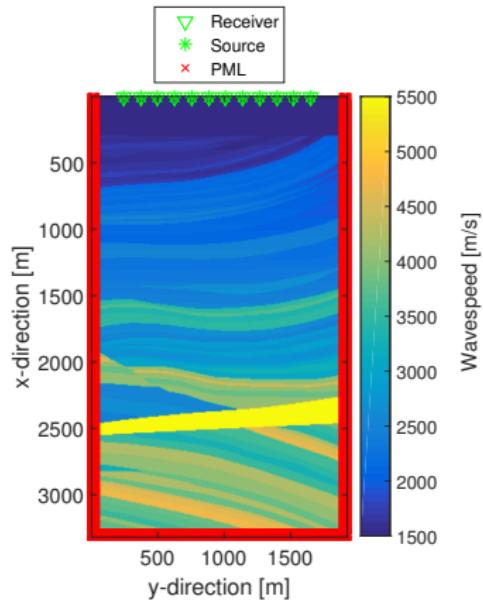
November 8, 2017

# Motivation

- Second order wave equation with wave operator A

$$Au - s^2 u = -\delta(x - x_S)$$

- Assume N grid steps in every spatial direction
- Scaling of surface seismic in 3D:
  - # Grid points  $O(N^3)$
  - # Sources  $O(N^2)$
  - # Frequencies  $O(N)$
  - Overall  $O(N^6)\psi(N^3)$



(a) Section of wave speed profile of the Marmousi model.

# Goal of this work

- **Simulate and compress** large scale wave fields in modern high performance computing environment  
**(parallel CPU and GPU environment)**
- Use projection based **model order reduction** to
  - Approximate transfer function
  - reduce # of frequencies needed to solve
  - reduce # of sources to be considered
  - reduce # number of grid points needed

# Introduction

- Simulating and compressing large scale wave fields

$$Au^{[l]} - s^2 u^{[l]} = -\delta(x - x_S^{[l]}), \quad (1)$$

- With the wave operator given by  $A \equiv \nu^2 \Delta$ , Laplace frequency  $s$
- We consider a Multiple-Input Multiple-Output problem
- Define fields  $U = [u^{[1]}, u^{[2]}, \dots, u^{[N_s]}]$  and sources  
 $B = [-\delta(x - x_S^{[1]}), -\delta(x - x_S^{[2]}), \dots, -\delta(x - x_S^{[N_s]})]$
- We are interested in the transfer function (Receivers and Sources coincide)

$$F(s) = \int B^H U(s) dx \quad (2)$$

- Open Domains

# Problem Formulation

- After finite difference discretization with PML

$$(A(s) - s^2 I)U = \hat{B}$$

- Step sizes inside the PML  $h_i = \alpha_i + \frac{\beta_i}{s}$
- Frequency dependent  $A(s)$  caused by absorbing boundary

$$Q(s)U = B \text{ with } Q(s) \in \mathbb{C}^{N \times N}$$

- $Q(s)$  properties
  - sparse
  - complex symmetric (reciprocity)
  - Schwarz reflection principle  $\overline{Q(s)} = Q(\bar{s})$
  - passive (nonlinear NR<sup>1</sup>  $\Re e < 0$ )

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<sup>1</sup>NR:  $\mathcal{W}\{A(s)\} = \{s \in \mathbb{C} : x^H A(s)x = 0 \quad \forall x \in \mathbb{C}^k \setminus \{0\}\}$

# Problem Formulation

- Transfer function from sources to receivers

$$F(B, s) = B^H Q(s)^{-1} B$$

- Reduced order modeling of transfer function over frequency range

$$F_m(B, s) = V_m B^H (V_m^H Q(s) V_m)^{-1} V_m^H B \text{ with } V_m \in \mathbb{C}^{N \times m}$$

- valid in a range of  $s$ , and easy to store

## Motivation

- FD grid overdiscretized w.r.t. Nyquist
- approximation  $F(B, s)$  to noise level
- PML introduces losses
- limited I/O map

# Outline

- ① Problem formulation
- ② Model order reduction – Rational Krylov subspaces
- ③ Phase-Preconditioning
- ④ Numerical Experiments
- ⑤ Conclusions

# Structure preserving rational Krylov subspaces

- Preserve: symmetry (w.r.t. matrix, frequency), passivity
- Block rational Krylov subspace approach  $\kappa = s_1, \dots, s_m$

$$\mathcal{K}^m(\kappa) = \text{span} \left\{ Q(s_1)^{-1} B, \dots, Q(s_m)^{-1} B \right\}$$

$$\mathcal{K}_{\Re}^{2m} = \text{span} \left\{ \mathcal{K}^m(\kappa), \mathcal{K}^m(\bar{\kappa}) \right\}$$

- Let  $V_m$  be a (real) basis for  $\mathcal{K}_{\Re}^m$  then with reduced order model (via Galerkin condition)

$$R_m(s) = V_m^H Q(s) V_m$$

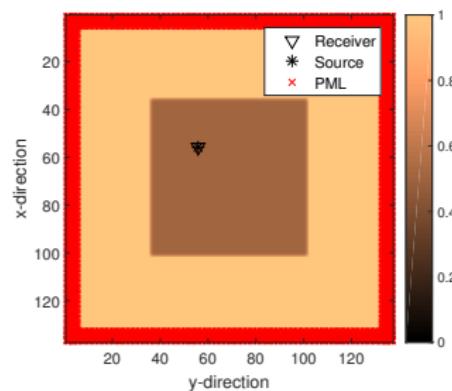
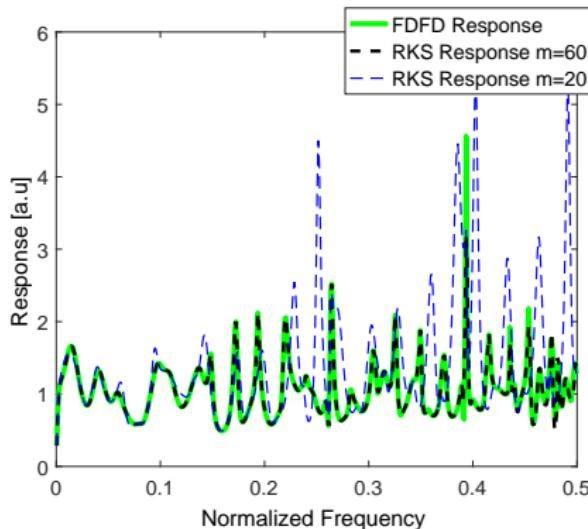
we approximate

$$F_m(s) = (V_m^H B)^H R_m(s)^{-1} V_m^H B,$$

# Structure preserving rational Krylov subspaces

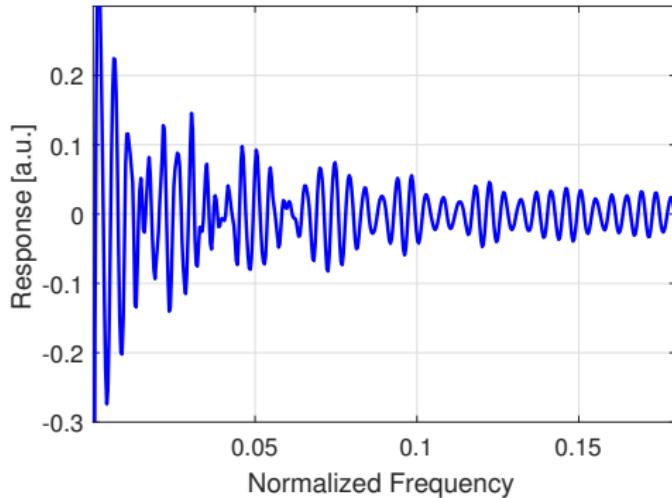
- Numerical Range:  $\mathcal{W}\{R_m(s)\} \subseteq \mathcal{W}\{Q(s)\}$   
**Proof:**  $x_m^H R_m(s) x_m = (V_m x_m)^H Q(s) (V_m x_m)$   
 $\Rightarrow R_m(s)$  is passive
- $F_m(s)$  is Hermite interpolant of  $F(s)$  on  $\kappa \cup \bar{\kappa}$   
 $Q(\kappa)^{-1} B \in \mathcal{K}_{\Re}^{2m}$  + uniqueness of Galerkin
- Schwarz reflection and symmetry hold as well

# RKS for a Resonant cavity



- RKS has excellent convergence if singular Hankel values of system decay fast (few contributing eigenvectors)
- $F_m(s)$  is a  $[2m - 1/2m]$  rational function

# Problem of RKS in Geophysics - Nyquist Limit



- Long travel times  $*\delta(t - T) \xrightarrow{\mathcal{F}} \exp(-sT)$ 
  - Nyquist sampling of  $\Delta\omega = \frac{\pi}{T}$
  - $F(s) = \int B^H Q(s)^{-1} B dx$  is oscillatory

# Filion Quadrature

- Filion quadrature deals with oscillatory integral

$$F(s) = \int \exp(st) f(t) dt$$

quadrature requires  $s\Delta t \ll 1$

$$F(s) \approx \Delta t \sum_n a_n \exp(s n \Delta t) f(n \Delta t)$$

- Filion quadrature makes  $a_n$  function of  $s\Delta t$

$$F(s) \approx \Delta t \sum_n a_n(s\Delta t) \exp(s n \Delta t) f(n \Delta t)$$

- $\Rightarrow$  Make projection basis  $s$  dependent
- $\Rightarrow$  Frequency dependence from asymptotic  $s \rightarrow i\infty$  (WKB)

# Phase-Preconditioning I - 1D

- We can overcome the Nyquist demand by splitting the wavefield into oscillatory and smooth part

$$u(s_j) = \exp(-s_j T_{\text{eik}}) c_{\text{out}}(s_j) + \exp(s_j T_{\text{eik}}) c_{\text{in}}(s_j). \quad (3)$$

- Oscillatory **phase term** obtained from high frequency asymptotics
- Eikonal equation  $|\nabla T_{\text{eik}}^{[l]}|^2 = \frac{1}{\nu^2}$
- Amplitudes  $c_{\text{out/in}}$  are smooth
- Motivated by Filon quadrature
  - Handle oscillatory part analytically
  - Quadrature with smooth amplitudes
- Note: Splitting not unique

# Phase-Preconditioning II

- Projection on frequency *dependent* Reduced Order Basis

$$\mathcal{K}_{\text{EIK}}^{2m}(\kappa, s) = \text{span}\{\exp(-sT_{\text{eik}}) c_{\text{out}}(s_1), \dots, \exp(-sT_{\text{eik}}) c_{\text{out}}(s_m), \\ \exp(sT_{\text{eik}}) c_{\text{in}}(s_1), \dots, \exp(sT_{\text{eik}}) c_{\text{in}}(s_m)\}$$

- Preserve Schwartz reflection principle

$$\mathcal{K}_{\text{EIK};R}^{4m}(\kappa, s) = \text{span}\{\mathcal{K}_{\text{EIK}}^{2m}(\kappa, s), \mathcal{K}_{\text{EIK}}^{2m}(\bar{\kappa}, s)\} \quad (4)$$

- equivalent to changing Operator
- Coefficients from Galerkin condition

$$u_m(s) = \sum_{i=1}^m \alpha_i(s) \exp(-sT_{\text{eik}}) c_{\text{out}}(s_i) + \sum_{i=1}^m \beta_i(s) \exp(sT_{\text{eik}}) c_{\text{in}}(s_i) + \dots$$

# Phase-Preconditioning III

- Non-uniqueness of splitting resolved by one-way WEQ

$$c_{\text{out}}(s_j) = \frac{\nu}{2s_j} \exp(-s_j T_{eik}) \left( \frac{s_j}{\nu} u(s_j) - \frac{\partial}{\partial |x - x_S|} u(s_j) \right), \quad (5)$$

$$c_{\text{in}}(s_j) = \frac{\nu}{2s_j} \exp(-s_j T_{eik}) \left( \frac{s_j}{\nu} u(s_j) + \frac{\partial}{\partial |x - x_S|} u(s_j) \right). \quad (6)$$

## Effects of Phase preconditioning on

- Number of Interpolation points
- Size of the computational Grid
- MIMO problems
- Computational Scheme

# Projection on frequency dependent space

- Let  $V_{m; \text{EIK}}(s)$  be a real basis of  $\mathcal{K}_{\text{EIK}; R}^{4m}(\kappa, s)$
- The reduced order model is given by

$$R_{m; \text{EIK}}(s) = V_{m; \text{EIK}}^H(s) Q(s) V_{m; \text{EIK}}(s).$$

- large inner products on GPU
- This preserves
  - symmetry
  - Schwarz reflection principle
  - passivity
  - Interpolation

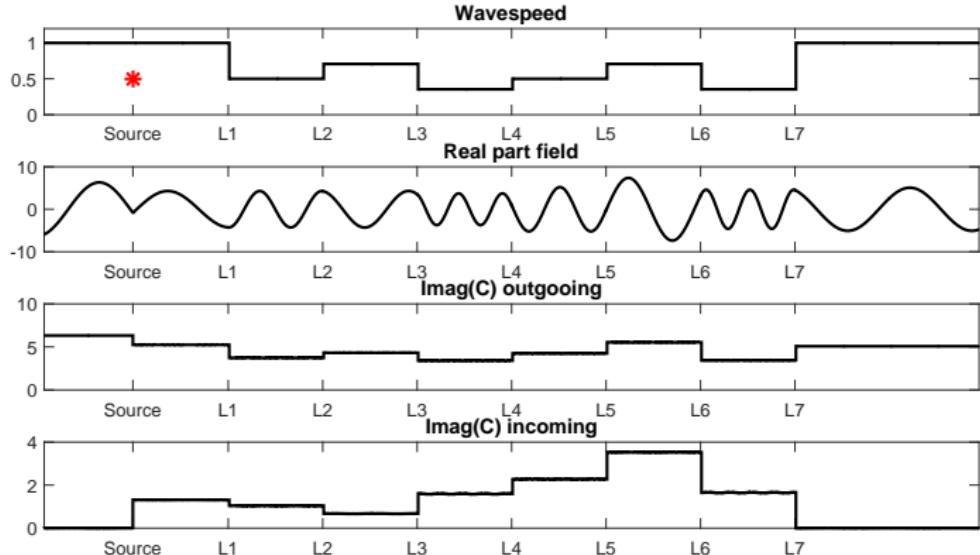
# Number of interpolation points needed

- Double interpolation of transfer function still holds

$$F_m(s) = F_m(s) \text{ and } \frac{d}{ds} F_m(s) = \frac{d}{ds} F(s) \text{ with } s \in \kappa \cup \bar{\kappa}. \quad (7)$$

- Number of interpolation point needed dependent on complexity medium, not latest arrival
- **Proposition:** Let a 1D problem have  $\ell$  homogenous layers . Then there exist  $m \leq \ell + 1$  non-coinciding interpolation points, such that the solution  $u_{m;EIK}(s) = u$ .

# Illustration of Proposition



- Amplitudes are constants in layers + left and right of source
- Basis is complete after  $\ell + 1$  iterations

# Phase-Preconditioning higher dimensions/MIMO

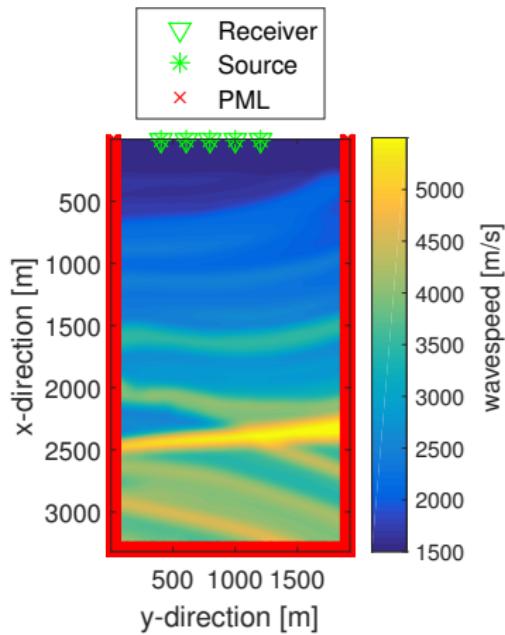
- Split with dimension specific function

$$u(s_j)^{[l]} = g(s_j T_{eik}^{[l]}) c_{\text{out}}(s_j)^{[l]} + g(-s_j T_{eik}^{[l]}) c_{\text{in}}(s_j)^{[l]}, \quad (8)$$

- $g(x)$  obtained from WKB approximation
- One way wave equations along  $\nabla T_{eik}$  used for decomposition
- In 2D is we use  $g(x) = \mathcal{K}_0(x)$  for outgoing
- Multiple  $T_{eik}^{[l]}$  for multiple sources  $[l]$  account for multiple direction

$$c_{\text{in}}(s_j) = \frac{s_j T}{\text{sign}(\Im m(s_j)) i \pi} \left[ \mathcal{K}_1(s_j T) u(s_j) + \mathcal{K}_0(s_j T) \frac{\nu^2}{s_j} \nabla T \cdot \nabla u(s_j) \right]$$

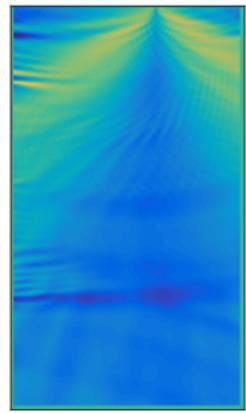
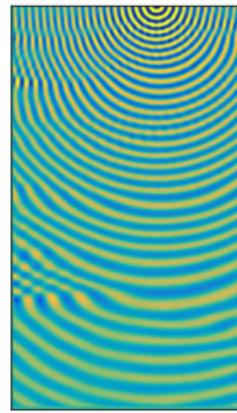
# Size of the computational Grid



(b) Section of the wave speed profile of the smoothed Marmousi model.

(c) Real part of the wavefield  $u^{[4]}$ .

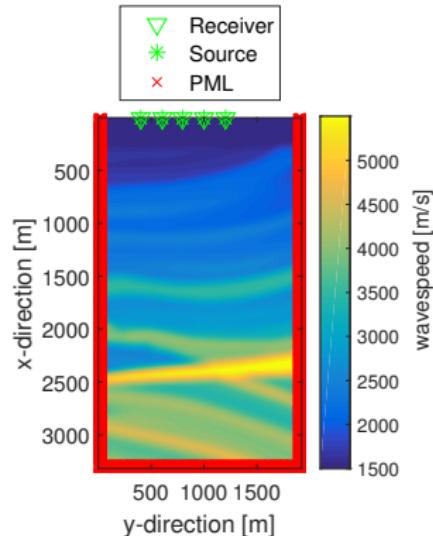
(d) Real part of the amplitude  $c_{\text{out}}^{[4]}$ .



# Numerical Experiments - I

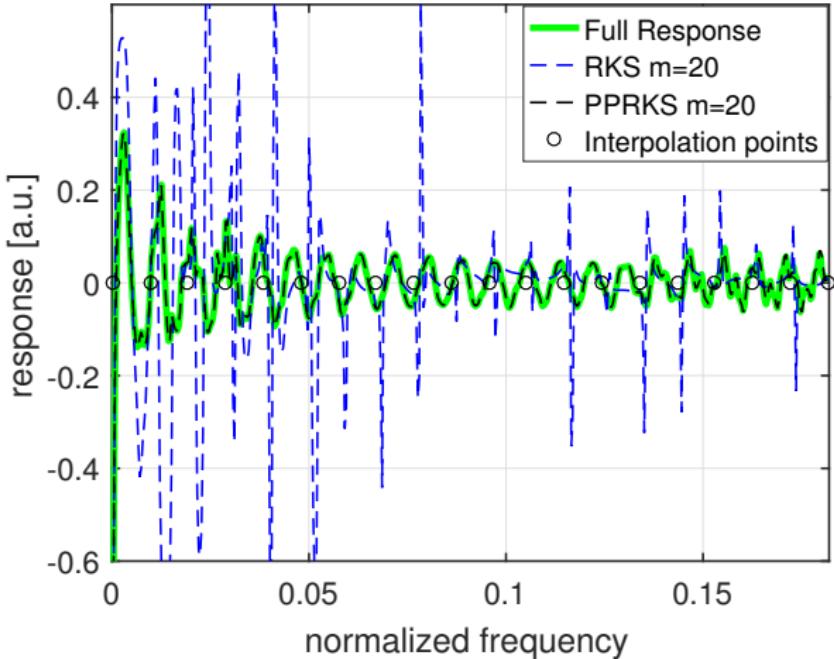
- Configurations (Neumann boundary condition on top)
- Layered medium
- Travel time dominated
- 5 Sources and 5 Receivers

$\Delta x$	4m
Comp. Size	829x480 points
Size	3160 m $\times$ 1920m
range $c$	1500 - 5500 m/s
Range Quadrature	0-40 Hz



(e) Section of the wave speed profile of the smoothed Marmousi model.

# Numerical Experiments

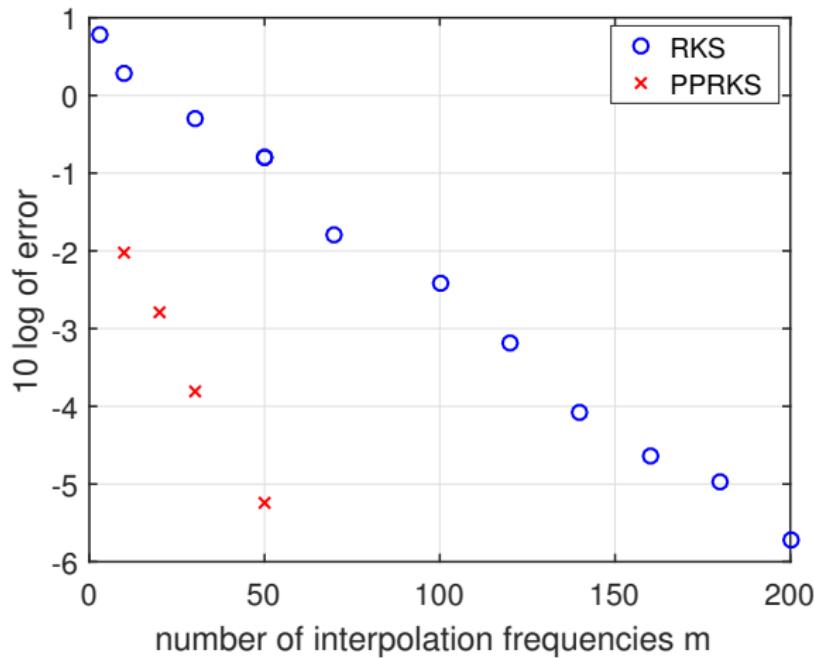


- Source 1 to Receiver 5
- PPRKS clearly outperforms RKS

(f) Real part of the frequency-domain transfer function

# Numerical Experiments I

- Time-domain convergence of the RKS and the PPRKS



# Computational Grid

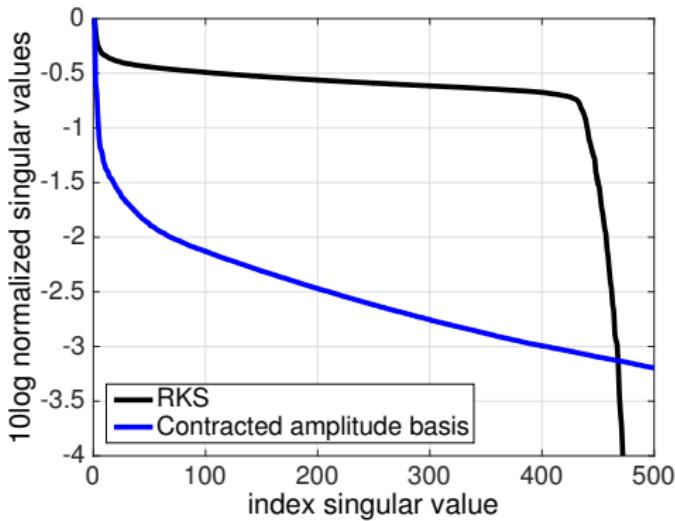
- Amplitudes  $c_{\text{in/out}}$  are much smoother than the wavefield
- ROM can extrapolate to high frequencies  
⇒ oscillatory part is handled analytically
- Two-grid approach:
- Amplitudes can be computed on coarse grid  $U_c = Q_{\text{course}}(s)^{-1} B_c$
- Interpolate amplitudes to fine grid
- Projection of operator and evaluation are performed on fine grid

$$F_{c;m}(s) = B^H \left\{ [V_{c;m}(s)]^H Q_{\text{fine}}(s) V_{c;m}(s) \right\}^{-1} B$$

- Solution gets gauged to the fine grid  
(no interpolation anymore)

# Phase-Preconditioning SVD

- Amplitudes are smooth in space and can become redundant
- Reduce amplitudes via SVD of  $[c_{\text{out}} \bar{c}_{\text{in}}] \Rightarrow c_{\text{SVD}}^j$
- Amplitudes have no source information



(h) Singular values of normalized  $(c_{\text{out}} \bar{c}_{\text{in}})$

# singular values larger than 0.01  
versus # sources with  $m = 40$

$N_{\text{src}}$	12	24	48	96
$[c_{\text{out}}, \bar{c}_{\text{in}}]$	69	72	73	73
$u$	457	833	1369	1741
$m \cdot N_{\text{src}}$	480	960	1920	3840

⇒ Reduction of sources

# Phase-Preconditioning SVD

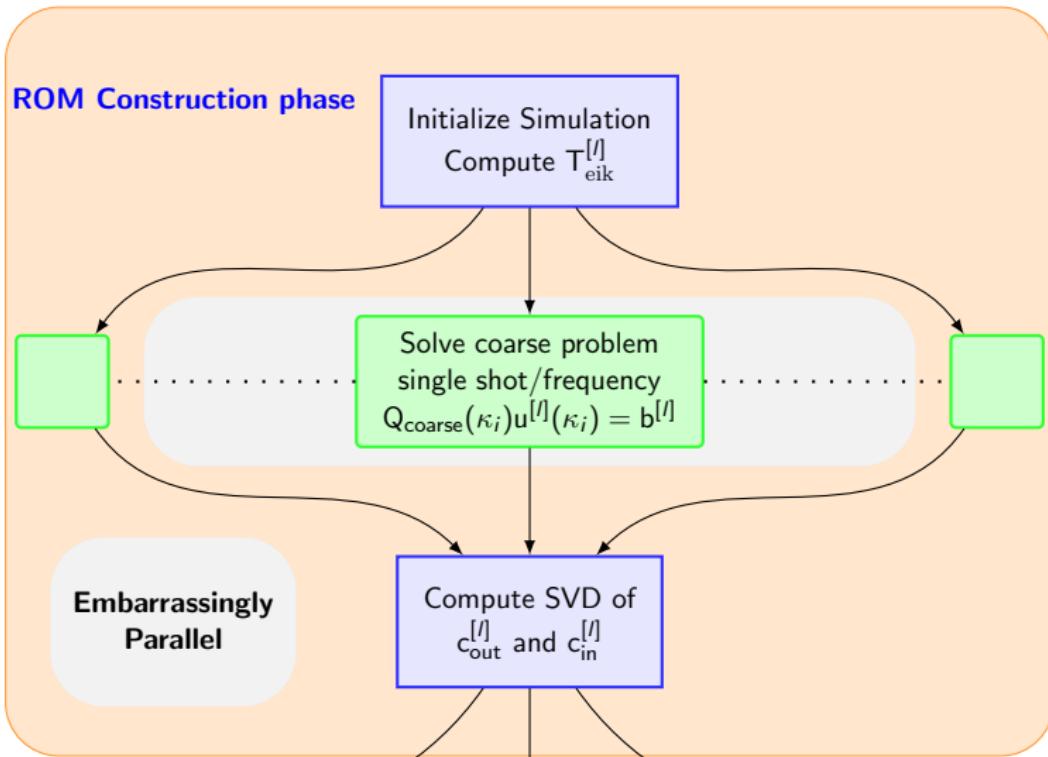
- Assume  $s \in i\mathbb{R}$  then we obtain

$$u_m^{[l]}(s) = \sum_{r=1}^{N_{\text{src}}} \sum_{j=1}^{M_{\text{SVD}}} \begin{bmatrix} a_{rj}^{[l]} \\ \alpha_{rj}^{[l]} \end{bmatrix}^T \begin{bmatrix} g(s T_{\text{eik}}^{[r]}) c_{\text{SVD}}^j \\ g(-s T_{\text{eik}}^{[r]}) \bar{c}_{\text{SVD}}^j \end{bmatrix} \quad (9)$$

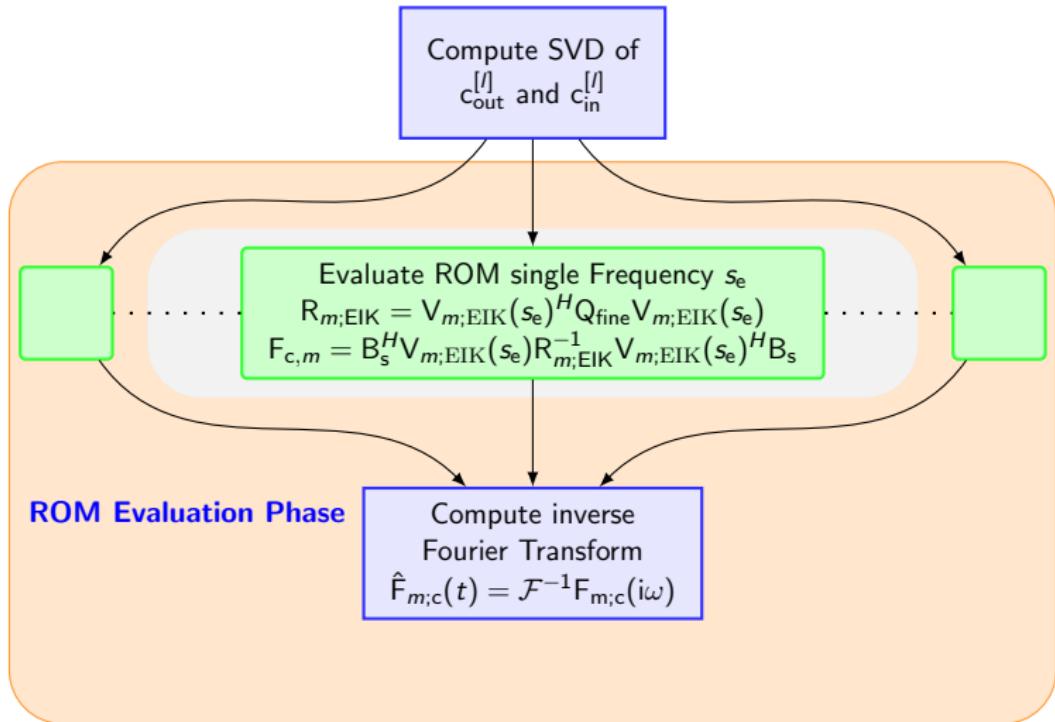
where  $M_{\text{SVD}} \ll 2mN_{\text{src}}$ .

- Coefficients from Galerkin condition
- $c_{\text{SVD}}^j$  is no longer source dependent

# Computational Scheme - Coarse Grid - CPU

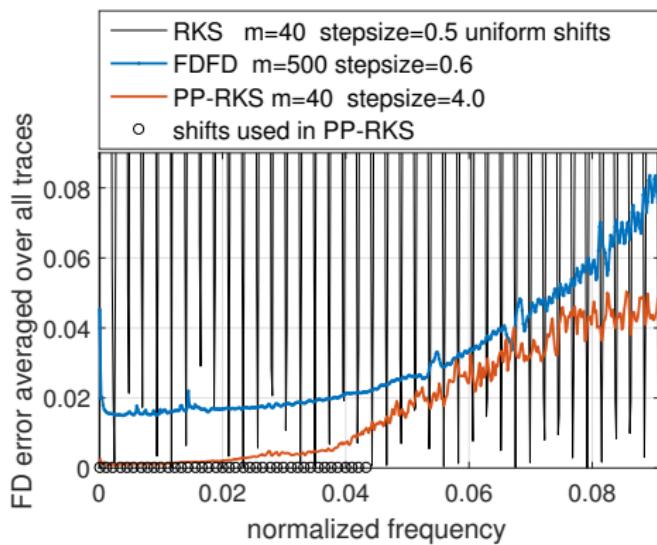


## Computational Scheme - Fine Grid - GPU

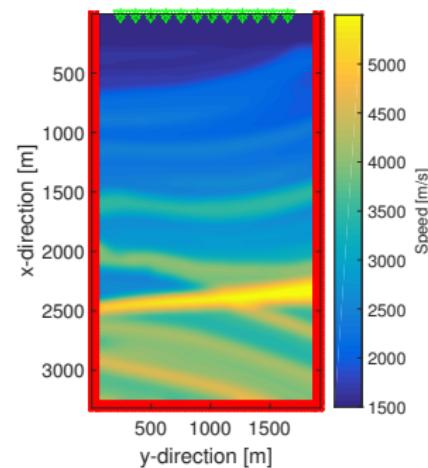


# Numerical Experiments - Grid Coarsening

- Coarsen the computation mesh by factor 16 (4 in each direction)
- Interpolation points until 5.5 ppw ( $m = 40$ ,  $N_{\text{src}} = 12$ ,  $M = 100$ )



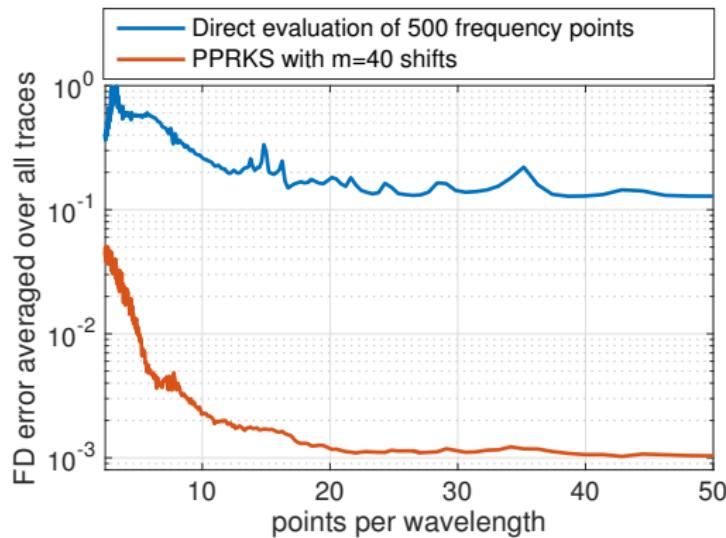
(i) Relative error  $\text{err}^{\text{average}}$



(j) Configuration

# Numerical Experiments - Grid Coarsening

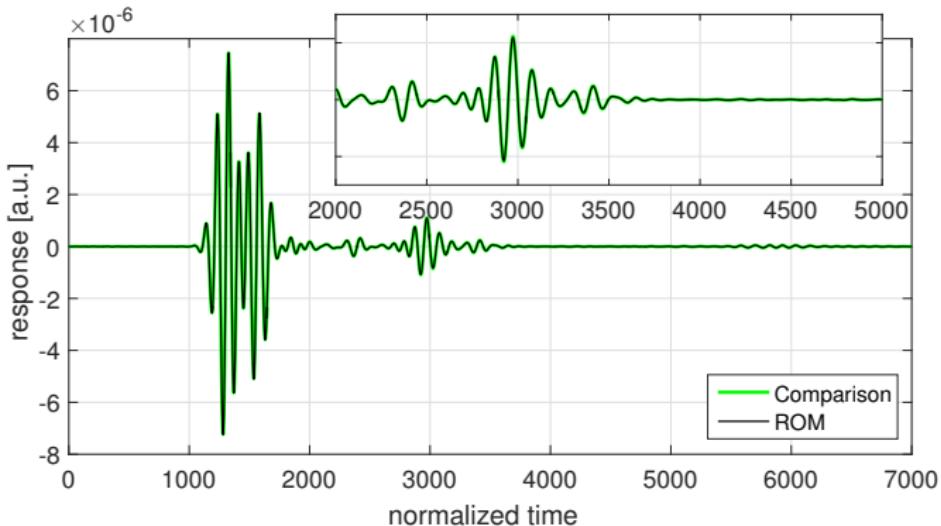
- Projection of fine operator gauges the ROM
- Direct evaluation of coarse operator not accurate



(k)  $\text{err}_{\text{ROM};\text{coarse}}^{\text{average}}$  versus  $\text{err}_{\text{FD};\text{coarse}}^{\text{average}}$

# Numerical Experiments - Grid Coarsening

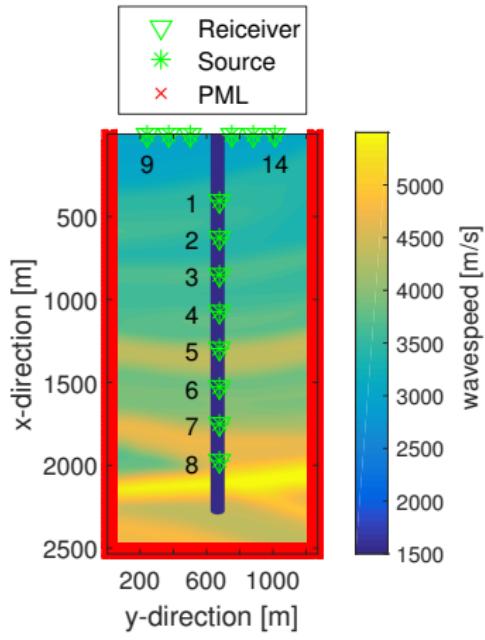
- Ricker Wavelet with cut-off frequency of 2.7 ppw on coarse grid



(I) Time domain trace from the left most source to the right most receiver after  $m = 40$  interpolation points.

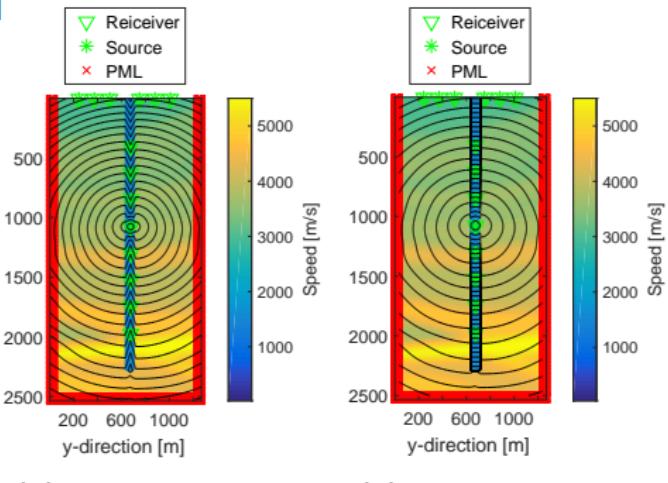
# Numerical Experiment III

- Resonant Borehole in smooth Geology
- Resonant behavior causes long runtimes
- 6 Surface- and 8 BH source-receiver pairs



(m) Simulated configuration.

# Numerical Experiments III

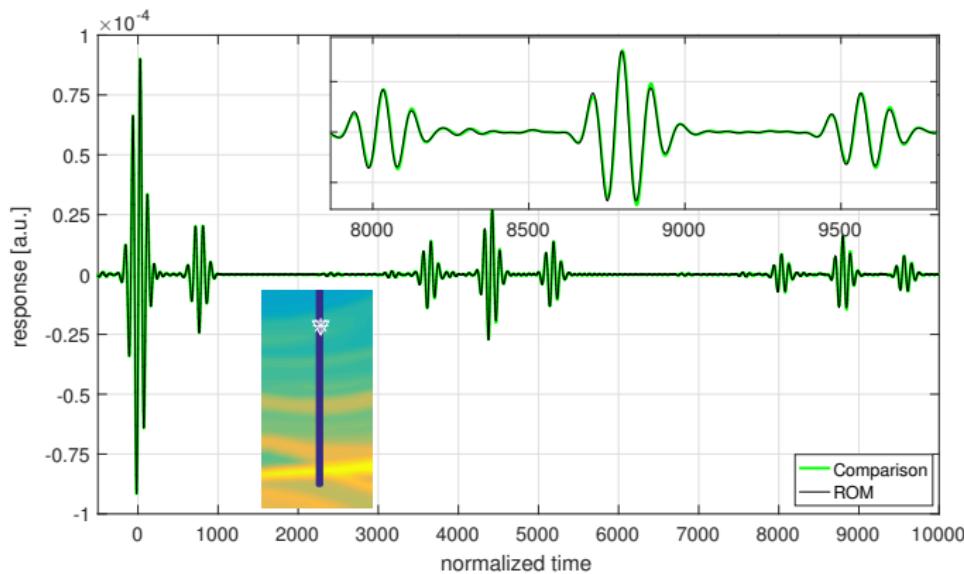


$$u^{[I]}(s_j) = g(s_j T_{eik}^{[I]}) c_{\text{out};eik}^{[I]}(s_j) + g(-s_j T_{eik}^{[I]}) c_{\text{in};eik}^{[I]}(s_j),$$
$$u^{[I]}(s_j) = g(s_j T_{eik;\text{CM}}^{[I]}) c_{\text{out};\text{CM}}^{[I]}(s_j) + g(-s_j T_{eik;\text{CM}}^{[I]}) c_{\text{in};\text{CM}}^{[I]}(s_j).$$

- $m = 40, N_{\text{src}} = 14, M_{\text{SVD}} = 30$
- $c_{\text{in/out};eik/\text{CM}}$

# Numerical Experiments III

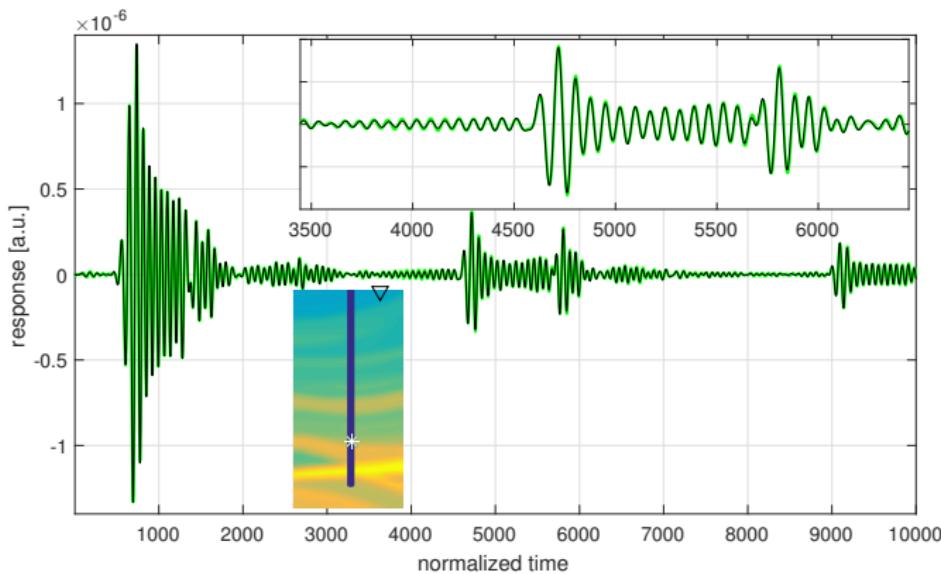
- Ricker Wavelet with cut-off frequency of 2.7 ppw on coarse grid



(p) Time-domain trace of the coinciding source receiver pair number 1 after  $m = 40$  interpolation points, together with the comparison solution.

# Numerical Experiments III

- Ricker Wavelet with cut-off frequency of 2.7 ppw on coarse grid



(q) Time-domain trace from source number 7 inside the borehole to the rightmost surface receiver number 14 after  $m = 40$  interpolation points.

# Conclusions

- All three challenges (Grid size, Nr of Sources, Nr of interpolation points) can be reduced with **phase preconditioning**
- Projection on frequency dependent basis allows ROM beyond the **Nyquist limit**
- Can be used for other oscillatory PDEs that have asymptotic solutions
- Work shifted from solvers to inner products
- Significantly compressed the ROM into coarse amplitudes

# Paper

V. Druskin, R. Remis, M. Zaslavsky and J. Zimmerling,  
*Compressing Large-Scale Wave Propagation Models via  
Phase-Preconditioned Rational Krylov Subspaces*, arXiv:1711.00942

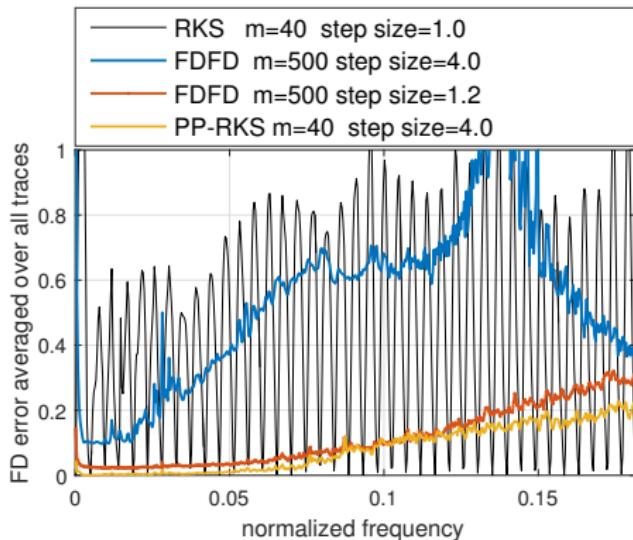
Thanks<sup>2</sup>

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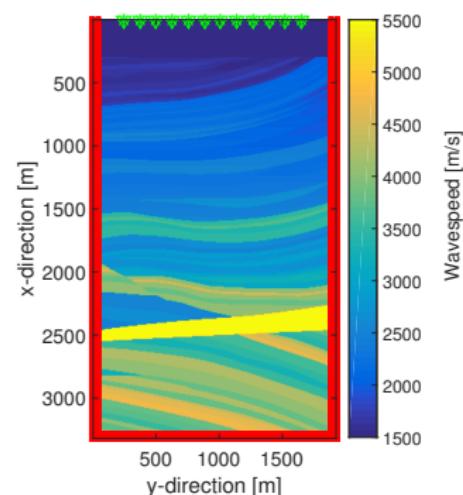
<sup>2</sup>STW (project 14222, **Good Vibrations**) and Schlumberger Doll-Research

# Numerical Experiments III

- Coarsen the computation mesh by factor 16 (4 in each direction)
- Interpolation points until 5.5 ppw ( $m = 40, N_{\text{src}} = 12, M = 150$ )



(g) Relative error  $\text{err}^{\text{average}}$

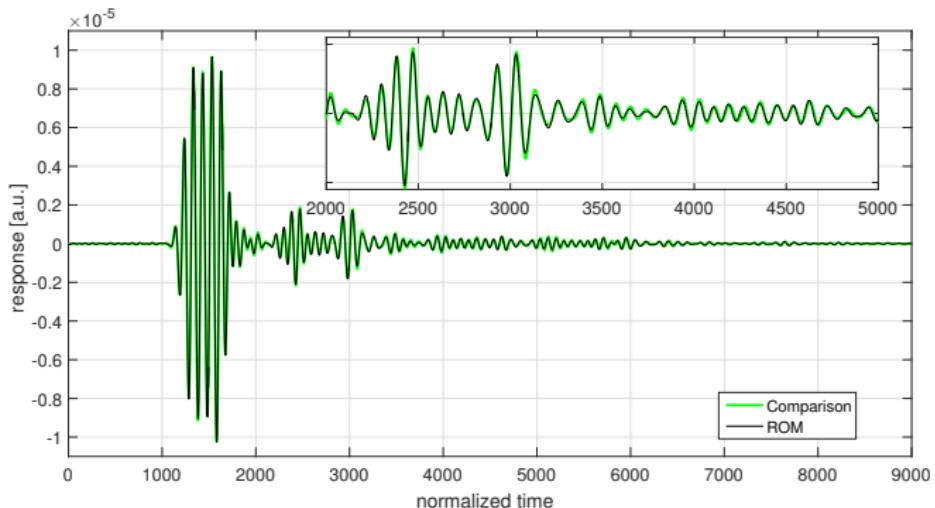


(h) Configuration

Figure: Marmousi test configuration with grid coarsening.

# Numerical Experiments III

- Ricker Wavelet with cut-off frequency of 2.7 ppw on coarse grid



(a) Time domain trace from the left most source to the right most receiver after  $m = 40$  interpolation points.

# Computational Complexity

- Cost of the basis computation and evaluation of the ROM
- Basis Computation on CPU<sup>3</sup>, Evaluation GPU<sup>4</sup>

Basis Computation comparison	Computation	Time	
Block solve fine grid	$Q_{\text{fine}}(s_i)^{-1}B$	10.3s	
Single solve fine grid	$Q_{\text{fine}}(s_i)^{-1}b$	4.1s	
Block solve coarse grid	$Q_{\text{coarse}}(s_i)^{-1}B$	0.6s	
Single solve coarse grid	$Q_{\text{coarse}}(s_i)^{-1}b$	0.2s	
Evaluation Step	Computation	Time	Scaling
Computing phase functions	$\exp(i\omega T_{\text{eik}})$	0.00546s	$N_{\text{src}}N_f$
Hadamard Products	$\exp(i\omega T_{\text{eik}}) c_{\text{SVD}}$	0.01496s	$M_{\text{SVD}}N_{\text{src}}N_f$
Galerkin inner product	$V_{m;\text{EIK}}(s_e)^H \cdot Q_{\text{fine}} V_{m;\text{EIK}}(s_e)$	1.752s	$N_f M_{\text{SVD}}^2 N_{\text{src}}^2$

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<sup>3</sup>Solved using UMFPACK v 5.4.0 on a 4-Core Intel i5-4670 CPU@3.40 GHz with parallel BLAS level-3 routines

<sup>4</sup>Double precision python implementation on an Nvidia GTX 1080 Ti

# Dispersion Correction

- At 5.5 ppw with a second order scheme we dispersion
- analytical travel time does not correspond to numerical
- use  $\nu'^{[l]}$  in decomposition to cancel highest  $s^2$  term

$$\exp\left(2sT_{\text{eik}}^{[l]}\right) \sum_{i=1}^k |D_{x_i} \exp\left(-sT_{\text{eik}}^{[l]}\right)|^2 = \frac{s^2}{\nu'^{[l]}{}^2} \quad (10)$$