# Evolution of a Scalable 3D Helmholtz Solver with Geophysical Applications

Russell J. Hewett Mathematics & CMDA, Virginia Tech

UMD Numerical Analysis Seminar

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- Laurent Demanet, MIT
- ► Adrien Scheuer, Universitè Catholique de Louvain

# Full Waveform Inversion



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seismic source + receivers $\rightarrow$ data	d
Earth's physical parameters	m
model physics (wave propagation)	$\mathcal{F}(m)$
full waveform inversion	$\min J(m) = \frac{1}{2}   d - \mathcal{F}(m)  _2^2$
gradient optimization	$m^{(k+1)} = m^{(k)} + f(\nabla J[m^{(k)}])$

## Full Waveform Inversion: Data



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# Full Waveform Inversion: Earth Models

#### Marmousi 2 Velocity



BP 2004 Velocity



# Full Waveform Inversion: Earth Models

#### SEAM Phase I Velocity (Fehler; SEG)



Polarized Traces & L-Sweeps

PDE constrained optimization in frequency domain

•  $\min J(m) = \frac{1}{2} ||d - \mathcal{F}(m)||_2^2$  s.t. Lu = f

Advantages:

No need to invert source time series

$$\hat{f}(\omega) = \mathsf{DFT}(f(t))$$

Only need specific frequency components

PDE constrained optimization in frequency domain

•  $\min J(m) = \frac{1}{2} ||d - \mathcal{F}(m)||_2^2$  s.t. Lu = f

Advantages:

Reduced memory and disk requirements in inverse problem

$$\delta m = -\langle q, \partial_{tt} u_0 \rangle_T = -\int_0^T q(x, t) \partial_{tt} u_0(x, t) dt$$

becomes

$$\delta m = -\left\langle q, -\omega^2 u_0 \right\rangle_{\Omega} = -\sum_{\omega} \hat{q}(x,\omega) - \omega^2 \hat{u}_0(x,\omega)$$

PDE constrained optimization in frequency domain

•  $\min J(m) = \frac{1}{2} ||d - \mathcal{F}(m)||_2^2$  s.t. Lu = f

Advantages:

- Multiple simultaneous right-hand sides
- ▶ With a factorization based method, only need to solve Helmholtz operator once per domain
- ► Compare to explicit time-stepping: "matvec" required for each time step for each source

PDE constrained optimization in frequency domain

•  $\min J(m) = \frac{1}{2} ||d - \mathcal{F}(m)||_2^2$  s.t. Lu = f

Advantages:

 $\blacktriangleright$  Heirarchichal frequency "sweeping"  $\Rightarrow$  Convergence guarantees



(E. Beretta, M.V. de Hoop, F. Faucher, O. Scherzer (SIMA 2016))



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Challenges for Frequency Domain Inversion ... it's all in the foward problem:

- Helmholtz in high frequency regime
- Helmholtz in 3D at high resolution
- Scalable Helmholtz in HPC environment

Take-home from this talk:

- ▶ With the right mix of tools, addressing all three is tractible
- Still need fast, parallelizable dense linear algebra
- ► Sub-linear complexity is achieved in parallel environments

Helmholtz at high frequency is hard

$$Hu = (-\omega^2 - \triangle)u = f + ABCs$$

- $\blacktriangleright$  Frequency  $\omega$  grows with n
- $\blacktriangleright$  Computational load N scales with  $n^d$

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### Classical dense direct methods in 3D

- memory-intensive
- hard to parallelize

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### Multigrid methods

- poor frequency scaling
- down-sampling oscillatory waves is hard

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### Classical iterative schemes

•  $n_{\mathrm{iter}}$  grows with  $\omega$ 

# Sweeping Solvers and Domain Decomposition Methods

### Sweeping Solvers/Preconditioners

- First O(N) claim (Engquist and Ying, 2010)
- ▶ First O(N) claim w/ domain decomposition (Stolk 2013)

# Sweeping Solvers and Domain Decomposition Methods

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Other domain-decomposition methods (DDMs):

- Multifrontal w/ HSS compression (Xia, et al., 2013)
- ▶ Hierarchical Poincare-Steklov methods (Gillman, et al., 2014)
- Common challenges:
  - Hazy scalability
  - Issues with rough media

### Sweeping Solvers/Preconditioners

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### Our approach: DDMs + sweeping w/ polarized traces

- Use direct methods distributed over tractable subproblems
- Glue with boundary integral formulations
- Embedded within iterative scheme



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Polarized Traces & L-Sweeps



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Polarized Traces & L-Sweeps



Polarization condition:

$$\begin{split} 0 &= -\int_{\Gamma} G(x,y)\partial_{n_y} u^{\uparrow}(y) ds_y \\ &+ \int_{\Gamma} \partial_{n_y} G(x,y) u^{\uparrow}(y) ds_y \end{split}$$



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Polarized Traces & L-Sweeps



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Polarized Traces & L-Sweeps

# Sweeping Algorithm



Zepeda-Nuñez, RJH, & Demanet, SEG, 2014

Zepeda-Nuñez & Demanet, JCP, 2016

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Polarized Traces & L-Sweeps

# Polarized Traces & A Sequential Bottleneck

- Assume local PDE is solved in the bulk Traces can be found by solving  $\underline{\mathbf{M}} \ \underline{\mathbf{u}} = \underline{\mathbf{f}} = \begin{bmatrix} \mathbf{v}_n^1 \\ \mathbf{v}_1^2 \\ \mathbf{v}_n^2 \\ \vdots \\ \mathbf{v}_1^L \end{bmatrix}$
- M is constructed from dense Green's function blocks...but is non-trivial to invert ►



# Polarized Traces & A Sequential Bottleneck

- Annihilation relation:
  - $\blacktriangleright$  If  $\mathbf{u}^{\uparrow}$  is an up-going wavefield, then the annihilator relations are true on the lower-half plane, i.e.

$$\mathcal{G}_i^{\downarrow,\ell}(\mathbf{u}_-^\uparrow,\mathbf{u}_1^\uparrow)=0,\qquad \text{for }i\geq 1.$$

 $\blacktriangleright$  If  $\mathbf{u}^{\downarrow}$  is a down-going wavefield, then the annihilator relations are true on the upper-half plane, i.e.

$$\mathcal{G}_i^{\uparrow,\ell}(\mathbf{u}_n^{\downarrow},\mathbf{u}_+^{\downarrow}) = 0, \qquad ext{for } i \leq n^\ell$$

## Polarized Traces & A Sequential Bottleneck

1. Seek to solve  $\underline{\mathbf{M}} \, \underline{\mathbf{u}} = \underline{\mathbf{f}}$
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2. Transform to underdetermined system

$$\begin{bmatrix} \mathbf{M} & \mathbf{M} \end{bmatrix} \begin{bmatrix} \mathbf{u}^{\downarrow} \\ \mathbf{u}^{\uparrow} \end{bmatrix} = -\mathbf{\underline{f}}$$

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3. Constrain with annihilation relations

$$\left[\begin{array}{cc} \underline{\mathbf{M}} & \underline{\mathbf{M}} \\ \underline{\mathbf{A}}^{\downarrow} & \underline{\mathbf{A}}^{\uparrow} \end{array}\right] \left[\begin{array}{c} \underline{\mathbf{u}}^{\downarrow} \\ \underline{\mathbf{u}}^{\uparrow} \end{array}\right] = - \left[\begin{array}{c} \underline{\mathbf{f}} \\ \underline{\mathbf{0}} \end{array}\right]$$

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4. Additional minor transformations and permutations

$$\begin{bmatrix} \underline{\mathbf{D}}^{\downarrow} & \underline{\mathbf{U}} \\ \underline{\mathbf{L}} & \underline{\mathbf{D}}^{\uparrow} \end{bmatrix} \underline{\underline{\mathbf{u}}} = \underline{\underline{\mathbf{f}}}$$

1. Seek to solve  $\underline{\mathbf{M}}\,\underline{\mathbf{u}}=\underline{\mathbf{f}}$ 

2. Transform to underdetermined system

$$\begin{bmatrix} \mathbf{\underline{M}} & \mathbf{\underline{M}} \end{bmatrix} \begin{bmatrix} \mathbf{\underline{u}}^{\downarrow} \\ \mathbf{\underline{u}}^{\uparrow} \end{bmatrix} = -\mathbf{\underline{f}}$$

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$$\left[\begin{array}{cc}\underline{\mathbf{M}} & \underline{\mathbf{M}} \\ \underline{\mathbf{A}}^{\downarrow} & \underline{\mathbf{A}}^{\uparrow}\end{array}\right] \left[\begin{array}{c}\underline{\mathbf{u}}^{\downarrow} \\ \underline{\mathbf{u}}^{\uparrow}\end{array}\right] = -\left[\begin{array}{c}\underline{\mathbf{f}} \\ \underline{\mathbf{0}}\end{array}\right]$$

4. Additional minor transformations and permutations

$$\begin{bmatrix} \underline{\mathbf{D}}^{\downarrow} & \underline{\mathbf{U}} \\ \underline{\mathbf{L}} & \underline{\mathbf{D}}^{\uparrow} \end{bmatrix} \underline{\underline{\mathbf{u}}} = \underline{\underline{\mathbf{f}}}$$

5. Final system of equations

$$\underline{\underline{\mathbf{M}}} \underline{\underline{\mathbf{u}}} = \underline{\underline{\mathbf{f}}}$$

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# $\blacktriangleright\ \ldots\underline{\mathbf{M}}$ is far easier to invert

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$$\blacktriangleright \underline{\mathbf{M}} = \left[ \begin{array}{cc} \underline{\mathbf{D}}^{\downarrow} & \mathbf{0} \\ \mathbf{0} & \underline{\mathbf{D}}^{\uparrow} \end{array} \right] + \left[ \begin{array}{cc} \mathbf{0} & \underline{\mathbf{U}} \\ \underline{\mathbf{L}} & \mathbf{0} \end{array} \right]$$

- Block diagonal, and block upper and lower triangular
  - Perfect for block Gauss-Seidel
- Embed Gauss-Seidel iteration into GMRES to achieve convergence independent of number of layers



# BP 2004 2D solution



#### Iteration 0

# BP 2004 2D solution



#### Iteration 1 (2 domain sweeps)

# BP 2004 2D solution



#### Iteration 2 (4 domain sweeps)

# The State of Method So Far

- $\blacktriangleright$  Explicit representation of  $\underline{\mathbf{M}}$
- Matrix blocks are concrete representations of the Green's function
- Green's function blocks are compressed using PLR format
- Green's functions can be computed off-line, in parallel
- Gauss-Seidel sweep is inherently sequential
- Sequential nature corresponds directly to the physics



# Challenges in Moving to 3D

- Green's function blocks: n (in 2D) vs  $n^2$  (in 3D)
- Explicit computation is impractical at scale
- ▶ PLR does not work as well for 2D Green's functions
- Sequential portion is still sequential
- Solution: Don't compute Green's functions. Solve local systems.
- Problem: Local systems are still computationally difficult.



# Can We Apply Polarized Traces Recursively?

- Solution: Use polarized traces to solve local systems.
- Problem: Same major sequential bottleneck.



Zepeda-Nuñez & Demanet, SISC, 2018

#### Domain

Zepeda-Nuñez, RJH, Demanet, & Scheuer, SEG, 2016

Zepeda-Nuñez, Scheuer, RJH, & Demanet, Geophysics, 2019



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# Sources of Parallelism: Layers

MPI: Parallelize over Layers

Zepeda-Nuñez, RJH, Demanet, & Scheuer, SEG, 2016 Zepeda-Nuñez, Scheuer, RJH, & Demanet, Geophysics, 2019

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Zepeda-Nuñez, RJH, Demanet, & Scheuer, SEG, 2016

Zepeda-Nuñez, Scheuer, RJH, & Demanet, Geophysics, 2019

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MPI: Multifrontal/Nested dissection

Zepeda-Nuñez, RJH, Demanet, & Scheuer, SEG, 2016

Zepeda-Nuñez, Scheuer, RJH, & Demanet, Geophysics, 2019

# OpenMP: Parallelize within MPI tasks



Zepeda-Nuñez, RJH, Demanet, & Scheuer, SEG, 2016

Zepeda-Nuñez, Scheuer, RJH, & Demanet, Geophysics, 2019

# Pipelining: Parallelizing the Sequential Part



# Pipelining: Parallelizing the Sequential Part



#### Homogeneous Problem



Polarized Traces & L-Sweeps

N	$50^{3}$	$100^{3}$	$100^{3}$	$200^{3}$	$200^{3}$	$400^{3}$	$400^{3}$	$400^{3}$
L	5	10	10	20	20	40	40	40
MPI Tasks	5	10	10	80	80	640	640	640
OMP Threads/Task	1	1	2	1	2	1	2	3
Total Cores	5	10	20	80	160	640	1280	1920
Total Nodes	1	1	2	5	10	80	80	128
Single rhs								
# GMRES Iterations	4	4	4	5	5	6	6	6
Initialization [s]	0.2	1.0	0.9	6.9	4.4	18.9	18.9	18.4
Factorization [s]	4.1	41.1	21.9	153.2	78.3	320.5	200.1	148.6
Online [s]	4.0	39.2	22.6	182.0	109.7	696.6	401.4	315.5
Avg. GMRES [s]	0.9	8.4	4.8	32.0	19.2	103.5	59.3	46.6
Pipelined rhs								
R (number of rhs)	5	10	10	20	20	40	40	40
Online [s]	15.8	189.4	106.2	1255.5	668.5	3994.2	2654.4	1878.1
Avg. GMRES [s]	3.4	40.6	22.7	223.8	118.6	599.9	401.0	283.0
Online/rhs [s]	3.2	18.9	10.6	62.8	33.4	99.9	66.4	47.0
Avg. GMRES/rhs [s]	0.7	4.1	2.3	11.2	5.9	15.0	10.0	7.1

#### Homogeneous Problem

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#### Smooth Heterogeneous Problem



Polarized Traces & L-Sweeps

N	$50^{3}$	$100^{3}$	$100^{3}$	$200^{3}$	$200^{3}$	$400^{3}$	$400^{3}$	$400^{3}$
L	5	10	10	20	20	40	40	40
MPI Tasks	5	10	10	80	80	640	640	640
OMP Threads/Task	1	1	2	1	2	1	2	3
Total Cores	5	10	20	80	160	640	1280	1920
Total Nodes	1	1	2	5	10	80	80	128
Single rhs								
# GMRES Iterations	5	5	5	5	5	6	6	6
Initialization [s]	0.2	1.1	1.0	7.3	4.6	21.3	21.2	20.8
Factorization [s]	3.8	41.1	21.8	156.0	79.4	323.7	204.5	151.5
Online [s]	4.6	45.9	26.1	202.2	106.9	717.0	400.1	314.5
Avg GMRES [s]	0.8	8.1	4.6	35.5	18.7	106.4	59.2	46.5
Pipelined rhs								
R (number of rhs)	5	10	10	20	20	40	40	40
Online [s]	17.1	225.1	118.8	1260.9	650.2	4085.0	2714.8	1872.1
Avg GMRES [s]	3.0	39.8	20.9	223.6	115.6	613.3	409.2	281.9
Online/rhs [s]	3.4	22.5	11.9	63.0	32.5	102.1	67.9	46.8
Avg GMRES/rhs [s]	0.6	4.0	2.1	11.2	5.8	15.3	10.2	7.0

#### Smooth Heterogeneous Problem

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#### Fault Problem



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Polarized Traces & L-Sweeps

N	$50^{3}$	$100^{3}$	$100^{3}$	$200^{3}$	$200^{3}$	$400^{3}$	$400^{3}$	$400^{3}$
L	5	10	10	20	20	40	40	40
MPI Tasks	5	10	10	80	80	640	640	640
OMP Threads/Task	1	1	2	1	2	1	2	3
Total Cores	5	10	20	80	160	640	1280	1920
Total Nodes	1	1	2	5	10	80	80	128
Single rhs								
# GMRES Iterations	4	5	5	5	5	6	6	6
Initialization [s]	0.4	1.1	1.0	7.3	4.7	20.4	20.3	21.0
Factorization [s]	3.8	40.4	22.1	152.2	79.9	317.6	199.5	152.5
Online [s]	3.7	46.2	26.2	188.5	109.8	713.2	395.8	315.6
Avg GMRES [s]	0.8	8.1	4.6	33.0	19.2	106.2	58.7	46.5
Pipelined rhs								
R (number of rhs)	5	10	10	20	20	40	40	40
Online [s]	13.7	226.7	122.4	1222.7	647.1	4031.6	2710.6	1838.9
Avg GMRES [s]	2.9	40.1	21.6	216.5	114.7	605.0	409.9	276.3
Online/rhs [s]	2.7	22.7	12.2	61.1	32.4	100.8	67.7	46.0
Avg GMRES/rhs [s]	0.6	4.0	2.2	10.8	5.7	15.1	10.2	6.9

#### Fault Problem

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SEAM Problem



N	$6.51 \cdot 10^{5}$	$5.16\cdot 10^6$	$4.12\cdot 10^7$	$4.12\cdot 10^7$
L	12	24	48	48
MPI Tasks	12	48	384	384
OpenMP Threads per Task	1	2	2	3
Total Cores	12	96	768	1152
Total Nodes	1	6	77	77
Single rhs				
# GMRES Iterations	4	5	6	6
Initialization [s]	0.6	2.3	10.4	10.7
Factorization [s]	15.2	46.5	111.4	97.9
Online [s]	21.4	85.6	269.8	228.4
Average GMRES [s]	4.6	14.9	40.0	33.7
Pipelined rhs				
R (number of rhs)	12	24	48	48
Online [s]	106.3	474.8	1527.1	1415.4
Average GMRES [s]	22.8	83.9	229.4	212.9
Online per rhs [s]	8.8	19.8	31.8	29.5
Average GMRES per rhs [s]	1.9	3.5	4.8	4.4

#### SEAM Problem

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**Pipelined Parallel Run-time complexity:**  $\mathcal{O}(\max(1, R/L)N \log N)$ 

Question: Can we better parallelize this preconditioner?

Problem: Serial nature of the sweeps

Problem: 2D memory growth due to planar slabs

Problem: Interface "communication" volume



Polarization condition:

$$\begin{split} 0 &= -\int_{\Gamma} G(x,y) \partial_{n_y} u^{\uparrow}(y) ds_y \\ &+ \int_{\Gamma} \partial_{n_y} G(x,y) u^{\uparrow}(y) ds_y \end{split}$$



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### Solution: L-sweeps



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#### Solution: L-sweeps



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Each propagation onto the next diagonal can is embarrassingly parallel on a cell-wise level!



## M O V I E! :)

Each propagation onto the next diagonal can is embarrassingly parallel on a cell-wise level!

 $\Rightarrow O(N/p) \underset{(\text{as long as } p = O(N^{1/d}))}{\text{complexity}}$ 



N	$\omega/2\pi$	p	$T_{\texttt{fact}}$	$N_{\texttt{it}}$	$T_{\texttt{it}}$	$T_{\texttt{total}}$
$202 \times 202$	20.1	2	1.09	2	0.66	2.63
$404 \times 404$	40.3	4	1.00	3	0.58	2.56
808  imes 808	80.7	8	1.41	3	1.26	6.02
$1616\times1616$	161.5	16	2.80	2	3.39	14.05
3232  imes 3232	323.1	32	4.41	3	5.47	27.47
$6464\times 6464$	646.3	64	8.34	4	11.09	67.74
$12928\times12928$	1292.7	128	15.66	5	22.39	160.88

#### Numerical Example: Homogeneous Velocity



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(without PML)	$\omega/2\pi$	q = r	BG1	BG2	with salt	with salt	model
$202 \times 202$	20.1	2	1	4	7	6	7
$404 \times 404$	40.3	4	2	4	9	9	9
$808 \times 808$	80.7	8	4	6	12	12	12
$1616\times1616$	161.4	16	5	6	15	15	15
$3232 \times 3232$	323.1	32	6	7	17	17	16
$6464 \times 6464$	646.3	64	7	7	19	19	19
$12928 \times 12928$	1292.7	128	8	8	21	21	20

RJH (Virginia Tech)

Polarized Traces & L-Sweeps



- max. 16 wavelengths in domain
- PML width:
  1.25 wavelengths
- ► 2 × 2 domain decomposition



Polarized Traces & L-Sweeps



- max. 32 wavelengths in domain
- PML width:
  1.5 wavelengths
- $4 \times 4$  domain decomposition





- max. 64 wavelengths in domain
- PML width:
  1.75 wavelengths
- ► 8 × 8 domain decomposition





- max. 128
  wavelengths in domain
- PML width:2 wavelengths
- ► 16 × 16 domain decomposition





- max. 256 wavelengths in domain
- PML width:2.25 wavelengths
- ► 32 × 32 domain decomposition





- max. 512 wavelengths in domain
- PML width:2.5 wavelengths
- ▶ 64 × 64 domain decomposition





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Polarized Traces & L-Sweeps

#### Numerical Example: High-contrast Waveguide



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Polarized Traces & L-Sweeps

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#### Numerical Example: High-contrast Waveguide

N			Contrast ratio					
(without PML)	$\omega/2\pi$	m = n	2	3	4	5	6	
$202 \times 202$	20.1	2	18	24	24	25	26	
$404 \times 404$	40.3	4	28	29	29	28	30	
808  imes 808	80.7	8	30	32	34	33	33	
$1616\times1616$	161.5	16	31	33	33	34	35	
$3232 \times 3232$	323.1	32	32	34	36	36	37	
$6464\times 6464$	646.3	64	32	34	35	36	36	

### Numerical Example: High-contrast Waveguide



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Polarized Traces & L-Sweeps

- ▶ There are serious challenges in optimizing parallelism in 3D
- Current implementation uses vertically extruded subdomains
- Consider it a quasi-2D domain decomposition

### Numerical Example: Homogeneous Velocity (3D)

N						
(without PML)	$\omega/2\pi$	p	$T_{\texttt{fact}}$	$N_{\texttt{it}}$	$T_{\texttt{it}}$	$T_{\texttt{total}}$
$26\times26\times26$	4.17	2	.04	4	1.34	6.52
$52 \times 52 \times 52$	8.50	4	5.54	6	5.30	37.17
78  imes 78  imes 78	12.83	6	12.42	6	12.80	89.76
$104\times104\times104$	17.17	8	22.91	6	23.27	163.62
$130\times130\times130$	21.50	10	37.53	7	36.47	292.33
$156\times156\times156$	25.83	12	52.47	7	51.62	417.08
$182\times182\times182$	30.17	14	71.71	8	68.92	627.23
$208\times208\times208$	34.50	16	96.14	7	91.65	743.37
$234\times234\times234$	38.83	18	124.64	8	116.08	1050.31
$260\times260\times260$	43.17	20	211.87	7	177.21	1438.12
$312\times312\times312$	51.83	24	314.93	8	263.16	2457.40
$416\times416\times416$	69.17	32	418.36	9	377.60	3992.63

#### Numerical Example: Homogeneous Velocity (3D)



RJH (Virginia Tech)

## Successful construction of a scalably parallelizable preconditioner for the high-frequency Helmholtz equation.

- ▶ O(N/p) complexity as long as  $p = O(N^{1/d})$
- Independent of the discretization
- Applicable to heterogeneous media
- Paper: https://arxiv.org/abs/1909.01467

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#### Next steps:

- ▶ O(N/p)-scaling in 3D where  $p = O(N^{2/3})$
- $\blacktriangleright$  several right-hand sides (O(1) scaling per right hand side?)