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The method of polarized traces for the 3D Helmholtz equation

FAST, ACCURATE AND SCALABLE SOLVERS FOR THE HIGH-FREQUENCY HELMHOLTZ EQUATION

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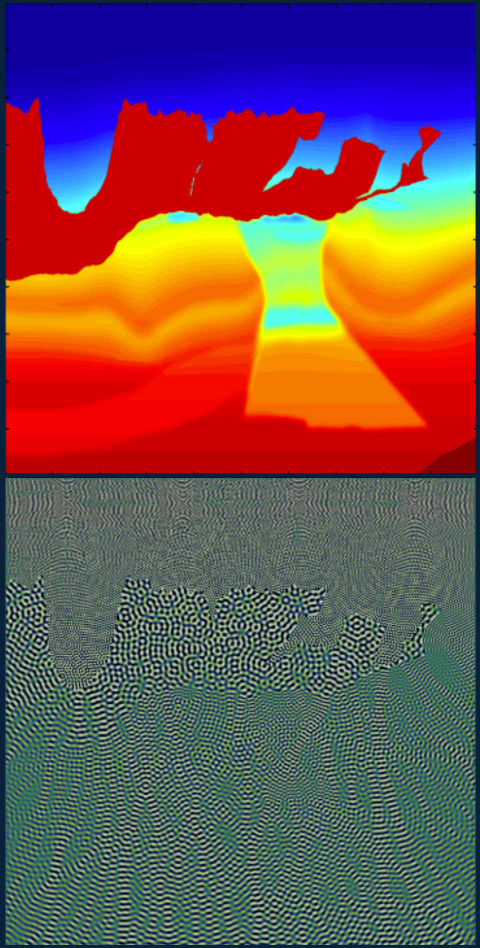
In collaboration with Leonardo Zepeda-Núñez, Matthias Taus, Russell Hewett and Laurent Demanet

TOTAL

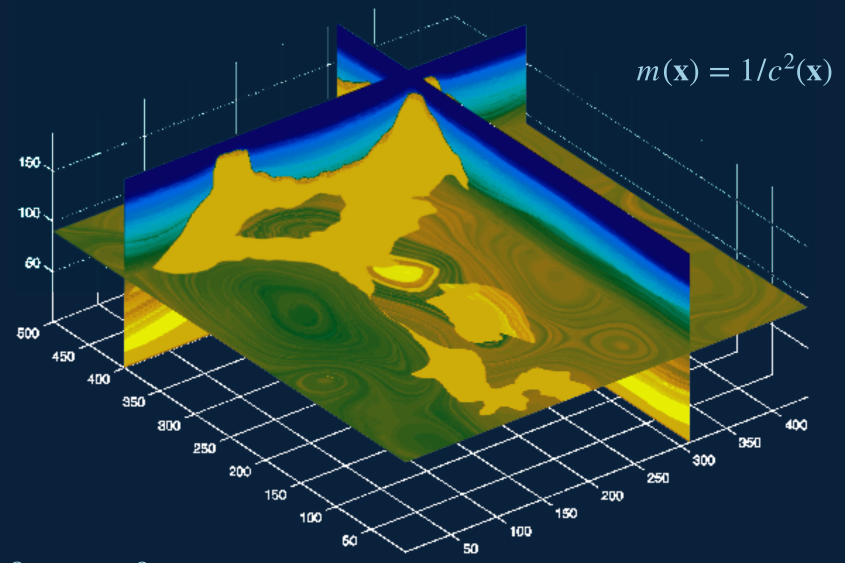
Outline

- The Helmholtz equation
- Complexity claims
- The method of polarized traces
- Implementation and numerical results
- Further developments



The Helmholtz equation

TARGET APPLICATIONS: INVERSE PROBLEMS



- 10^8 to 10^9 unknowns
- 50+ wavelengths across the domain
- 10^3 to 10^4 sources

→ Need for a scalable solver!

HELMHOLTZ EQUATION

$$(\nabla^2 + \omega^2 m(\mathbf{x}))\ u(\mathbf{x}) = f_s(\mathbf{x}) \text{ in } \Omega$$

absorbing b.c. at $\partial\Omega$

Sources: $f_s\ ,\quad s = 1, \ldots, R$

After discretization

$$\mathbf{H}\ \mathbf{u} = \mathbf{f}_s$$

Structured discretization: $N = n^d$

High frequency regime: $\omega \sim n$

Why is it hard to solve?

- Unbounded domain
- The discretization is in general not stable, $N \gtrsim \omega^d$
  (FD: pollution error; SE & IE: dense system; A-HDG: high interconnectivity)
- The complexity of many solvers grows faster than N
  - Classical iterative methods are slow: N_{iter} grows with ω
  - Classical direct methods are memory-intensive and hard to parallelize

	2D	3D
Operations	$O(N^{3/2})$	$O(N^2)$
Memory	$O(N \log N)$	$O(N^{4/3})$

$\rightarrow$ **method of polarized traces: combination of iterative and direct solvers**

- Very active field of research over the last decade
  Gander and Zhang, 2019

Scalability

COMPLEXITY IS NOT JUST A FUNCTION OF N

P: number of processors

Distribute the input / output

$\rightarrow$ can expect not just $O(N)$, but $O(N/P)$ even for large P

Zepeda-Núñez and Demanet, 2016; 2018: Online complexity $O(N/P)$, $P = O(N^{1/5})$ (2D)
Taus *et al.*, 2019: Online complexity $O(N/P)$, $P = O(N^{1/d})$ (2D and 3D)

R: number of right-hand sides (sources)

Handle several hrs at once

$\rightarrow$ can expect not just $O(RN)$, but $O(N)$ even for large R

Zepeda-Núñez *et al.*, 2019: Online complexity $O(N)$, $R = O(N^{1/3})$ (3D)

The method of polarized traces

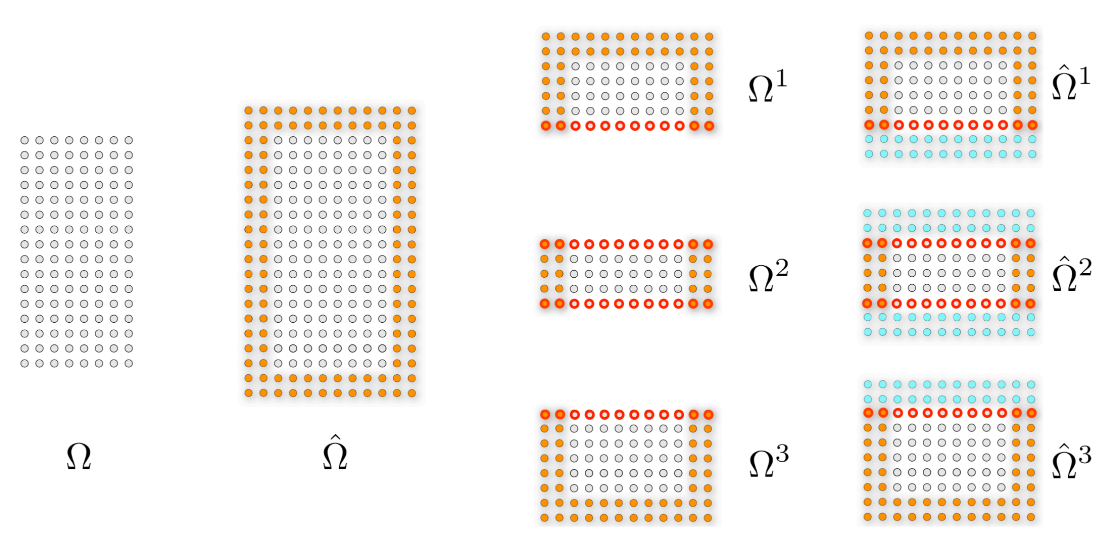
Zepeda-Núñez and Demanet, 2016

POLARIZED TRACES

$\equiv$ domain decomposition method with transmission boundary condition

Polarization: decompose $u = u^{\uparrow} + u^{\downarrow}$

Traces: restrict $u^{\uparrow}$ and $u^{\downarrow}$ on the interfaces Γ_i



LOCAL FORMULATIONS

Discretized local problem in layer l

$$\mathbf{H}^l\ \mathbf{u}^l = \mathbf{f}_s^l$$

(PML used as absorbing b.c.)

REDUCTION TO SURFACE INTEGRAL EQUATION

Coupling the subdomains using the Green's representation formula within each layer

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

to solve iteratively

The method of polarized traces

Zepeda-Núñez and Demanet, 2016

PRECONDITIONING WITH POLARIZED TRACES

Introducing the polarized wavefield

$$\underline{\mathbf{u}} = \underline{\mathbf{u}}^{\uparrow} + \underline{\mathbf{u}}^{\downarrow}\,; \quad \underline{\underline{\mathbf{u}}} = \begin{bmatrix} \underline{\mathbf{u}}^{\uparrow} \\ \underline{\mathbf{u}}^{\downarrow} \end{bmatrix}$$

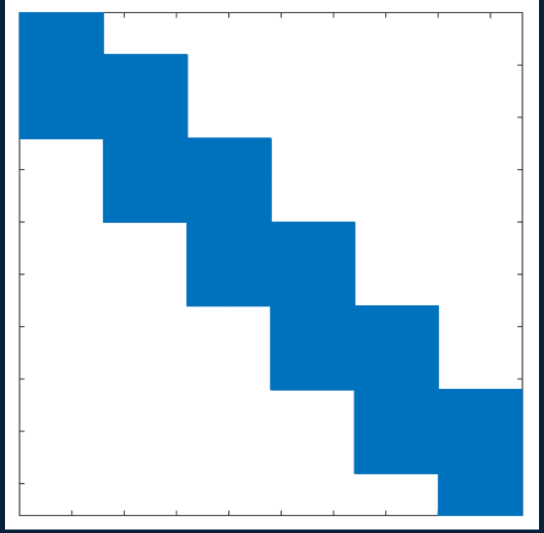
and imposing annihilation/polarization conditions (with some permutations and algebraic operations)

$$\underline{\underline{\mathbf{M}}}\,\underline{\underline{\mathbf{u}}} = \underline{\underline{\mathbf{f}}}_s\,; \quad \underline{\underline{\mathbf{M}}} = \begin{bmatrix} \underline{\mathbf{D}}^{\downarrow} & \underline{\mathbf{U}} \\ \underline{\mathbf{L}} & \underline{\mathbf{D}}^{\uparrow} \end{bmatrix}$$

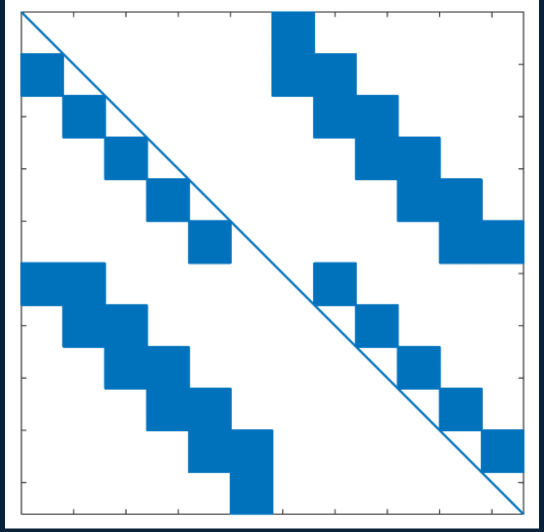
$$\rightarrow \mathbf{P}\underline{\underline{\mathbf{M}}}\,\underline{\underline{\mathbf{u}}} = \mathbf{P}\underline{\underline{\mathbf{f}}}_s$$

where the preconditioning matrix is $\mathbf{P} = \begin{bmatrix} \underline{\mathbf{D}}^{\downarrow} & \mathbf{0} \\ \underline{\mathbf{L}} & \underline{\mathbf{D}}^{\uparrow} \end{bmatrix}^{-1}$

$\underline{\underline{\mathbf{M}}}$



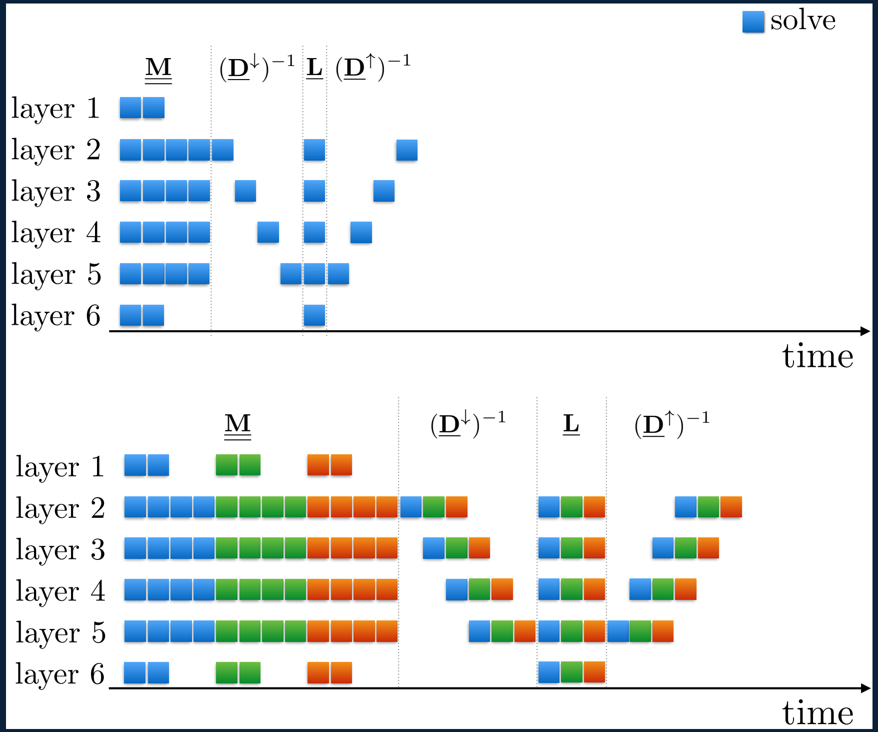
$\underline{\underline{\mathbf{M}}}$



Parallelization strategies

PIPELINING THE MANY RHS

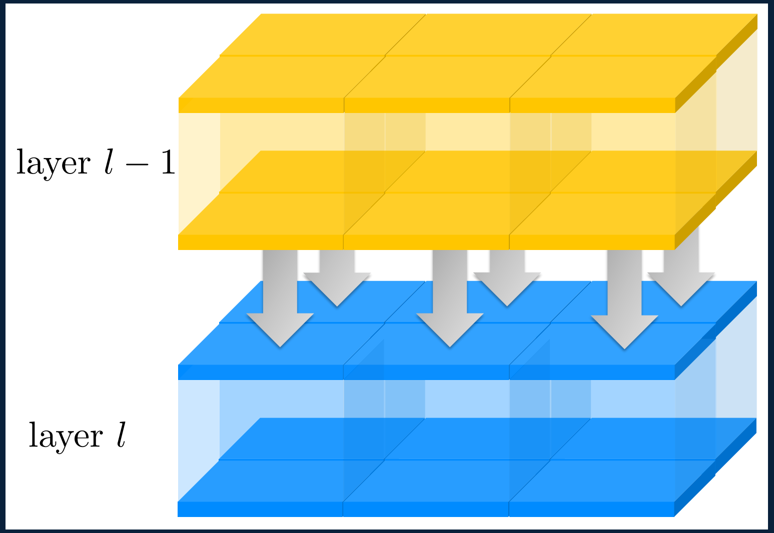
Pipelining allows us to process multiple right sides simultaneously, each at different levels of progress through the sweeps, which helps to balance the computational load on the layers, reducing the idle time and increasing the computational efficiency.



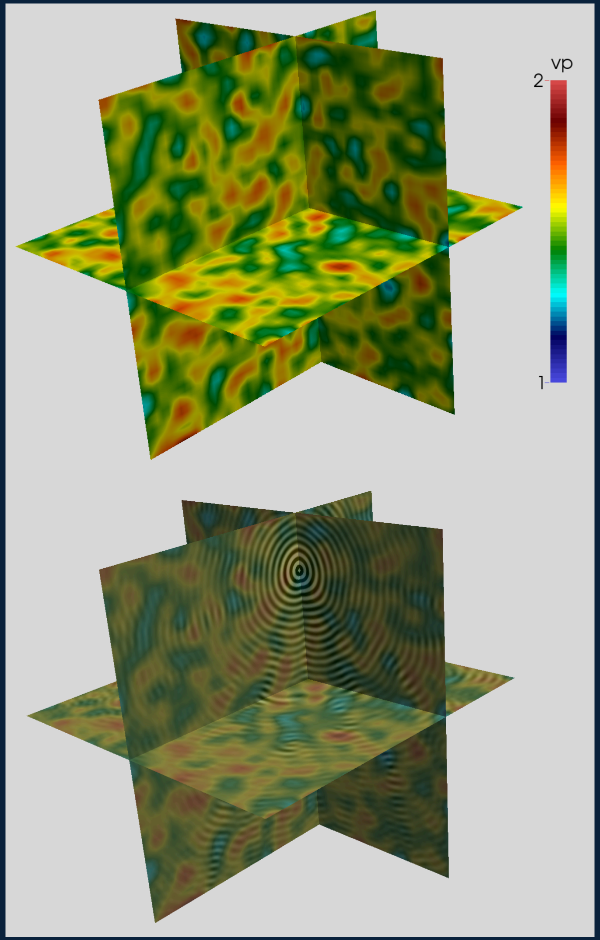
PARALLEL MULTIFRONTAL LOCAL SOLVES & COMMUNICATION PATTERNS

High-performance distributed linear algebra library to solve the local problems within each layer (in this work STRUMPACK)

Each slab is divided into $O(n^2)$ cubes, and the parallel tasks associated with that slab are divided evenly and contiguously amongst the cubes.



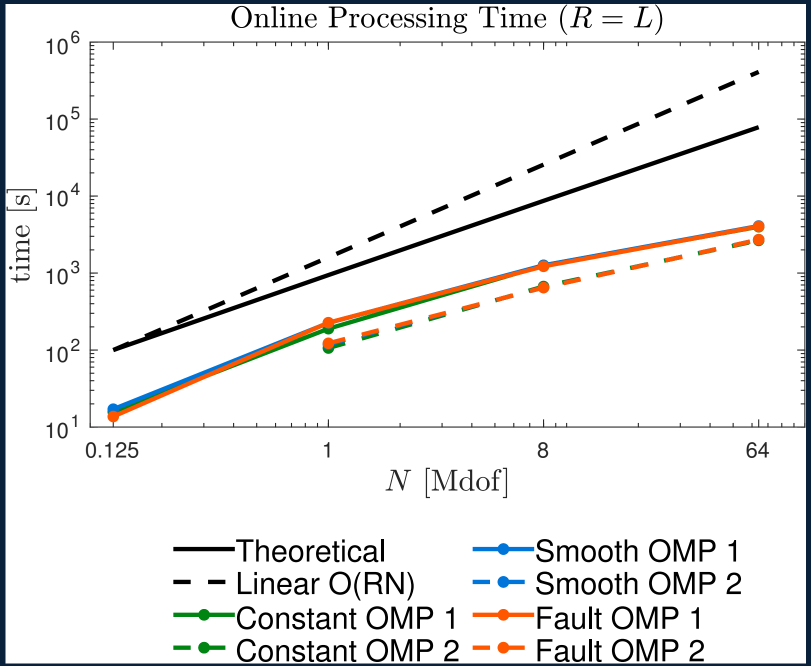
Smooth heterogeneous domain



Complexity: $O(N)$ for $R \sim N^{1/3}$

$N_{\text{it}} \sim \log \omega$

N	L	R	N_{cores}	N_{it}	T (s)
50^3	5	5	5	5	17.1
100^3	10	10	10	5	225.1
200^3	20	20	80	5	1260.9
400^3	40	40	640	6	4086.0

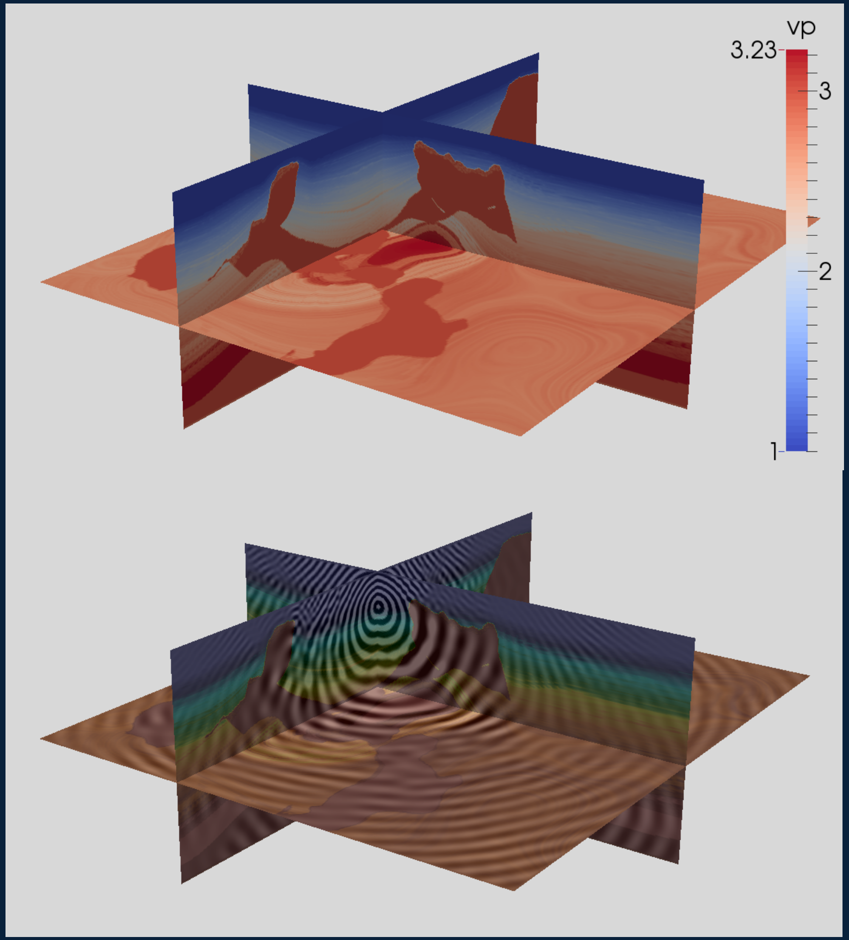


Contrast $m_{\max}/m_{\min} \sim 5$

Size $400 \times 400 \times 400$

40 layers

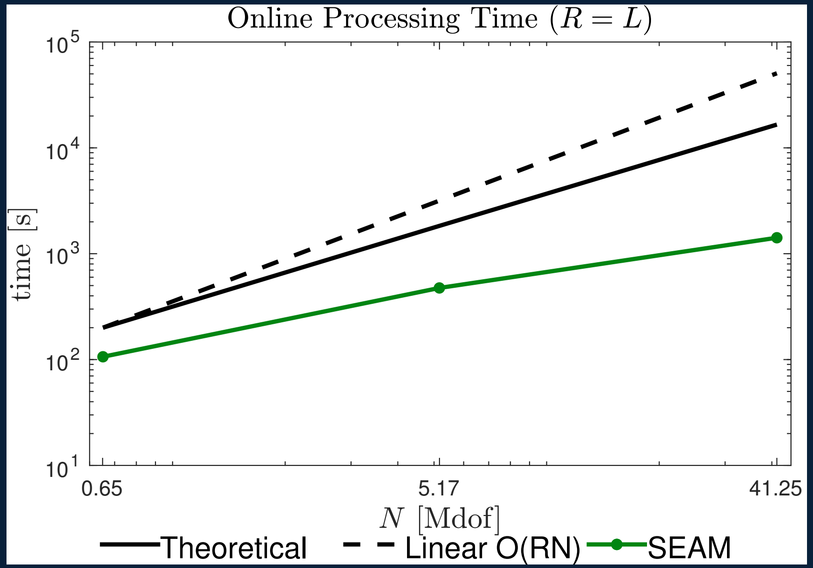
SEAM model



Complexity: $O(N)$ for $R \sim N^{1/3}$

$N_{\text{it}} \sim \log \omega$

N	L	R	N_{cores}	N_{it}	T (s)
$6.51 \cdot 10^5$	12	12	12	4	106.3
$5.16 \cdot 10^6$	24	24	96	5	474.8
$4.12 \cdot 10^7$	48	48	768	6	1415.4



Contrast $m_{\max}/m_{\min} \sim 10$

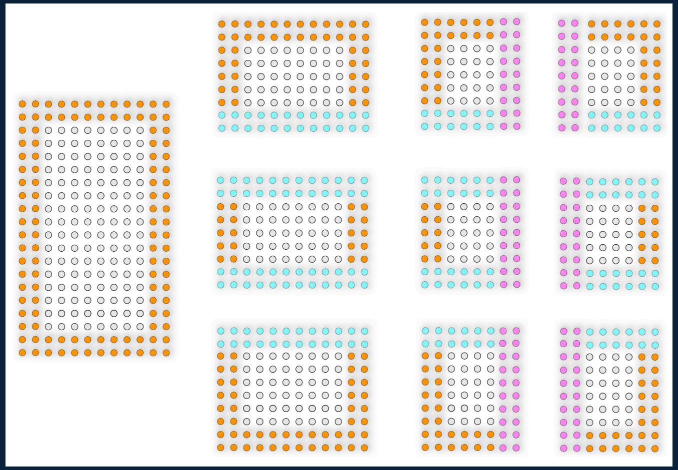
Size $188 \times 438 \times 501$

48 layers

Further developments

NESTED POLARIZED TRACES

Two-level nested domain decomposition: a layered partition on the outer level and a further decomposition of each layer in cells at the inner level.



Online complexity $O(N/P)$, $P = O(N^{1/5})$ (2D)

Zepeda-Núñez and Demanet, 2018

L-SWEEPS

Information propagates in 90º cones induced by a checkerboard domain decomposition (instead of the 180º cone in which information flows in a layered decomposition)

Online complexity $O(N/P)$, $P = O(N^{1/3})$ (2D)

Taus *et al.*, 2019

Take-home messages

- Successful construction of a fast, accurate and scalably parallelizable preconditioned for the high-frequency Helmholtz equations
  - Applicable to heterogeneous media
  - Weakly dependent on the frequency ($O(\log \omega)$)
  - Legacy direct solvers in the subdomains

- P: number of processors

  $O(N/P)$ complexity as long as $P = O(N^{1/d})$

- R: number of right-hand sides (sources)

  $O(N)$ complexity as long as $R = O(N^{1/d})$

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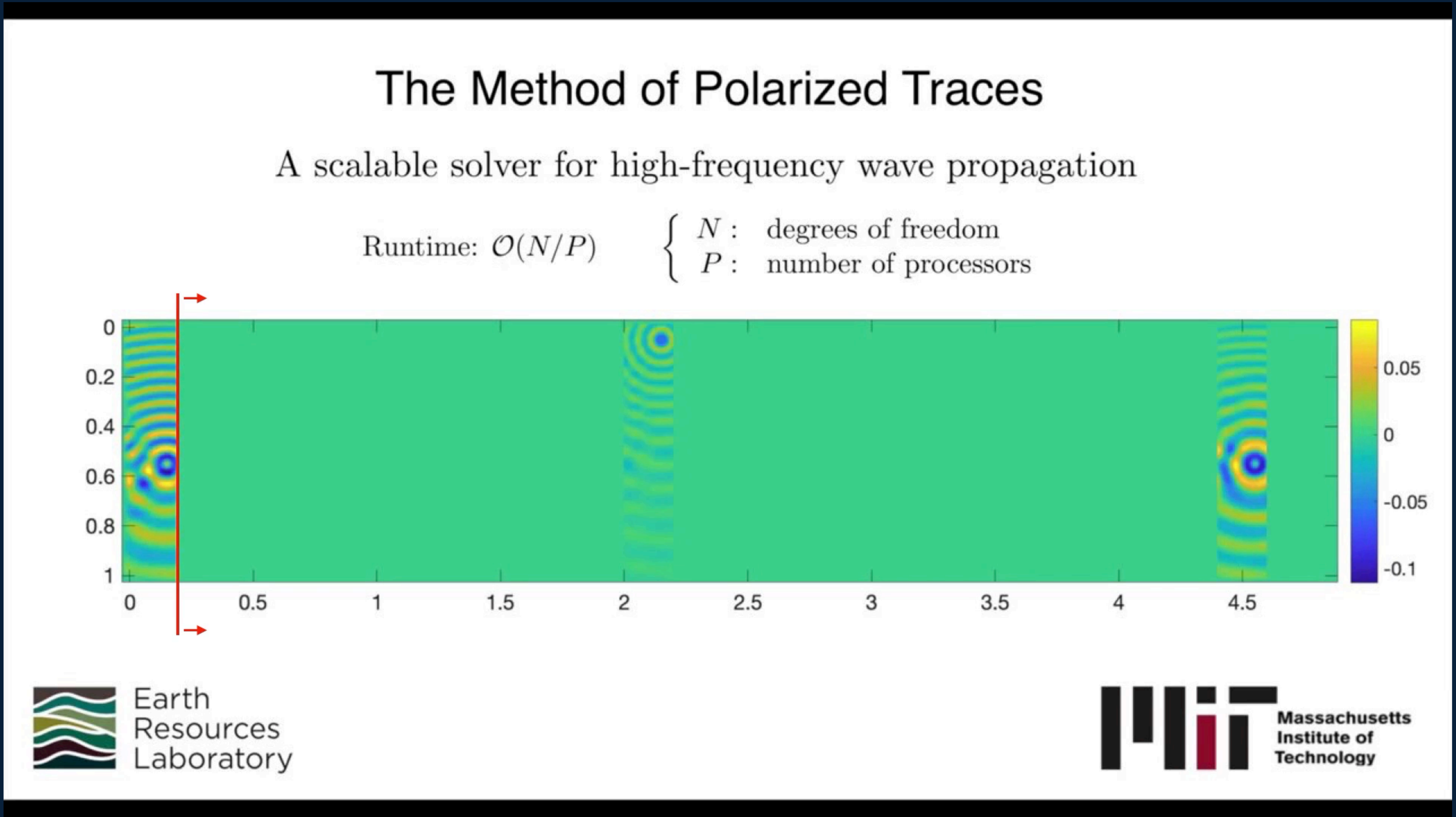
Movie :-)


The Method of Polarized Traces
A scalable solver for high-frequency wave propagation
Runtime: $\mathcal{O}(N/P)$
N : degrees of freedom
P : number of processors
0
0.2
0.4
0.6
0.8
1
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
0.05
0
-0.05
-0.1
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References

POLARIZED TRACES

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