Recent methods for solving the high-frequency Helmholtz equation on a regular mesh

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Overview

- We study the Helmholtz equation

$$(-\Delta - k(x)^2)u(x) = f(x), \qquad k(x) = \frac{\omega}{c(x)},$$

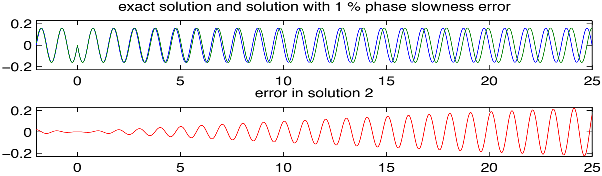
  mostly on rectangular domains with absorbing layers (e.g. PML).
- Three ideas to improve solvers
  - An FD method very small numerical dispersion on coarse meshes
  - Improved two-grid and multigrid methods
  - Domain decomposition
- Justification using analytical and numerical results
- A hybrid solver

Numerical dispersion

Numerical dispersion leads to propagating wave solutions $e^{i\xi_{\mathrm{FD}}\cdot x}$ with wavenumber errors

$$\|\xi_{\mathrm{FD}}(\theta)\| \neq k.$$

Leads to large errors in solution:



Relative wave number errors should be very small, e.g.

$$e(\theta) \stackrel{\mathrm{def}}{=} \left| \frac{\|\xi_{\mathrm{FD}}(\theta)\|}{k} - 1 \right| \lesssim 10^{-4}, \qquad \text{for each direction } \theta = \frac{\xi_{\mathrm{FD}}}{\|\xi_{\mathrm{FD}}\|} \in S^{d-1}!$$

Discretizations for small numerical dispersion

- High-order finite elements (on regular and unstructured meshes)
- High-order finite differences with long stencils
- $3 \times 3 \times 3$ cubic stencils (compact stencil).
  - QS-FEM (2-D), is optimal in 2-D, (Babuska et al. 1995)
  - 6-th order FD (Sutmann, 2007; Turkel et al., 2013)
  - Optimized FD (Jo, Shin, Suh 1998; Operto et al 2007; ...)
- **Plan**:
  - A new optimized compact stencil method
  - Comparison of phase errors (except unstructured FE)
  - Geometrical optics analysis and numerical example

Finite difference Helmholtz operators, constant k

Let $(h\mathbb{Z})^d$ be our mesh, and $x = h\alpha$, with $\alpha \in \mathbb{Z}^d$ the meshpoints. A compact stencil discrete Helmholtz operator P has matrix elements

$$p_{\alpha,\beta} = \frac{1}{h^2} f_{\alpha-\beta}(hk), \qquad \alpha, \beta \in \mathbb{Z}^d$$

for some functions f_γ that are nonzero for $\gamma \in \{-1, 0, 1\}^d$.

Acts multiplicatively on plane wave $e^{ix\cdot\xi}$. Factor is given by the symbol

$$P(\xi) = h^{-2} \sum_\gamma f_\gamma(hk) e^{ih\gamma\cdot\xi}.$$

Assumption The symbol $P(\xi)$ is like that of the continuous operator $H(\xi) = \xi^2 - k^2$, in the sense that

(i) $P(\xi)$ has a zero-set Z_P that is the boundary of a convex set containing the origin

(ii) $\frac{\partial P}{\partial \xi} \neq 0$ on Z_P

The limit $x \to \infty$

Theorem (S., cf. Lighthill 1960) The outgoing solution to $Pu = \delta$ satisfies

$$u(x) = (2\pi)^{-\frac{d-1}{2}} e^{-\frac{(d-1)\pi i}{4}} \|x\|^{-\frac{d-1}{2}} \frac{i\, K(\xi_+)^{-1/2}}{\|\partial P/\partial\xi(\xi_+)\|} e^{ix\cdot\xi_+} + O(\|x\|^{-1/2-d/2}),$$

where d is dimension, $K(\xi)$, $\xi \in Z_P$ is (generalized) Gaussian curvature of Z_P and $\xi_\pm(x)$ denote the maxima $\arg\max_{\xi\in Z_P} \pm x\cdot\xi$.

Consequences

- Z_P should be close to the set $\|\xi\| = k$ to minimize phase errors
- To obtain (close to) correct amplitudes, we solve

  $$Pv = \tilde{Q}\delta, \qquad u = \hat{Q}v$$

  where the order zero operators $\tilde{Q}$ and $\hat{Q}$ have matrix elements and symbols

  $$\tilde{q}_{\alpha,\beta} = \tilde{g}_{\alpha-\beta}(hk), \qquad \tilde{Q}(\xi) = \sum_\gamma \tilde{g}_\gamma(hk)e^{ih\gamma\cdot\xi}, \qquad \hat{Q} \text{ similar}$$

  such that $\left.\frac{\tilde{Q}(\xi)\hat{Q}(\xi)}{\|\partial P/\partial\xi(\xi)\|}\right|_{\xi\in Z_P} \approx \frac{1}{2k}$.

A parameterized finite difference operator

We define a discrete operator with 5 parameter functions $\alpha_j = \alpha_j(\frac{hk}{2\pi})$

$$P = -D_{xx} \otimes I_{y,z}^{(2)} - D_{yy} \otimes I_{x,z}^{(2)} - D_{zz} \otimes I_{x,y}^{(2)} - k^2 I^{(3)}$$

where

$$D_{xx} = h^{-2} \begin{bmatrix} -1 & 2 & -1 \end{bmatrix}$$

$$I^{(2)} = \alpha_4 \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \frac{\alpha_5}{4} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} + \frac{1 - \alpha_4 - \alpha_5}{4} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix}$$

$I^{(3)} =$ similar in 3-D with coefficients $\alpha_1, \alpha_2, \alpha_3$

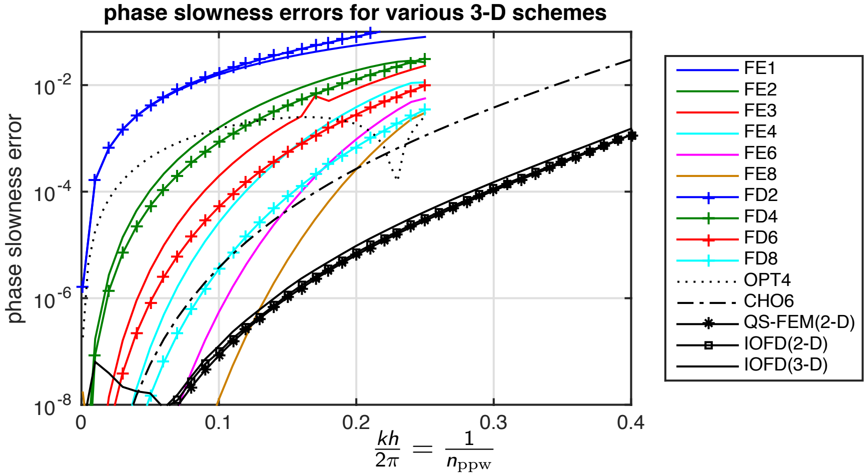
Optimal coefficients

- $\alpha_j(\frac{hk}{2\pi})$ depends on $\frac{hk}{2\pi} = \frac{1}{\text{ppw}}$ via Hermite interpolation on 9 control points.
- carefully minimize phase errors at approximately 400 angles and 40 values of $\frac{hk}{2\pi}$ for ≥ 2.5 points per wavelength

$\frac{hk}{2\pi}$	α_1	$\frac{\partial\alpha_1}{\partial(1/G)}$	α_2	$\frac{\partial\alpha_2}{\partial(1/G)}$	α_3	$\frac{\partial\alpha_3}{\partial(1/G)}$	α_4	$\frac{\partial\alpha_4}{\partial(1/G)}$	α_5	$\frac{\partial\alpha_5}{\partial(1/G)}$
0.0000	0.635413	-0.000228	0.210638	0.016303	0.172254	-0.014072	0.710633	-0.006278	0.245303	0.019576
0.0500	0.635102	-0.015578	0.210152	-0.023424	0.171912	-0.005802	0.709821	-0.047764	0.245148	0.021398
0.1000	0.634166	-0.034804	0.208167	-0.043396	0.171146	-0.012462	0.707374	-0.070981	0.244762	0.007493
0.1500	0.632093	-0.054496	0.205348	-0.065935	0.170031	-0.022145	0.703359	-0.088202	0.245160	0.009937
0.2000	0.628341	-0.103457	0.201605	-0.069385	0.169740	0.001893	0.698813	-0.092327	0.245687	0.012201
0.2500	0.622526	-0.133896	0.197423	-0.098212	0.169475	-0.002559	0.694726	-0.066617	0.246454	0.016791
0.3000	0.614611	-0.183988	0.192414	-0.115398	0.168690	-0.005589	0.692615	-0.011177	0.247743	0.029213
0.3500	0.603680	-0.255991	0.186819	-0.120930	0.167581	-0.015564	0.694109	0.077605	0.250098	0.059733
0.4000	0.588498	-0.356326	0.180737	-0.132266	0.166640	-0.001852	0.700902	0.199685	0.254352	0.106049

- We set $\hat{Q} = \tilde{Q} = Q$ and also find coefficients for Q on a cubic stencil.

Comparison of relative phase errors



QS-FEM (2-D)(Babuska et al., 1995) and IOFD (2-D and 3-D) have the smallest dispersion errors with few points per wavelength.

Classical geometrical optics

- Consider smoothly varying k (c is C^2 or smoother)
- In classical geometrical objects the ansatz is $u = A(x)e^{i\omega\Phi(x)}$

$$(-\Delta - \frac{\omega^2}{c^2})A(x)e^{i\omega\Phi(x)} = \left[\omega^2 A\left((\nabla\Phi)^2 - \frac{1}{c^2}\right) + \omega(\ldots) + O(1)\right]e^{i\omega\Phi(x)}.$$

- In terms of the symbol $\tilde{H}(x,\xi) = \xi^2 - \frac{1}{c(x)^2}$ we find the equations

$$\tilde{H}(x, \nabla\Phi(x)) = 0 \qquad \text{(eikonal equation)}$$

$$\sum_j (L_{\tilde{H},\Phi})_j \frac{\partial A}{\partial x_j} + \frac{1}{2}(\operatorname{div} L_{\tilde{H},\Phi})A + (t - 1/2)\sum_j \frac{\partial^2 \tilde{H}}{\partial x_j \partial \xi_j} A = 0 \quad \text{(transport eq.)}$$

where $\left(L_{\tilde{H},\Phi}\right)_j = \frac{\partial \tilde{H}}{\partial \xi_j}(x, \nabla\Phi)$ (Duistermaat, 1996)

- Point source solutions, are obtained by choosing appropriate initial conditions for A and Φ.

Geometrical optics for discrete Helmholtz operators

- Asymptotics for $\omega \to \infty$, $\omega h =$ constant (variable k)
- The symbol becomes $P(x,\xi) = h^{-2} \sum_\gamma f_\gamma(hk(x)) e^{ih\gamma\cdot\xi}$
- We consider the discretization

$$p_{\alpha,\beta} = \frac{1}{h^2} f_{\alpha-\beta}(hk((1-t)\alpha h + t\beta h)),$$

for $t \in \{0, 1/2, 1\}$. This is the t-quantization of $P(x,\xi)$

$$\mathrm{Op}_t(P(x,\xi))u(x) \stackrel{\mathrm{def}}{=} (2\pi)^{-d} \sum_{y\in(h\mathbb{Z})^d} \int_{[-\pi/h,\pi/h]^d} P(x+t(y-x),\xi) e^{i(x-y)\cdot\xi} u(y)\, d\xi$$

- Using Taylor expansions of the phase functions the same eikonal and transport equations in terms of $P(x,\xi)$ are obtained.

Variable k results

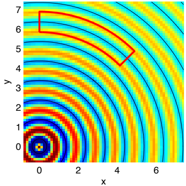
- Correct geometrical optics phase and amplitude result if
  (i) $P(x,\xi)$ has same zeros as $H(x,\xi) = \xi^2 - k(x)^2$
  (ii) $t = 1/2$ is used in the quantization
  (iii) $\tilde{Q} = \hat{Q} \stackrel{\mathrm{def}}{=} Q$ and $Q(\xi)$ satisfies

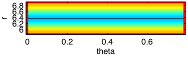
$$\left.\frac{Q(\xi)^2}{\|\partial P/\partial\xi(\xi)\|}\right|_{\xi\in Z_P} = \frac{1}{2k}$$

  (same equation as before)
- Small phase errors (proportional to distance from source) and amplitude errors result if the equalities are satisfied only approximately
- The dispersion minimizing scheme can provide accurate solutions if the velocity $c(x)$ is smooth

Simulations at constant k (2-D)

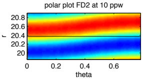
Polar plots



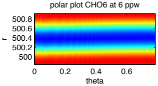


(spline interpolation)

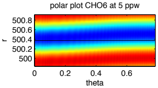
FD2, 10ppw, 20wl



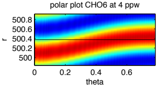
CHO6, 6ppw, 500wl



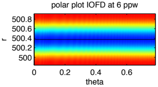
CHO6, 5ppw, 500wl



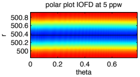
CHO6, 4ppw, 500wl



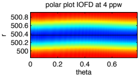
IOFD, 6ppw, 500wl



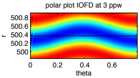
IOFD, 5ppw, 500wl



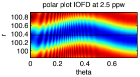
IOFD, 4ppw, 500wl



IOFD, 3ppw, 500wl



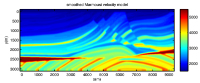
IOFD, 2.5ppw, 100wl



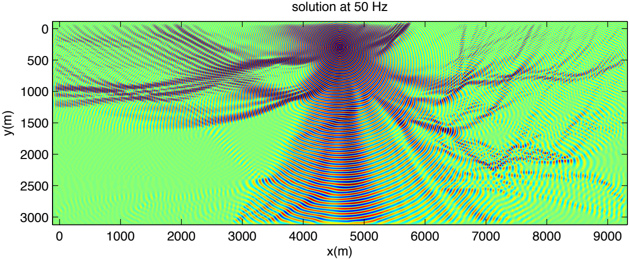
Smoothed Marmousi example

Compare a IOFD solution at 6 ppw with a FE4 solution 12 ppw.

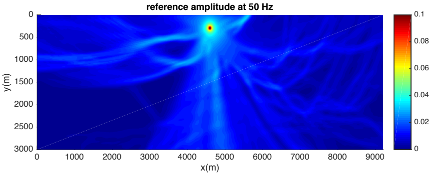
Velocity: Smoothed Marmousi model

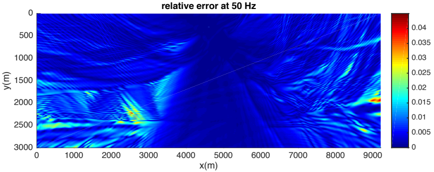


Solution at 50 Hz



Reference amplitude and relative local error at 50 Hz





Local error mostly < 1 %

Multigrid for Helmholtz equations

- Multigrid was developed for elliptic problems were it is highly efficient
- For time-harmonic problems using standard multigrid, a relatively fine discretization $\gtrsim$10 points per wavelength at the coarse level is required
- Elliptic and shifted-Laplacian preconditioners use multigrid: The multigrid scheme of a complex-shifted operator acts as a preconditioner. (Bayliss et al, 1983; Erlannga, Oosterlee, Vuik, 2004; Calandra, Gratton et al., 2013; ...). Typically requires many iterations.
- **Idea** (S. et al 2014): Optimized discretizations on a coarse mesh can be used to speed up the solution process for a finer mesh discretization.

Multigrid with optimized coarse discretizations

- **Plan today**:
  - Local Fourier analysis to choose parameters and compare methods
  - analyze weakly damped Helmholtz operators on infinite domain $H = -\Delta - ((1 + \alpha i)k)^2$
    e.g. $\alpha = 0.01$ corresponds to a damping of 6.28%/cycle
  - A numerical example with damping only at the boundary
- Two-grid method for an approximate solution was obtained by testing different parameter choices using local Fourier analysis:
  - Simple iterative solver (smoother) (3 times ω-Jacobi, $\omega \approx 0.7$)
  - Compute residual, restrict to coarse mesh, solve on coarse mesh, interpolate back to fine mesh
  - Simple iterative solver again
  - Apply this as a preconditioner for GMRES

Local Fourier analysis of the two-grid method

Local Fourier analysis is a standard method in multigrid analysis (Trottenberg et al., 2001)

Let h be the fine mesh distance, $2h$ coarse mesh distance.
We consider Fourier-Bloch waves on cells of size $2h$

$$u(x_1 + j_1 2h, x_2 + j_2 2h) = e^{i(j_1\xi_1 + j_2\xi_2)} u(x_1, x_2).$$

Operators are block diagonal on a Fourier-Bloch basis

In such a basis, the action of multigrid on the residual is given by 4×4 matrices

$$M_h^{2h}(\xi) = S(\xi)^{\nu_2} K_h^{2h}(xi) S(\xi)^{\nu_1}$$
$$K_h^{2h}(\xi) = I - R_h(\xi) \left(P_{\text{coarse},2h}(\xi)\right)^{-1} R_h(\xi) P_{\text{fine},h}(\xi)$$

where $S(\xi)$ is the action of one iteration of ω-Jacobi on the residual, $R_h^T(\xi)$ and $R_h(\xi)$ are for interpolation and restriction and $P_{\mathrm{coarse,2h}}(\xi)$ and $P_{\mathrm{fine,h}}(\xi)$ are Helmholtz operator symbols.

Two-grid convergence factor

Two-grid convergence factor

$$\rho = \sup_{\xi \in [-\frac{\pi}{2h}, \frac{\pi}{2h}]^2} \text{SpectralRadius}(M_h^{2h}(\xi)).$$

Numerical computation of convergence factors (S. et al, 2014)

FD5-optimized matching FD5

coarse ppw	$\alpha =$ 1.25e-3	$\alpha =$ 0.005
3	0.634	0.439
3.5	0.228	0.204
4	0.170	0.156
6	0.079	0.079
8	0.067	0.067

FD5-Galerkin

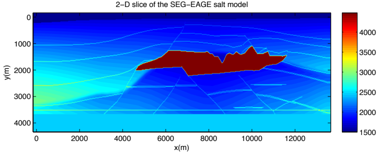
coarse ppw	$\alpha =$ 0.005	$\alpha =$ 0.02
6	> 1	> 1
7	> 1	> 1
8	> 1	0.896
10	> 1	0.588
12	> 1	0.415

(IOFD at fine and coarse levels slightly outperforms FD5-optimized.)

Two-grid iteration count

Iterations for residual reduction by 10^{-6} with "sponge" bdy conditions.

2-D slice of SEG-EAGE model

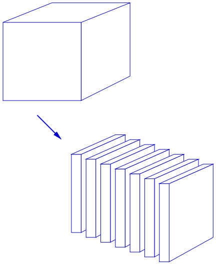


	constant 2400×2400		salt model 2700×836	
ppw fine	freq	its	freq	its
5	480	29	60	18
6	400	8	50	8
8	300	5	37.5	6
10	240	4	30	5

- Multigrid with optimized FD at the coarse level works, downto ~ 3 ppw at the coarse level.
- However, in 3-D, the coarse level linear system can remain large

Double sweep domain decomposition

- Get solution by solving a sequence of subdomain problems
- artificial boundaries should not introduce reflections
- coupling s.t. incoming waves in domain j are outgoing waves in domains $j \pm 1$



- Schwartz type methods involve coupling through numerical absorbing boundary conditions (Benamou, Després 1997; Gander et al., 2007; ...)
- Sweeping methods (Engquist, Ying, 2010) use very thin subdomains with PML on one side
- **Idea:** (S., 2013, 2017)
  - subdomains with PML layers on both sides (cf. Schadle, 2007)
  - coupling via source terms involving single and double potentials
  - Forward and backward sweep with shifted domain boundaries

Domain decomposition method in 1-D

Robin boundary value problem

$$
\begin{aligned}
&Au = f \text{ for } 0 < x < L, && A = -\partial_{xx} - k^2, \\
&\partial_x u(0) + iku(0) = h_1, && -\partial_x u(L) + iku(L) = h_2.
\end{aligned}
$$

Let $0 = b_0 < b_1 < \ldots < b_J = L$ be domain boundaries, and $A^{(j)}$ the Helmholtz operator on $[b_{j-1} - \epsilon, b_j + \epsilon]$ with Robin boundary conditions as above.

Upward sweep

1. For $j = 1, 2, \ldots, J$, solve $v^{(j)}$ from

$$
P^{(j)} v^{(j)} = I_{x \in [b_{j-1}, b_j]} f + T_+^{(j)} v^{(j-1)}
$$

$$
T_+^{(j)} v^{(j-1)} = \begin{cases} 0 & \text{if } j = 1 \\ P^{(j-1)} H(b_{j-1} - x) v^{(j-1)} + H(b_{j-1} - x) P^{(j-1)} v^{(j-1)} & \text{otherwise} \end{cases}
$$

2. Define an approximate solution $v(x) = \sum_{j=1}^{J} I_{x \in [b_{j-1}, b_j]}(x)\, v^{(j)}(x)$

Domain decomposition method in 1-D (cont'd)

Downward sweep:

- Define new domain boundaries $0 = \tilde{b}_0 < \tilde{b}_1 < \ldots < \tilde{b}_J = L$, such that $b_j \neq \tilde{b}_k$ for any j, k.
- The downward sweep acts on the residual $g = f - Pv$ to produce an approximate solution w to $Pg = w$.
  The "double sweep" approximate solution is $u = v + w$.
- The downward sweep is similar to the upward sweep.

Remarks on the 1-D problem

- The source transfer term $T_+ v^{(j-1)}$ is a sum of single and double potentials

$$
\begin{aligned}
T_+^{(j)} v^{(j-1)} &= P^{(j-1)} H(b_{j-1} - x) v^{(j-1)} + H(b_{j-1} - x) P^{(j-1)} v^{(j-1)} \\
&= a\delta(x - b_{j-1}) + b\delta'(x - b_{j-1})
\end{aligned}
$$

  and causes only forward propagating waves
- The solution formula for the 1-D Helmholtz equation gives that

$$
\begin{aligned}
v(x) &= \frac{i}{2k} \int_0^x e^{ix(x-s)} f(s)\, ds \\
&\qquad + \frac{i}{2k} \int_x^{b_l} e^{-ik(x-s)} f(s)\, ds \qquad \text{for } x \in (b_{l-1}, b_l) \\
u(x) &= \text{exact solution} \\
&= \frac{i}{2k} \int_0^x e^{ix(x-s)} f(s)\, ds + \frac{i}{2k} \int_x^L e^{-ik(x-s)} f(s)\, ds
\end{aligned}
$$

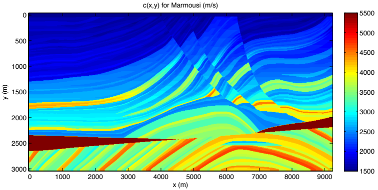
Discretization and extension to 3-D

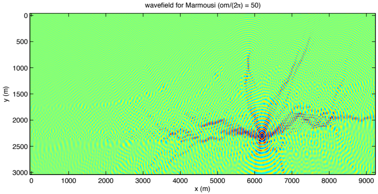
- The above description is straightforwardly extended to the discrete 2-D and 3-D cases (with domain decomposition along the x_1 axis)
- In this case the domain boundaries b_j are chosen halfway between grid points, and $\tilde{b}_j = b_j + 1$ or $\tilde{b}_j = b_j - 1$.
- There is a two grid-cell overlap between subdomains j and $j \pm 1$.
- At the internal boundaries, PML layers are added to simulate absorbing boundaries. PML means that

$$\frac{\partial}{\partial x_1} \text{ is replaced by } \frac{1}{1 + i\omega^{-1}\sigma(x_1)} \frac{\partial}{\partial x_1}.$$

  with σ_1 increasing quadratically into the x_1-boundary layers.
- At the external boundaries, PML layers, or classical damping layers can be used.
- upward and downwardsweep can be done in parallel (X-sweep)

2-D Marmousi example





$N_x \times N_y$	h (m)	$\frac{\omega}{2\pi}$ (Hz)	Number of x-subdomains				
			3	10	30	100	300
600×212	16	12.5	4	5	6		
1175×400	8	25	5	6	7		
2325×775	4	50	6	6	7	9	
4625×1525	2	100	6	6	7	8	
9225×3025	1	200		7	8	9	8^*

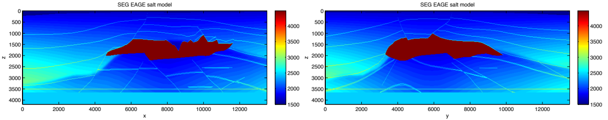
Results from S., 2013.

A hybrid solver

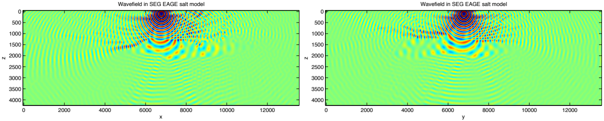
- **Idea** (S., 2017): In the two-grid method, the coarse level solver can be replaced by a domain decomposition preconditioner.
- Parallel 3-D implementation
  - Linux cluster with 64 GB per node, 16 cores/node, up to 16 nodes at surfsara.nl.
  - Cartesian mesh decomposition for multigrid
  - Subdomain solves done on 8 to 32 cores using MUMPS
  - Subdomains must be solved consecutively: Pipeline solution process to keep all nodes busy

Example: SEG-EAGE Salt model

Velocity: SEG-EAGE salt model, $676 \times 676 \times 210$ points, $h = 20$ m.



Solution for $f = 12.5$ Hz: xz and yz slices



frequency	6.25	7.87	9.91	12.5
size	338x338x106	426x426x132	536x536x166	676x676x210
# dof	$1.3 \cdot 10^7$	$2.5 \cdot 10^7$	$5.0 \cdot 10^7$	$1.0 \cdot 10^8$
cores	32	64	128	256
# of rhs.	1	2	4	8
iterations	12	12	13	15
time/rhs.	26	35	45	73

Fast compared to methods in the literature!

Discussion

- Sizeable efficiency gains in some Helmholtz problems
- Variants of sweeping domain decomposition have been applied to finite element discretizations, EM and elastic waves (Tsuji et al. 2014; Vion, Geuzaine, 2014; ...).
  The key point is the reduced memory use compared to the direct method.
- Sweeping domain decomposition remains difficult to parallellize
- Multigrid with optimized finite differences can combine
  - fine sampling for accurate discretization
  - very coarse sampling in the costly part of the solver

  Direct generalization to FE fails.
  Can we extend this to more general meshes?

THANK YOU