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

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Overview

- We study the Helmholtz equation

\[-\Delta - k(x)^2)u(x) = f(x), \quad k(x) = \frac{\omega}{c(x)},\]

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 $e^{i\xi_{\text{FD}} \cdot x}$ with wavenumber errors

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

Leads to large errors in solution:

![Graph showing exact solution and solution with 1% phase slowness error](image)

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

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

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

for some functions $f_{\gamma}$ 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 $\arg \max_{\xi \in Z_P} x \cdot \xi$.

**Consequences**

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

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

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

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

such that

$$\left. \left| \frac{\tilde{Q}(\xi)\hat{Q}(\xi)}{\|\partial P/\partial \xi(\xi)\|} \right|_{\xi \in Z_P} \approx \frac{1}{2k}. \right.$$
A parameterized finite difference operator

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

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

where

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

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

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

- $\alpha_j \left( \frac{hk}{2\pi} \right)$ 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 $\geq 2.5$ points per wavelength

<table>
<thead>
<tr>
<th>$\frac{hk}{2\pi}$</th>
<th>$\alpha_1$</th>
<th>$\frac{\partial \alpha_1}{\partial (1/G)}$</th>
<th>$\alpha_2$</th>
<th>$\frac{\partial \alpha_2}{\partial (1/G)}$</th>
<th>$\alpha_3$</th>
<th>$\frac{\partial \alpha_3}{\partial (1/G)}$</th>
<th>$\alpha_4$</th>
<th>$\frac{\partial \alpha_4}{\partial (1/G)}$</th>
<th>$\alpha_5$</th>
<th>$\frac{\partial \alpha_5}{\partial (1/G)}$</th>
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<tbody>
<tr>
<td>0.0000</td>
<td>0.635413</td>
<td>-0.000228</td>
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<td>0.172254</td>
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<td>0.245303</td>
<td>0.019576</td>
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<td>-0.005589</td>
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<td>0.700902</td>
<td>0.199685</td>
<td>0.254352</td>
<td>0.106049</td>
</tr>
</tbody>
</table>

- 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

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

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

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

- Point source solutions, are obtained by choosing appropriate initial conditions for $A$ and $\Phi$. 
Geometrical optics for discrete Helmholtz operators

- Asymptotics for $\omega \to \infty$, $\omega h = \text{constant}$ (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 $P(x, \xi)$

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

- 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) $P(x, \xi) \text{ has same zeros as } H(x, \xi) = \xi^2 - k(x)^2$
  
  (ii) $t = 1/2$ is used in the quantization
  
  (iii) $\tilde{Q} = \hat{Q} \text{ def } Q \text{ and } Q(\xi) \text{ satisfies}$

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

  (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

FD2, 10ppw, 20wl

CHO6, 6ppw, 500wl

IOFD, 6ppw, 500wl

IOFD, 5ppw, 500wl

IOFD, 4ppw, 500wl

IOFD, 3ppw, 500wl

IOFD, 2.5ppw, 100wl

(spline interpolation)
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 ≥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 $\omega$-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 $4 \times 4$ matrices

$$M_h^{2h}(\xi) = S(\xi)^{\nu_2} K_h^{2h}(\xi) S(\xi)^{\nu_1}$$

$$K_h^{2h}(\xi) = I - R_h(\xi) (P_{\text{coarse}, 2h}(\xi))^{-1} R_h(\xi) P_{\text{fine}, h}(\xi)$$

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

<table>
<thead>
<tr>
<th>FD5-optimized matching FD5</th>
<th>FD5-Galerkin</th>
</tr>
</thead>
<tbody>
<tr>
<td>coarse ppw</td>
<td>coarse ppw</td>
</tr>
<tr>
<td></td>
<td>$\alpha =$</td>
</tr>
<tr>
<td></td>
<td>1.25e-3</td>
</tr>
<tr>
<td>3</td>
<td>0.634</td>
</tr>
<tr>
<td>3.5</td>
<td>0.228</td>
</tr>
<tr>
<td>4</td>
<td>0.170</td>
</tr>
<tr>
<td>6</td>
<td>0.079</td>
</tr>
<tr>
<td>8</td>
<td>0.067</td>
</tr>
<tr>
<td></td>
<td>0.005</td>
</tr>
<tr>
<td>6</td>
<td>&gt; 1</td>
</tr>
<tr>
<td>7</td>
<td>&gt; 1</td>
</tr>
<tr>
<td>8</td>
<td>&gt; 1</td>
</tr>
<tr>
<td>10</td>
<td>&gt; 1</td>
</tr>
<tr>
<td>12</td>
<td>&gt; 1</td>
</tr>
</tbody>
</table>

(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.

Multigrid with optimized FD at the coarse level works, downto $\sim 3$ 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

\[ Au = f \text{ for } 0 < x < L, \quad A = -\partial_{xx} - k^2, \]
\[ \partial_x u(0) + iku(0) = h_1, \quad -\partial_x u(L) + iku(L) = h_2. \]

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

\[
P^{(j)} v^{(j)} = \int_{x \in [b_{j-1}, b_j]} f + T^{(j)} v^{(j-1)}
\]
\[
T^{(j)} v^{(j-1)} = \begin{cases} 
0 & \text{if } j = 1 \\
\int_{x \in [b_{j-1}, b_j]} P^{(j-1)} H(b_{j-1} - x) v^{(j-1)} + H(b_{j-1} - x) P^{(j-1)} v^{(j-1)} & \text{otherwise}
\end{cases}
\]

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 $g = f - P \nu$ to produce an approximate solution $w$ to $Pg = w$.
  The “double sweep” approximate solution is $u = \nu + w$.
- 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

$$T_+^{(j)} v^{(j-1)} = P^{(j-1)} H(b_{j-1} - x) v^{(j-1)} + H(b_{j-1} - x) P^{(j-1)} v^{(j-1)}$$

$$= a \delta(x - b_{j-1}) + b \delta'(x - b_{j-1})$$

and causes only forward propagating waves

The solution formula for the 1-D Helmholtz equation gives that

$$v(x) = \frac{i}{2k} \int_0^x e^{ix(s-x)} f(s) \, ds$$

$$+ \frac{i}{2k} \int_x^{b_l} e^{-ik(x-s)} f(s) \, ds \quad \text{for } x \in (b_{l-1}, b_l)$$

$$u(x) = \text{exact solution}$$

$$= \frac{i}{2k} \int_0^x e^{ix(s-x)} f(s) \, ds + \frac{i}{2k} \int_x^L e^{-ik(x-s)} f(s) \, ds$$
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 $\sigma_1$ 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

<table>
<thead>
<tr>
<th>$N_x \times N_y$</th>
<th>$h$ (m)</th>
<th>$\frac{\omega}{2\pi}$ (Hz)</th>
<th>Number of $x$-subdomains</th>
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</thead>
<tbody>
<tr>
<td>600 $\times$ 212</td>
<td>16</td>
<td>12.5</td>
<td>4  5  6</td>
</tr>
<tr>
<td>1175 $\times$ 400</td>
<td>8</td>
<td>25</td>
<td>5  6  7</td>
</tr>
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<td>2325 $\times$ 775</td>
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<tr>
<td>4625 $\times$ 1525</td>
<td>2</td>
<td>100</td>
<td>6  6  7  8</td>
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<tr>
<td>9225 $\times$ 3025</td>
<td>1</td>
<td>200</td>
<td>7  8  9  8*</td>
</tr>
</tbody>
</table>

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

Fast compared to methods in the literature!

<table>
<thead>
<tr>
<th>frequency size</th>
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<th>7.87</th>
<th>9.91</th>
<th>12.5</th>
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<td>338x338x106</td>
<td>426x426x132</td>
<td>536x536x166</td>
<td>676x676x210</td>
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<tr>
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<td>2.5 \cdot 10^7</td>
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<tr>
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<tr>
<td># of rhs.</td>
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<td>8</td>
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<tr>
<td>iterations</td>
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<td>12</td>
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<td>15</td>
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<tr>
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<td>35</td>
<td>45</td>
<td>73</td>
</tr>
</tbody>
</table>

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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 parallelize
- 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