Scalable solvers for the Helmholtz probem

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Aim and Impact

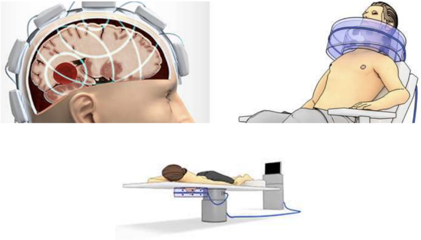
- Contribute to broad research on parallel scalable iterative solvers for time-harmonic wave problems
- This presentation: matrix-free parallelization
  - Complex shift Laplace Preconditioner (CSLP)
  - Deflation methods
  - Parallel performance

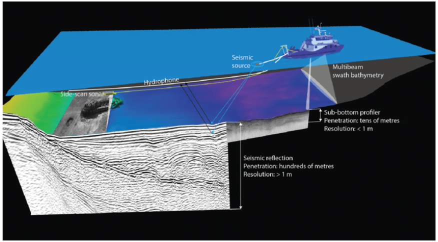
Introduction - the Helmholtz Problem

The Helmholtz equation (describing time-harmonic waves) + BCs

$$-\Delta u(\mathbf{x}) - k(\mathbf{x})^2 u(\mathbf{x}) = g(\mathbf{x}), \text{ on } \Omega \subseteq \mathbb{R}^n$$

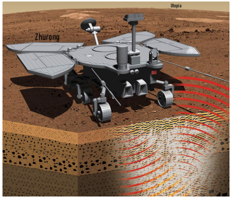
- $k(\mathbf{x})$ is the wavenumber, $k(\mathbf{x}) = (2\pi f)/c(\mathbf{x})$, where f is the frequency and c is the acoustic velocity of the media
- Applications in **seismic exploration**, medical imaging, antenna synthesis, etc.



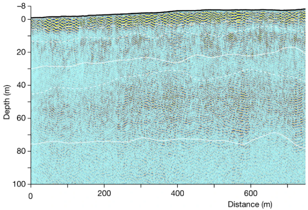


Larisa, High-performance implementation of Helmholtz equation with absorbing boundary conditions. http://www.math.chalmers.se/~larisa/www/MasterProjects/HelmholtzABSbc.pdf
M. Jakobsson, et al (2016). Mapping submarine glacial landforms using acoustic methods. Geological Society.

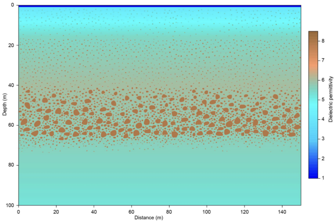
Introduction



(a) Zhurong rover



(b) The radar imaging profile



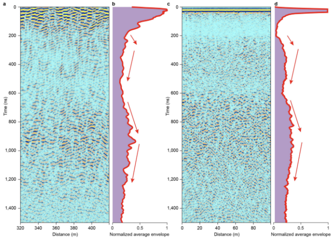
(c) Numerical model

Solve the

Helmholtz equation

$\longleftrightarrow$

Adjust model



(d) Observed data vs. simulation

Li, C., Zheng, Y., Wang, X. et al. (2022) Layered subsurface in Utopia Basin of Mars revealed by Zhurong rover radar. Nature.

Introduction - Challenges

- Linear system from discretization

$$Au = b$$

  - A is real, sparse, symmetric, normal, and **indefinite**; **non-Hermitian** with Sommerfeld BCs
- Direct solver or iterative solver
- **Accuracy and pollution error** ($k^3h^2 < 1$): finer grid (3D) $\Rightarrow$ larger linear system
  - Memory-efficient methods; High-Performance Computing (HPC)
- **Negative & positive eigenvalues**: larger wavenumber $\Rightarrow$ more iterations
  - Preconditioner: Complex Shifted Laplace Preconditioner (CSLP)
  - (Higher-order) Deflation
- **Parallelism**

Aim

- A wavenumber-independent convergent and parallel scalable solver

Introduction - Metrics

- Convergence metric:
  - Krylov-based solvers, GMRES-type: the number of iterations (#iter); IDR(s): the number of matrix-vector multiplications (#Matvec)
- Scalability:
  - Strong scaling: the number of processors is increased while the problem size remains constant
  - Weak scaling: the problem size increases along with the number of tasks, so the computation per task remains constant
  - Wall-clock time: t_w; number of processors: np
  - Speedup: $S_p = \dfrac{t_{w,r}}{t_{w,p}}$, $E_P = \dfrac{S_p}{np/np_r} = \dfrac{t_{w,r} \cdot np_r}{t_{w,p} \cdot np}$

Introduction - Numerical Models

- Model problems on a rectangular domain Ω with boundary $\Gamma = \partial\Omega$

$$-\Delta u(\mathbf{x}) - k(\mathbf{x})^2 u(\mathbf{x}) = \delta\left(\mathbf{x} - \mathbf{x}_0\right), \text{ on } \Omega$$

$$\frac{\partial u(\mathbf{x})}{\partial \vec{n}} - \mathrm{i}k(\mathbf{x})u(\mathbf{x}) = 0, \text{ on } \Gamma$$

  - Constant wavenumber: $k(\mathbf{x}) = k$
  - Non-constant wavenumber: Wedge, Marmousi problem, 3D SEG/EAGE Salt Model, etc.
- Finite-difference discretization on a uniform grid with grid size h. (2D example)
  - Laplace operator: $-\Delta_h \mathbf{u} \approx \dfrac{-u_{i,j-1} - u_{i-1,j} + 4u_{i,j} - u_{i+1,j} - u_{i,j+1}}{h^2}$
  - Sommerfeld BCs: a ghost point

$$\frac{\partial u}{\partial \vec{n}}(0, y_j) - \mathrm{i}k(0, y_j)u(0, y_j) \approx \frac{u_{0,j} - u_{2,j}}{2h} - \mathrm{i}k_{1,j}u_{1,j} = 0 \Rightarrow u_{0,j} = u_{2,j} + 2h\mathrm{i}k_{1,j}u_{1,j}$$

- Preconditioned Krylov subspace solver: Flexible GMRES for complex system
- Preconditioner: Geometric multigrid/multilevel methods

Introduction - Numerical Models

Stencil notation

- Laplace operator:

$$[-\Delta_h] = \frac{1}{h^2} \begin{bmatrix} 0 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 0 \end{bmatrix}$$

- "Wavenumber operator":

$$[\mathcal{I}_h \mathbf{k}^2] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & k_{i,j}^2 & 0 \\ 0 & 0 & 0 \end{bmatrix} \overset{const}{=} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} k^2$$

- $A\mathbf{u} = \mathbf{b}$:

$$[A_h] = [-\Delta_h] - [\mathcal{I}_h \mathbf{k}^2]$$

Framework - Matrix-free operations

- Perform computations with a matrix without explicitly forming or storing the matrix
  $\Rightarrow$ Reduce memory requirements

Matrix-vector multiplication

If a matrix can be represented by a so-called stencil notation

$$[A] = \begin{bmatrix} a_{-1,1} & a_{0,1} & a_{1,1} \\ a_{-1,0} & a_{0,0} & a_{1,0} \\ a_{-1,-1} & a_{0,-1} & a_{1,-1} \end{bmatrix},$$

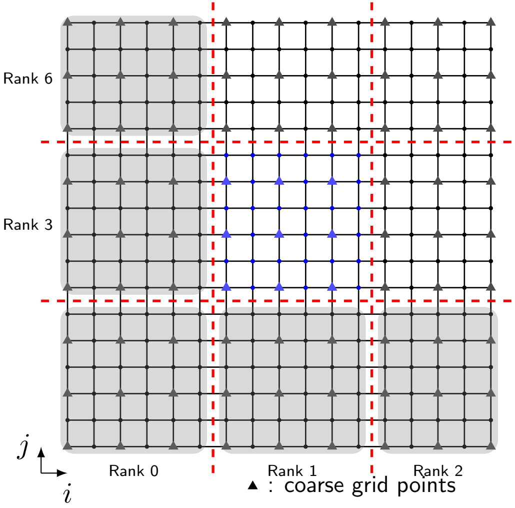
Then $\mathbf{v} = A\mathbf{u}$ can be computed by

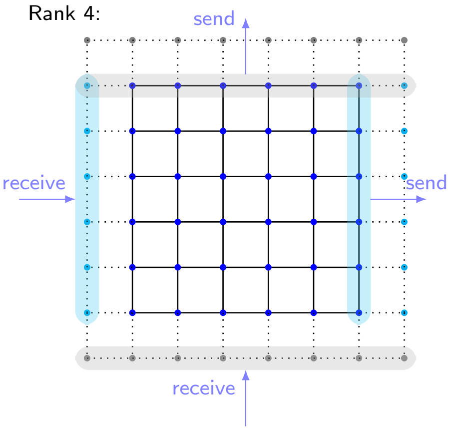
$$v_{i,j} = \sum_{p=-1}^{1} \sum_{q=-1}^{1} a_{p,q} u_{i+p,j+q}$$

with the help of a ghost point on the physical boundary and one overlapping grid point.

Framework - Distributed data structure

- Vector $\mathbf{u} \Leftarrow$ 2D array: u(1:Nx,1:Ny) $\Leftarrow$ each sub-domain: u(1−LAP:nx+LAP,1−LAP:ny+LAP)
- Operations (*e.g.* matvec, dot-product, vector update) perform on each u(1:nx,1:ny) simultaneously





CSLP

- Speed up convergence of Krylov subspace methods by Preconditioning
- Solve $M^{-1}Au = M^{-1}b$
- Complex Shifted Laplace Preconditioner (CSLP)

$$M_h = -\Delta_h - (\beta_1 - \beta_2 \mathrm{i})\,\mathcal{I}_h \mathbf{k}^2,\ (\beta_1, \beta_2) \in [0,1]\,, \quad e.g.\ \beta_1 = 1, \beta_2 = 0.5$$

  - ☑ Stencil notation

- Solve $Mx = u$ by multigrid method (V-cycle) $\Rightarrow x \approx M^{-1}u$
  - **Vertex-centered** coarsening based on the **global** grid
  - Damped Jacobi smoother (easy to parallelize)
  - Full-weight restriction I_h^{2h} & linear interpolation I_{2h}^h

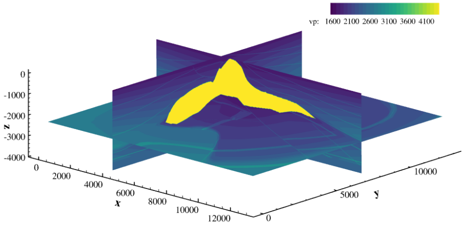
$$[I_h^{2h}] = \frac{1}{16}\begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}_h^{2h}, \quad [I_{2h}^h] = \frac{1}{4}\left]\begin{matrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{matrix}\right[_{2h}^{h}$$

  - Coarse-grid operator obtained by **re-discretization**
    - ☑ Stencil notation: $[M_{2h}]$ similar to $[M_h]$

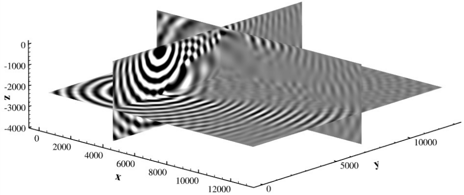
Parallel CLSP-preconditioned Krylov solver

3D SEG/EAGE Salt Model

- Real large-size domain $12\,800\,\mathrm{m} \times 12\,800\,\mathrm{m} \times 3840\,\mathrm{m}$
- High heterogeneity: the velocity varies from $1500\,\mathrm{m\,s^{-1}}$ to $4482\,\mathrm{m\,s^{-1}}$
- Grid size $641 \times 641 \times 193$



(a) Velocity distribution



(b) Pattern of wave field at $f = 5\,\mathrm{Hz}$

Figure: 3D SEG/EAGE Salt Model

Parallel CLSP-preconditioned Krylov solver

- Parallel CSLP-preconditioned IDR(4) for 3D SEG/EAGE Salt Model with grid size $641 \times 641 \times 193$ at $f = 5\,\text{Hz}$

Table: Performance on DelftBlue [1]

npx × npy × npz	Nodes	#Matvec	t(s)	Sp	Ep
6×4×2	1	413	897.25		
6×8×2	2	423	510.56	1.76	0.88
6×8×4	4	423	298.86	3.00	0.75
9×8×4	6	404	203.31	4.41	0.74

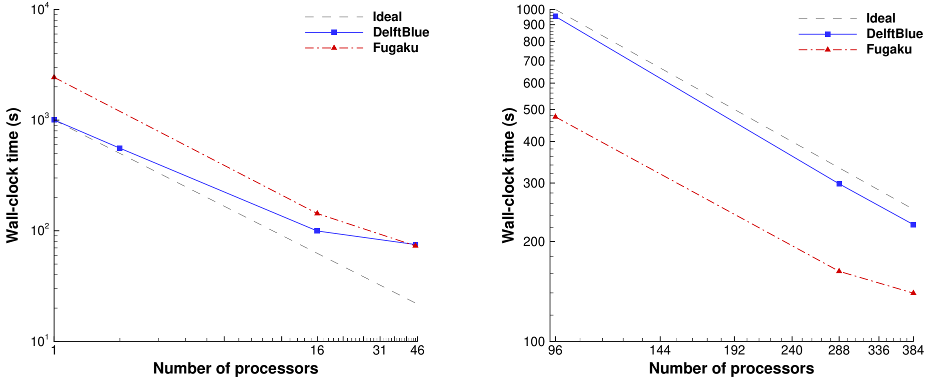
Table: Performance on Magic Cube [2]

npx × npy × npz	Nodes	#Matvec	t(s)	Sp	Ep
4 × 4 × 2	1	405	505.14		
4 × 4 × 4	2	418	287.60	1.76	0.88
8 × 8 × 2	4	390	155.64	3.25	0.81

- Good parallel performance
- Effective on different platforms

[1] DHPC, DelftBlue Supercomputer (Phase 1) `https://www.tudelft.nl/dhpc/ark:/44463/DelftBluePhase1`
[2] Supercomputer Magic Cube III: `https://www.ssc.net.cn/en/resource-hardware.html`

Parallel CLSP-preconditioned Krylov solver



(a) Single compute node (b) Multiple compute nodes

Figure: Strong scaling[1]. 3D model problem with ~ 100 million unknowns, #Matvec $\simeq 850$

[1] Supercomputer Fugaku: `https://www.r-ccs.riken.jp/en/fugaku/`. Riken International HPC Summer School 2022 is acknowledged

CSLP - Cons

- Increasing $k \Rightarrow$ eigenvalues move fast towards origin
- Too many iterations for high frequency
- Project unwanted eigenvalues to zero $\Rightarrow$ Deflation

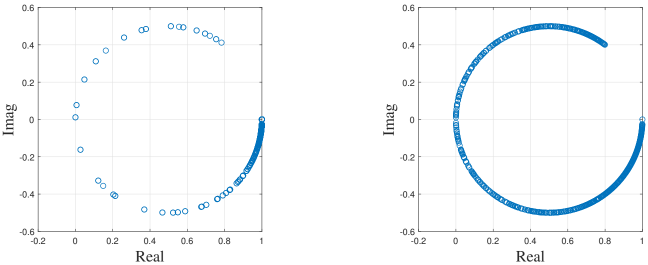


Figure: $\sigma\left(M_{(1,0.5)}^{-1}A\right)$ for $k=20$ (left) and $k=80$ (right)

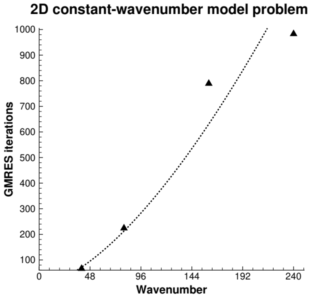


Figure: #Iter increases with k

Deflation - introduction

- Project unwanted eigenvalues to zero $\Rightarrow$ Deflation
- Deflation preconditioning: solve $PA\hat{u} = Pb$

$$P = I - AQ, \quad \text{where } Q = ZE^{-1}Z^T, \quad E = Z^TAZ$$

$$A \in \mathbb{R}^{n\times n}, Z \in \mathbb{R}^{m\times n}$$

- Columns of Z span deflation subspace
- Ideally Z contains eigenvectors
- In practice approximations: inter-grid vectors from multigrid
- Adapted Deflation Variant 1 (A-DEF1): $P_{A-DEF1} = M^{-1}_{(\beta_1,\beta_2)}P + Q$
  - Combined with the standard preconditioner CSLP
- Use CSLP-preconditioned GMRES to solve the coarse grid problem (obtain E^{-1}) approximately
- Linear approximation basis deflation vectors $\rightarrow$ **higher-order** deflation vectors (Adapted Preconditioned DEF, **APD**)
  - wavenumber-independent convergence

Two-level deflation - overall algorithm

- Flexible GMRES-type methods $\rightarrow$ allow for variable preconditioner

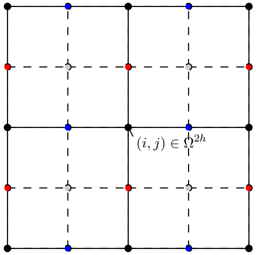
Algorithm Two-level deflation FGMRES

Choose u_0 and dimension k of the Krylov subspace.
Define $(k+1) \times k\bar{H}_k$ and initialize to zero
Compute $r_0 = b - Au_0$, $\beta = ||r_0||$, $v_1 = r_0/\beta$;
for $j = 1, 2, ..., k$ or until convergence **do**
  $\hat{v}_j = Z^T v_j$ ▷ Precondition starts
  $\tilde{v} \approx E^{-1}\hat{v}$ ▷ Solved by GMRES approximately, preconditioned by CSLP, **tol=**10^{-1}
  $t = Z\tilde{v}$
  $s = At$
  $\tilde{r} = v_j - s$
  $r \approx M^{-1}\tilde{r}$ ▷ Approximated by one multigrid V-cycle
  $x_j = r + t$ ▷ Precondition ends
  $w = Ax_j$
  for $i := 1, 2, ..., j$ **do**
    $h_{i,j} = (w, v_i)$
    $w := w - h_{i,j}v_i$
  end for
  $h_{j+1,j} := ||w||_2$, $v_{j+1} = w/h_{j+1,j}$; $X_k = [x_1, ..., x_k]$; $\bar{H}_k = \{h_{i,j}\}_{1 \le i \le j+1, 1 \le j \le m}$
end for
$u_k = u_0 + X_k y_k$ where $y_k = \arg\min_y \left|\left|\beta e_1 - \bar{H}_k y\right|\right|$

Higher-order deflation vectors

- 2D: the higher-order interpolation & restriction has 5×5 stencil
  - **Two overlapping** grid points are needed

$$[Z] = \frac{1}{64} \left] \begin{matrix} 1 & 4 & 6 & 4 & 1 \\ 4 & 16 & 24 & 16 & 4 \\ 6 & 24 & 36 & 24 & 6 \\ 4 & 16 & 24 & 16 & 4 \\ 1 & 4 & 6 & 4 & 1 \end{matrix} \right[_{2h}^{h}, \quad [Z^T] = \frac{1}{64} \left[\begin{matrix} 1 & 4 & 6 & 4 & 1 \\ 4 & 16 & 24 & 16 & 4 \\ 6 & 24 & 36 & 24 & 6 \\ 4 & 16 & 24 & 16 & 4 \\ 1 & 4 & 6 & 4 & 1 \end{matrix} \right]_{h}^{2h}$$



•••• : fine grid points $\in \Omega^h$
• : coarse grid points $\in \Omega^{2h}$

Figure: The allocation map of interpolation operator

Matrix-free two-level deflation

$$P = I - AQ, \quad \text{where } Q = ZE^{-1}Z^T, \quad E = Z^T AZ$$

- With matrix constructed, $E = Z^T AZ$, so-called Galerkin Coarsening

Matrix-free coarse grid operation $y = Ex$?

- Straightforward Galerkin Coarsening operator;

$$x_1 = Zx, \; x_2 = A_h x_1, \; y = Z^T x_2 \Rightarrow y = Ex$$

  - unacceptable computational cost for consideration of multilevel method

- Re-discretization:
  - **ReD-$\mathcal{O}$2**: The same as the fine grid
  - **ReD-$\mathcal{O}$4**: Fourth-order re-discretization of the Laplace operator

$$[E] = \frac{1}{12 \cdot (2h)^2} \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -16 & 0 & 0 \\ 1 & -16 & 60 & -16 & 1 \\ 0 & 0 & -16 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix} - \mathcal{I}_{2h}\mathbf{k}_{2h}^2$$

Matrix-free two-level deflation

ReD-Glk: Re-discretized scheme (stencil) from the result of Galerkin coarsening

$$[-\Delta_{2h}] = \frac{1}{(2h)^2} \cdot \frac{1}{256} \begin{bmatrix} -3 & -44 & -98 & -44 & -3 \\ -44 & -112 & 56 & -112 & -44 \\ -98 & 56 & 980 & 56 & -98 \\ -44 & -112 & 56 & -112 & -44 \\ -3 & -44 & -98 & -44 & -3 \end{bmatrix}$$

$$\Rightarrow -\Delta_{2h} u_{2h} = -4\frac{\partial^2 u}{\partial x^2} - 4\frac{\partial^2 u}{\partial y^2} - (\frac{13}{48}\frac{\partial^4 u}{\partial x^4} + \frac{1}{2}\frac{\partial^4 u}{\partial x^2 \partial y^2} + \frac{13}{48}\frac{\partial^4 u}{\partial y^4})(\mathbf{2h})^{\mathbf{2}} + \mathcal{O}(h^4)$$

$$[\mathcal{I}_{2h}\mathbf{k}_{2h}^2] = \frac{1}{64^2} \begin{bmatrix} 1 & 28 & 70 & 28 & 1 \\ 28 & 784 & 1960 & 784 & 28 \\ 70 & 1960 & 4900 & 1960 & 70 \\ 28 & 784 & 1960 & 784 & 28 \\ 1 & 28 & 70 & 28 & 1 \end{bmatrix} \mathbf{k}_{2h}^2$$

$$\Rightarrow [E] = [-\Delta_{2h}] - [\mathcal{I}_{2h}\mathbf{k}_{2h}^2]$$

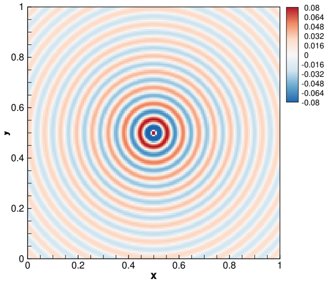
? Boundary conditions - ReD-$\mathcal{O}$2 on the boundary grid points

Convergence - Constant wavenumber

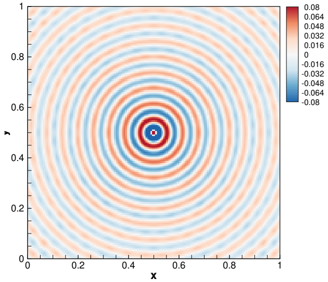
Table: The number of iterations required by using APD-GMRES.

Grid size	k	kh	ReD-$\mathcal{O}2$	ReD-$\mathcal{O}4$	ReD-Glk
65 $\times$ 65	40	0.625	**20**	**17**	**9**
129 $\times$ 129	80	0.625	**30**	**18**	**9**
257 $\times$ 257	160	0.625	**87**	**19**	**9**
513 $\times$ 513	320	0.625	**>100**	**23**	**10**
129 $\times$ 129	40	0.3125	**18**	**18**	**7**
257 $\times$ 257	80	0.3125	**19**	**18**	**7**
513 $\times$ 513	160	0.3125	**21**	**18**	**7**
1025 $\times$ 1025	320	0.3125	**28**	**20**	**6**
2049 $\times$ 2049	640	0.3125	**53**	**23**	**6**

"$>$" indicates it does not converge to the specified residual tolerance (10^{-6}) within a certain number of iterations.



(a) Exact solution



(b) $kh = 0.625$

- $Ex = Z^T A_h Z x$: #iter=**7** for $kh = 0.625$, **5** for $kh = 0.3125$
- ReD-$\mathcal{O}4$ better than ReD-$\mathcal{O}2$
- ReD-Glk: close to wavenumber independence

Convergence - 2D Wedge

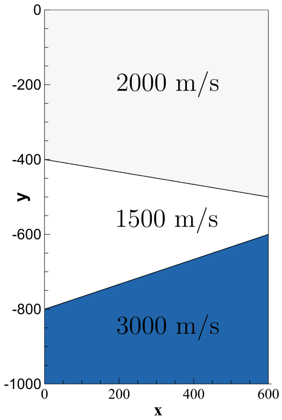


Figure: Wedge problem

Convergence - 2D Wedge

Table: The number of iterations required by using APD-GMRES.

Grid size	f	kh	ReD-$\mathcal{O}2$	ReD-$\mathcal{O}4$	ReD-Glk
$73\times$ 121	10	0.35	**22**	**22**	**9**
$145\times$ 241	20	0.35	**28**	**27**	**9**
$289\times$ 481	40	0.35	**31**	**29**	**9**
$577\times$ 961	80	0.35	**37**	**30**	**9**
$1153\times$ 1921	160	0.35	$>$**50**	**34**	**8**

"$>$" indicates it does not converge to the specified residual tolerance (10^{-6}) within a certain number of iterations.

- $Ex = Z^T A_h Z x$: #iter=**6**
- ReD-$\mathcal{O}4$ better than ReD-$\mathcal{O}2$
- ReD-Glk: wavenumber independence although it is derived from constant wavenumber

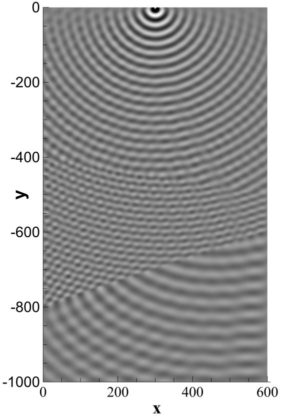
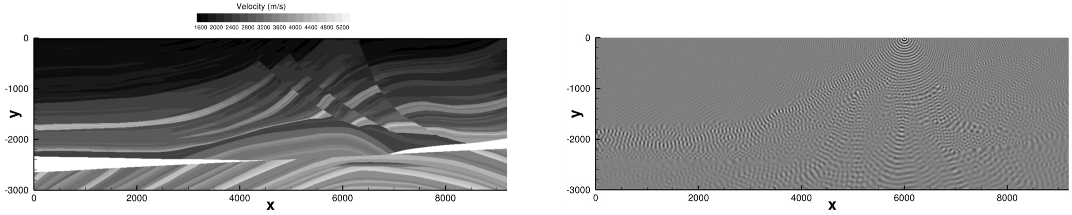


Figure: Waves pattern at 80 Hz

Convergence - Marmousi



(a) Marmousi problem (b) Wave pattern at $f = 40$ Hz

Table: The number of iterations required by using APD-GMRES.

Grid size	f	kh	ReD-$\mathcal{O}$2	ReD-$\mathcal{O}$4	ReD-Glk
737 $\times$ 241	10	0.5236	**38**	**30**	**11**
1473$\times$ 481	20	0.5236	**71**	**34**	**11**
2945$\times$ 961	40	0.5236	$>$**50**	**50** ($>$2500)	**12**

- $Ex = Z^T A_h Z x$: #iter=7
- Similar convergence properties for highly heterogeneous media
- ReD-Glk: close to wavenumber independence

Parallel performance - Weak scaling

- Preconditioned GCR
- APD using ReD-Glk
- DelftBlue, GNU Fortran 8.5.0, Open MPI 4.1.1

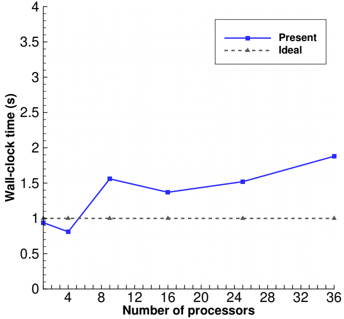


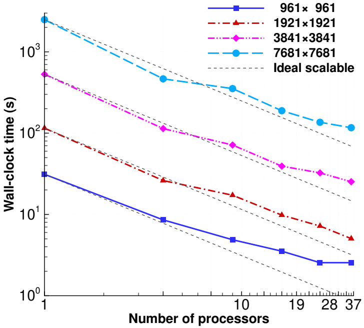
Figure: Weak scaling for constant-wavenumber problem with $k = 100$ and a grid size of 160×160 per processes.

Table: Weak scaling for model problems with non-constant wavenumber.

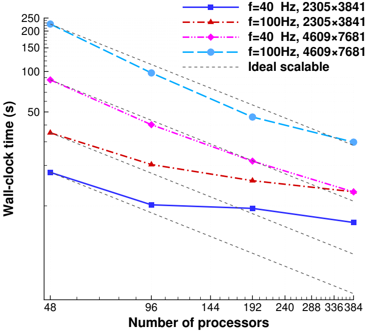
grid size	np	#iter	CPU time (s)
	Wedge, $f = 40$ Hz		
577×961	6	10 (46)	4.86
1153×1921	24	10 (43)	5.75
	Marmousi, $f = 10$ Hz		
737×241	3	11 (63)	10.55
1473×481	12	10 (58)	12.08
2945×961	48	10 (58)	17.72

Close to weak scalability

Parallel performance - Strong scaling



(a) Constant-wavenumber problem with $k = 200$



(b) Wedge problem with $f = 40$ Hz and $f = 100$ Hz

Figure: Strong scaling

Good strong scalability for large problems (larger computation/communication ratio)

Multilevel Deflation

- Apply two-level method **recursively**
- **Re-discretization scheme** derived from Galerkin coarsening for **both** E and M
  - The size of the stencil remains 7×7 for level > 3
  - Need three overlapping grid points
  - Truncate on the near-boundary grid points, not need extra boundary schemes
- **V-cycle**: Only one FGMRES iteration per **coarse** level except for the **coarsest** level, *i.e.* $m = 1$ in line 4
  - CSLP: Krylov iterations instead of multigrid
    - Max $\mathcal{O}(N^{0.25})$ iterations or tol$=10^{-1}$
    - Small complex shift: $1/k_{max}$
  - Coarsening **remains on indefinite levels**
  - Coarsest level: solved by CSLP-GMRES, tol$=10^{-1}$

Algorithm Recursive two-level deflated FGMRES: `TLADP-FGMRES(A, b)`

1: Determine the current level l and dimension m of the Krylov subspace
2: Initialize u_0, compute $r_0 = b - Au_0$, $\beta = ||r_0||$, $v_1 = r_0/\beta$;
3: Define $\bar{H}_m \in \mathbb{C}^{(m+1)\times m}$ and initialize to zero
4: **for** $j = 1, 2, ..., m$ or until convergence **do**
5:     $\hat{v}_j = Z^T v_j$ ▷ Restriction
6:     **if** $l + 1 == l_{max}$ **then** ▷ Predefined coarsest level l_{max}
7:         $\tilde{v} \approx E^{-1}\hat{v}$ ▷ Approximated by CSLP-FGMRES
8:     **else**
9:         $l \leftarrow l + 1$
10:         $\tilde{v} \leftarrow$`TLADP-FGMRES(E,` $\hat{v}$`)` ▷ Apply two-level deflation recursively
11:     **end if**
12:     $t = Z\tilde{v}$ ▷ Interpolation
13:     $s = At$
14:     $\tilde{r} = v_j - s$
15:     $r \approx M^{-1}\tilde{r}$ ▷ CSLP, by multigrid method or Krylov iterations
16:     $x_j = r + t$
17:     $w = Ax_j$
18:     **for** $i := 1, 2, ..., j$ **do**
19:         $h_{i,j} = (w, v_i)$
20:         $w \leftarrow w - h_{i,j}v_i$
21:     **end for**
22:     $h_{j+1,j} := ||w||_2$, $v_{j+1} = w/h_{j+1,j}$
23:     $X_m = [x_1, ..., x_m]$, $\bar{H}_m = \{h_{i,j}\}_{1\le i\le j+1, 1\le j\le m}$
24: **end for**
25: $u_m = u_0 + X_m y_m$ where $y_m = \arg\min_y ||\beta e_1 - \bar{H}_m y||$
26: **Return** u_m

Multilevel deflation - 'incomplete' V-cycle

Table: The number of outer iterations required to solve the Wedge problems by using **V-cycle** multilevel APD-FGMRES. For $kh = 0.17$, the coarse-grid systems become negative definite starting from the 5th level.

Grid size	f (Hz)	3 levels	4 levels	5 levels
289$\times$ 481	20	5	7	7
577$\times$ 961	40	6	7	8
1153$\times$ 1921	80	6	7	10
2305$\times$ 3841	160	7	8	12

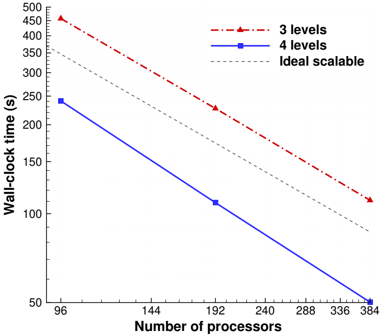


Figure: Strong scaling for Wedge problem with $f = 40$ Hz and a grid size of 4609×7681.

Coarsening **remains** on **indefinite** levels:

- close to wavenumber independence
- Good strong scalability

What about coarsening to **negative definite** levels?

Multilevel deflation - a robust and efficient variant

For the scenario of coarsening to **negative definite** levels:

- A **tolerance** for **the second level (L2)** (instead of one FGMRES iteration)
  - L2 tol=1×10^{-1} $\rightarrow$ close to constant outer iterations
  - L2 tol=3×10^{-1} $\rightarrow$ extra outer iterations but **reduced computation time** ✔
- **One** FGMRES iteration for **the other coarse levels** including the coarsest level
- CSLP: **the first and second** levels: multigrid method (one V-cycle); **the other** coarse levels: Krylov iterations (GMRES), tol=1×10^{-1}

Table: Number of outer FGMRES-iterations and **sequential** CPU time required to solve the Marmousi problem. For $kh = 0.54$, the coarse-grid systems become **negative definite** starting from the **3rd level**. In parentheses are the number of iterations to solve the second-level grid system.

f (Hz)	Grid size	Two-level, L2 tol=1×10^{-1}		Five-level, L2 tol=1×10^{-1}		Five-level, L2 tol=3×10^{-1}	
		Outer #iter (L2 #iter)	CPU time (s)	Outer #iter (L2 #iter)	CPU time (s)	Outer #iter (L2 #iter)	CPU time (s)
10	737×241	11 (64)	23.15	11 (13)	18.57	13 (7)	12.67
20	1473×481	11 (141)	224.21	11 (24)	108.03	15 (15)	84.06
40	2945×961	12 (381)	4354.83	13 (50)	1084.42	18 (29)	816.38

Multilevel deflation - complexity analysis

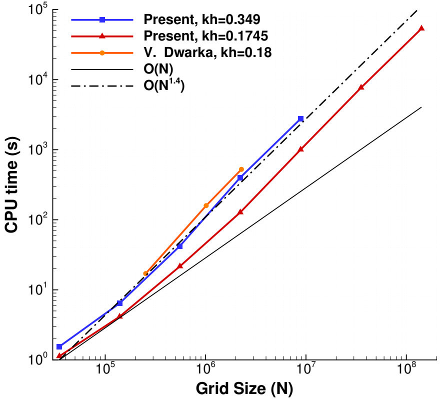


Figure: Complexity analysis of the multilevel APD preconditioned Krylov subspace method. Evolution of the **sequential** computational time versus problem size. Wedge model problem.

Table: The number of outer iterations required to solve the Wedge problems with $kh = 0.17$ by using the multilevel APD-FGMRES.

Six-level deflation, L2 tol=3×10^{-1}		
Grid size	f (Hz)	Outer #iter (L2 #iter)
289× 481	20	11 (3)
577× 961	40	12 (4)
1153× 1921	80	12 (7)
2305× 3841	160	13 (13)
4609× 7681	320	14 (27)
9217× 15361	640	17 (47)

- The number of iterations **weakly** depends on the frequency
- The computational time behaves asymptotically as $N^{1.4}$

Multilevel deflation - parallel performance

Table: The number of iterations required and computation time, along with the resulting speedup (Sp) and parallel efficiency (Ep), to solve the Wedge problem with a grid size 4609×7681 and $f = 320\,\text{Hz}$ by using the parallel multilevel (six-level) APD-FGMRES on one compute node of DelftBlue.

np	Grid points per processor	#iter	DelftBlue Phase 1* CPU time (s)	DelftBlue Phase 1* Sp	DelftBlue Phase 1* Ep	Delftblue Phase 2** CPU time (s)	Delftblue Phase 2** Sp	Delftblue Phase 2** Ep
1	35401729	14	5996.43	-	-	4064.63	-	-
2	17700865	14	3034.40	1.98	0.99	2029.36	2.00	1.00
6	5900288	14	1097.27	5.46	0.91	686.19	5.92	0.99
12	2950144	14	574.84	10.43	0.87	343.05	11.85	0.99
24	1475072	14	319.71	18.76	0.78	186.67	21.77	0.91
48	737536	14	203.49	29.47	0.61	120.29	33.79	0.70
64	553152	14	-	-	-	100.19	40.57	0.63

* Phase 1 (June 2022): 2x Intel XEON E5-6248R **24**C 3.0GHz, 192GB

** Phase 2 (Jan. 2024): 2x Intel XEON E5-6448Y **32**C 2.1GHz, 256 GB

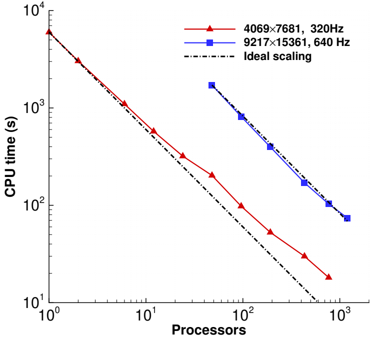


Figure: Strong scaling for Wedge problem

Good strong scalability for massively parallel computing

Conclusions and Perspectives

- Parallel CSLP preconditioned Krylov solvers (2D/3D)
- Parallel two-level deflation preconditioned Krylov solvers (2D)
- Matrix-free implementation with wavenumber-independent convergence
- Parallel framework with fairly good weak and strong scaling
- Robust parallel multilevel deflation for high-frequency heterogeneous problems
- Generalize to large-scale 3D applications

Further reading:

- Dwarka, V., Vuik, C.: Scalable convergence using two-level deflation preconditioning for the Helmholtz equation, SIAM Journal on Scientific Computing, 42(2020), A901-A928.
- Dwarka, V., Vuik, C.: Scalable multi-level deflation preconditioning for highly indefinite time-harmonic waves, Journal of Computational Physics, 469(2022), 111327.
- Chen, J., Dwarka, V., Vuik, C.: A matrix-free parallel solution method for the three-dimensional heterogeneous Helmholtz equation, Electronic Transactions on Numerical Analysis, 59 (2023), 270–294.
- Chen, J., Dwarka, V., Vuik, C.: A matrix-free parallel two-level deflation preconditioner for the two-dimensional Helmholtz problems, `https://doi.org/10.48550/arXiv.2308.06152`.

Q&A

Thanks!