Fast Solution Methods for Wave Propagation Problems

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with: N. Bootland, I. Graham, P. Jolivet, C. Ma, S. F. Nataf, S. Operto, R. Scheichl, P.-H. Tournier

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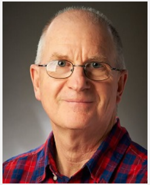
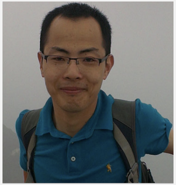
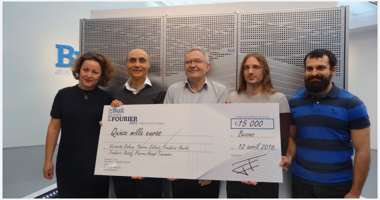


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Resources (slides and notes) from
`https://github.com/vicdolean/domain-decomposition-notes`

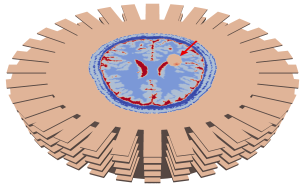
Outline

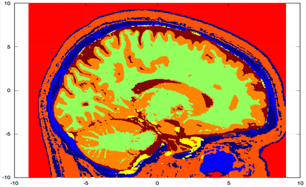
How to solve Helmholtz equation efficiently (part 1)

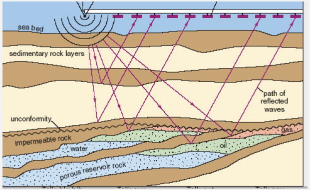
What about Maxwell? (part 2)

How to solve Helmholtz equation efficiently (part 1)

Wave propagation in heterogeneous media







Maxwell's equations

Medical imaging: reconstruct the permittivity ε

$$\nabla \times (\mu^{-1}\nabla \times \mathbf{E}) - \omega^2 \varepsilon \mathbf{E} = \mathbf{J}$$

- $\mathbf{E}$ is the electric field
- $\mu > 0$ is the magnetic permeability
- $\varepsilon > 0$ is the electric permittivity, ω is the frequency

Helmholtz equation

Seismic imaging: reconstruct material properties of subsurface

$$-\Delta u - (\omega^2 / c^2) u = f,$$

- $c^2 = \rho c_P^2$,
- ρ is the density,
- c_P is the speed of longitudinal waves.

AIM (a holistic approach)

Propose a combination of **discretisation** + **solvers** in frequency domain

Helmholtz equation

Hermann von Helmholtz (1821-1894)

physicist, physician, philosopher

Time-harmonic wave equation

$$-\Delta u - k^2 u = f$$

Scalar wave equation ($c(x)$ local speed)

$$\partial_{tt} v - c^2(x)\Delta v = F(x,t),$$

If $F(x,t) = f(x)e^{-i\omega t}$ (mono-chromatic) then

$$v(x,t) = u(x)e^{-i\omega t}$$

which leads to

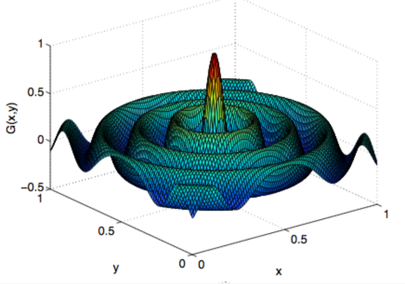
$$-\Delta u - n(x)^2\omega^2 u = f,$$

where $n(x) = \frac{1}{c(x)}$ is the **index of refraction**, $k^2 = n^2\omega^2$ is called **wave number**.

Remark

If k is small, Helmholtz is a perturbation of the Laplace's problem, otherwise the solution is highly oscillatory $\rightsquigarrow$ **mathematical** and **numerical** difficulties.

Why the high-frequency problem is hard? (Accuracy and pollution)



How to discretise well

- After discretisation **maximise** accuracy and **minimise** the number of degrees of freedom (#DoF)
- If $h\omega$ is kept constant the error increases with $\omega \rightsquigarrow$ **pollution error** [Babuska, Sauter, SINUM, 1997]
- FEM discretisations: for quasi-optimality we need [Melenk, Sauter, SINUM, 2011]

$$h^p \omega^{p+1} \lesssim 1$$

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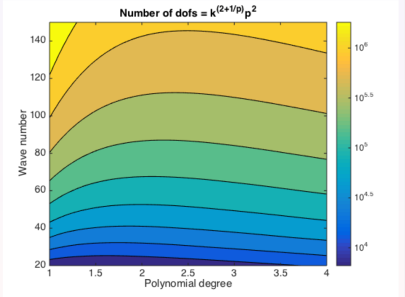

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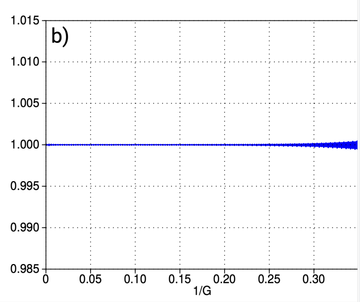
Consequences

- **High-frequency solution** u oscillates at a scale $1/\omega \Rightarrow h \sim \frac{1}{\omega} \rightsquigarrow$ large #DoF.
- **Pollution effect** requires $h \ll \frac{1}{\omega}$, $h \sim \omega^{-1-1/p}$, with p the finite element order $\rightsquigarrow$ even larger #DoF.
- Trade-off: **number of points per wavelength** (ppwl) $G = \frac{\lambda}{h} = \frac{2\pi}{\omega h}$ and polynomial degree $\rightsquigarrow$ **dispersion analysis** (measuring the ratio between the numerical and physical wave speeds).

Discretisation methods (pros and cons)

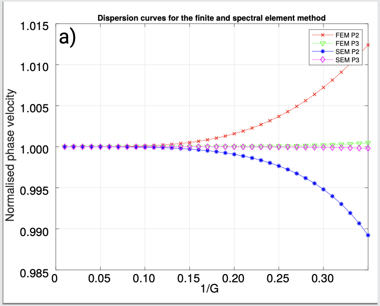
Finite differences (FD)

- Can reach high-order accuracy while minimising the number of unknowns and **maximising sparsity**
- Can **optimise dispersion** through adaptive coefficients



Finite elements (FE)

- Unstructured meshes: element size adapted to local wavelengths **(h-adaptivity)**
- Tetrahedral meshes can **conform to complex boundaries** (topography, sea bottom, salt bodies)

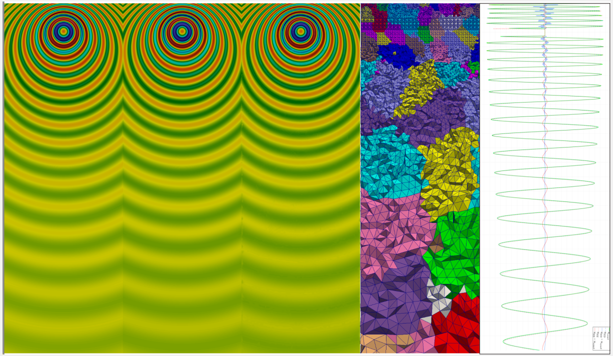


A hidden story of complexity and accuracy (Finite differences vs. Finite elements)

Test case: 2 km $\times$ 4 km $\times$ 12 km, $c(x, y, z) = c_0 + \alpha \times z$ with c_0=1 km/s, source at 1 km depth, frequency 8 Hz.

[Kuvshinov and Mulder, 2006] FD grid (h=31.25 m) with 4 ppwl, adapted tetrahedral FE grid.

			#dof (M)		Error norm	
$\alpha(s^{-1})$	$\lambda_{min}(m)$	$\lambda_{max}(m)$	FD	FE	FD	FE
0.8	125	1200	13	28	0.0079	0.034
2	125	3125	13	16	0.044	0.034



(a) FD solution.
(b) Analytical solution.
(c) FE solution.
(d) FE mesh.

(e) Comparison between (a-c) along a vertical profile cross-cutting source position.

Efficient solution of the discretised problem

A large linear system to solve $Au = b$

- A is symmetric but **indefinite or non-Hermitian.**
- A can become **arbitrarily ill-conditioned**
- A is getting larger with increasing ω: its size **n** grows like $\omega^{(1+1/p)d}$.

Solution in **optimal time** using solvers with **good parallel properties** and **robust w.r.t heterogeneities**

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Landscape of linear solvers

- **Direct solvers**: MUMPS, SuperLU, PastiX, UMFPACK, PARDISO
- **Iterative methods (Krylov)**: CG, BiCGStab, MINRES, GMRES ...

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Conventional iterative methods fail... [Ernst, Gander (2012)]]

... and direct solvers $\rightsquigarrow$ complexity and memory issues

Gauss	$d = 1$	$d = 2$	$d = 3$
dense matrix	$\mathcal{O}(\mathbf{n^3})$	$\mathcal{O}(\mathbf{n^3})$	$\mathcal{O}(\mathbf{n^3})$
using band structure	$\mathcal{O}(\mathbf{n})$	$\mathcal{O}(\mathbf{n^2})$	$\mathcal{O}(\mathbf{n^{7/3}})$
using sparsity	$\mathcal{O}(\mathbf{n})$	$\mathcal{O}(\mathbf{n^{3/2}})$	$\mathcal{O}(\mathbf{n^2})$

One and two-level methods

Solve the preconditioned $A\mathbf{u} = \mathbf{b}$, i.e. $M^{-1}A\mathbf{u} = M^{-1}\mathbf{b}$ by GMRES

The one-level preconditioner

$$\boxed{M^{-1} = \sum_{j=1}^{N} R_j^T D_j A_j^{-1} R_j}, \text{ where}$$

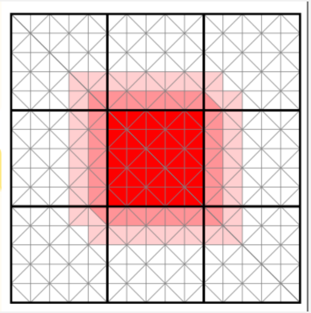
R_j	$\Omega \to \Omega_j$	**restriction operator**
R_j^T	$\Omega_j \to \Omega$	**prolongation operator**
D_j		**partition of unity matrix**.

Definition of the local matrices A_j $(k = \frac{\omega}{c})$

A_j is the stiffness matrix of the local **Robin problem**

$$\begin{aligned} (-\Delta - k^2)(u_j) &= f && \text{in } \Omega_j \\ \left(\frac{\partial}{\partial n_j} + ik\right)(u_j) &= 0 && \text{on } \partial\Omega_j \setminus \partial\Omega. \end{aligned}$$

$$\Omega = \cup_{j=1}^{N} \Omega_j$$



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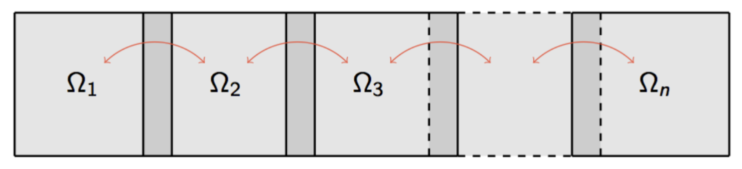
One level is not enough (only neighbouring subdomains communicate)



Solve the preconditioned $A\mathbf{u} = \mathbf{b}$, i.e. $M^{-1}A\mathbf{u} = M^{-1}\mathbf{b}$ by GMRES

The two-level (additive) preconditioner

$$\boxed{M_2^{-1} = \sum_{j=1}^{N} R_j^T D_j A_j^{-1} R_j + M_0^{-1}}, \text{ where}$$

R_j	$\Omega \to \Omega_j$	**restriction operator**
R_j^T	$\Omega_j \to \Omega$	**prolongation operator**
D_j		**partition of unity matrix**.

Definition of the local matrices A_j $(k = \frac{\omega}{c})$

A_j: stiffness matrix of the local **Robin problem**

$$\begin{array}{rcll} (-\Delta - k^2)(u_j) & = & f & \text{in } \Omega_j \\ \left(\frac{\partial}{\partial n_j} + ik\right)(u_j) & = & 0 & \text{on } \partial\Omega_j \setminus \partial\Omega. \end{array}$$

How to add a second level or coarse information Z

$M_0^{-1} = ZE^{-1}Z^*$	is the coarse space correction
$Z, E = Z^*AZ$	matrix spanning the coarse space and the coarse matrix

Remark: Hybrid variants of the preconditioner are also possible.

An example of coarse space for Helmholtz

How to choose the coarse information Z? [Graham, Spence, Vainikko, Math. Comp., 2017]

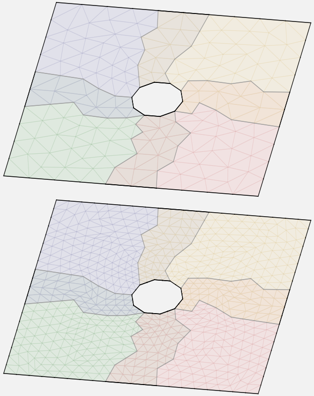
The grid coarse space (Grid CS)

- is based on a **geometrical** coarse mesh of diameter H_{coarse}
- R_0^T interpolation matrix from the fine to the coarse grid
- $Z = R_0^T$ matrix spanning the coarse space
- $E = Z^T A Z$ stiffness matrix on the coarse grid

Theory for absorptive problem: $-\Delta - (k^2 + i\xi)$

- For scalability and robustness w.r.t to the frequency we need $H_{coarse} \sim k^{-\alpha}$, $0 < \alpha <= 1$.
- $|\xi| \sim k^2$ and $\delta \sim H_{coarse}$, then weighted GMRES will converge with the number of iterations **independent of the wavenumber**.

Is the grid CS optimal for heterogeneous problems?



Bonazzoli, Dolean, Graham, Spence, Tournier. Domain decomposition preconditioning for the high-frequency time-harmonic Maxwell [...] Math. Comp., 2019.

Summary of available results

Two-level DD preconditioner

Solve $A\mathbf{u} = \mathbf{b}$, i.e. $M_2^{-1}A\mathbf{u} = M_2^{-1}\mathbf{b}$ by GMRES. DD preconditioner based on N domains of diameter $\sim H$.

$$\boxed{M_2^{-1} = \sum_{j=1}^{N} R_j^T D_j A_j^{-1} R_j + Z(Z^* A Z)^{-1} Z^*}$$

Different CS according to the choice of Z:

- **Grid CS**: $Z = R_0^T$ with R_0^T **interpolation matrix** from the fine to the coarse grid.
- **DtN CS** : solve $\mathrm{DtN}_{\Omega_j}(u_{\Gamma_j}^l) = \lambda^l u_{\Gamma_j}^l$, Z is formed from **local harmonic extensions** ($\mathcal{H}$) of modes, **weighted** (D_j) and **extended globally** $R_j^T D_j \mathcal{H} u_{\Gamma_j}^l$
- **Δ-GenEO** (**$\mathcal{H}_k$-GenEO**): solve $L_j \mathbf{u}_j^l = \lambda^l D_j L_j D_j \mathbf{u}_j^l$ ($\widetilde{B}_j \mathbf{u}_j^l = \lambda^l D_j B_{j,k} D_j \mathbf{u}_j^l$), Z is formed from **weighted** (D_j) and **extended globally** modes $R_j^T D_j \mathbf{u}_{\Gamma_j}^l$

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Advantages and available results

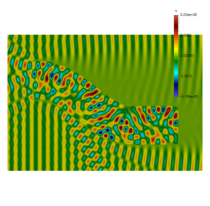
- ⊕ **Grid CS**: Theoretical/numerical results absorptive problem, robustness for $H \sim k^{-\alpha}, 0 < \alpha \leq 1$.
- ⊕ **Δ-GenEO** : Theoretical/numerical results and robustness for **mild heterogeneities** and **low frequencies**.
- ⊕ **$\mathcal{H}_k$-GenEO** : Theoretical/numerical results and robustness for **high frequencies** in **the indefinite case**.

Bootland, Dolean, Graham, Ma, Scheichl. Overlapping Schwarz methods with GenEO coarse spaces for indefinite and nonself-adjoint problems, IMAJNA, 2022.

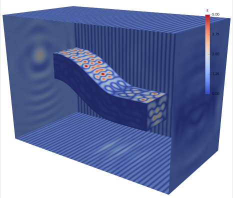
Numerical comparison: benchmark problems

Numerical tests with open source libraries and DSL: Freefem (`https://freefem.org`), ffddm (`https://doc.freefem.org/documentation/ffddm`), hpddm (`https://github.com/hpddm/`)

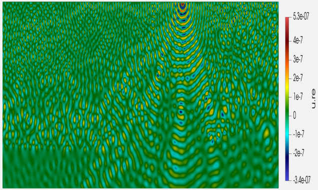
Cobra cavity 2d



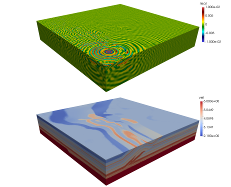
Cobra cavity 3d



Marmousi



Overthurst



			Grid CS		H-GenEO		DtN	
Problem	d	freq	5 ppwl	10 ppwl	5 ppwl	10 ppwl	5 ppwl	10 ppwl
Marmousi	2D	low	✓	✓	✓	✓	✓✓	✓✓
		high	✓✓	✓	✗	✓✓	✓	✓
COBRA Cavity	2D	low	✓	✓	✗	✗	✓✓	✓✓
		high	✗	✓	✗	✗	✓✓	✓✓
COBRA Cavity	3D	low	✓	✓✓	✗	✗	✓✓	✓
		high	✗	✓✓	✗	✗	✓✓	✓
Overthrust	3D	low	✓	✓	✗	✓	✓	✓
		high	✓	✓	✗	✓	✓	✓

Bootland, Dolean, Jolivet, Tournier A comparison of coarse spaces for Helmholtz problems in the high frequency regime, CAMWA, 2021.

Geophysical benchmarks

Overview

We only consider isotropic acoustic media with constant density 1

Models	$c_m(m/s)$	$c_M(m/s)$	f(Hz)	$\lambda_m(m)$	$\lambda_M(m)$	G_m	G_M	N_λ
Homogeneous	1500	1500	7.5	200	200	4	4	100
Linear	1500	8500	7.5	200	1133	4	22.7	50
Overthrust	2179	6000	10	218	600	4.4	12	50
GO_3D_OBS	1500	8639.1	3.75	400	2303.8	4	23	255

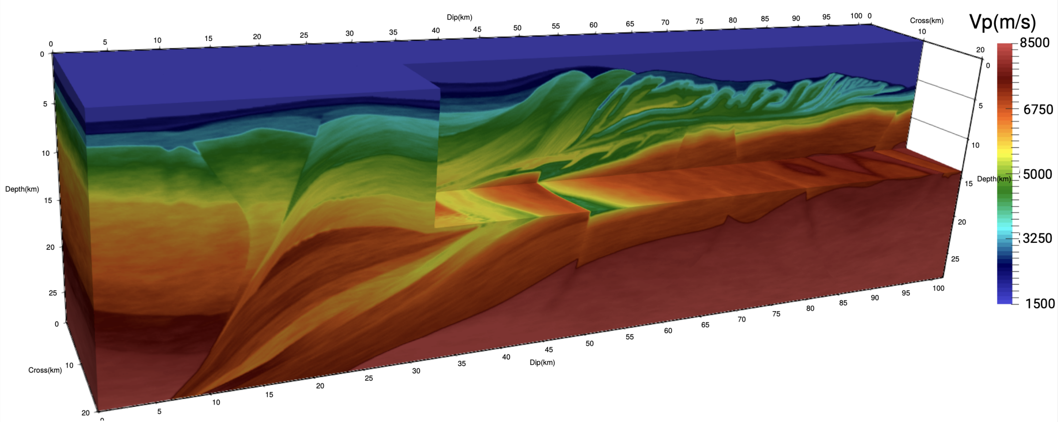
c_m, c_M: Minimum and maximum wavespeeds. f: Frequency. λ_{min}, λ_{max}: Minimum and maximum wavelength. G_{min}, G_{max}: Smallest and highest G. N_λ: Maximum number of propagated wavelengths.

- **Homogeneous**: 10 km $\times$ 20 km $\times$ 10 km, constant velocity
- **Linear**: 10 km $\times$ 20 km $\times$ 10 km, velocity increases linearly in the y direction
- **Overthrust**: the SEG/EAGE overthrust model, 20 km $\times$ 20 km $\times$ 4.65 km
- **GO_3D_OBS**: the 3D GO_3D_OBS **crustal geomodel** , designed to assess seismic imaging techniques for deep crustal exploration. Selected target of dimensions **20 km** $\times$ **102 km** $\times$ **28.4 km**

Tournier, Jolivet, Dolean, Aghamiry, Operto, Riffo: 3D finite-difference and finite-element frequency-domain wave simulation [...], Geophysics, 2022.

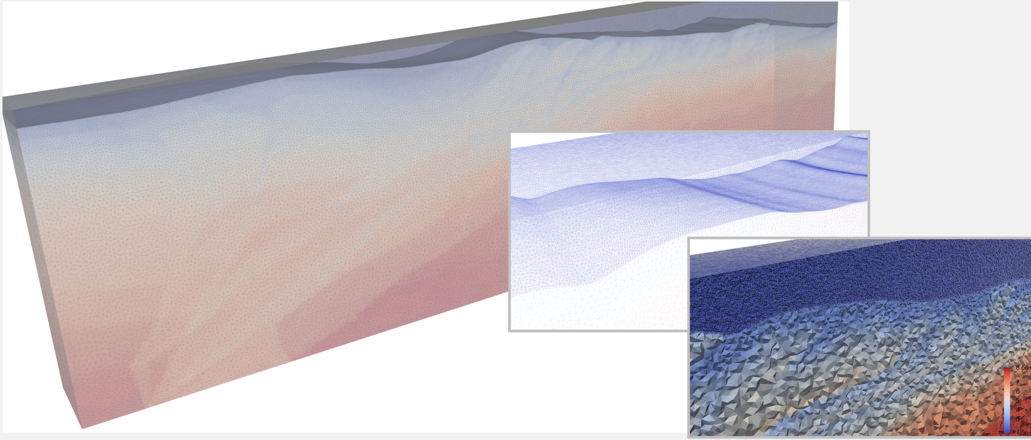
The crustal model

Velocity field



The crustal model

Adapted mesh



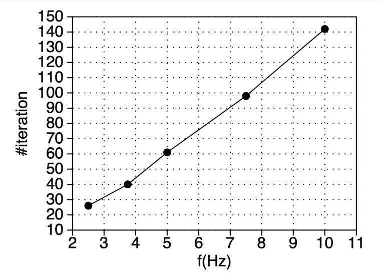
Explicit meshing of the interior boundary surface corresponding to the bathymetry. At 3.75 Hz, the adapted mesh has 132 million elements while the homogeneous mesh has 402.4 million ⇝ **coarsening factor of 3**

Numerical results

Weak scalability w.r.t. frequency

GO_3D_OBS with finite differences:

f(Hz)	#dof(10^6)	#cores	#it	ovl	T_f(s)	T_s(s)	T_{tot}(s)	E_w
2.5	21.4	60	26	3	52.5	24.8	77.3	1
3.75	67.5	360	40	3	21.9	18.6	40.5	1.003
5	153.5	875	61	3	20.9	26.0	46.9	0.811
7.5	500.1	2450	98	4	26.7	60.8	87.5	0.506
10	1160.6	9856	142	5	15.1	70.8	85.9	0.297



Linear increase of the iteration count with the frequency

- Factorisation time: T_f
- Solver time: T_s
- Weak scaling parallel efficiency
$$E_w = \frac{\left[T_{tot}^{(ref)} \times \#cores^{(ref)} / \#dof^{(ref)}\right]}{[T_{tot} \times \#cores / \#dof]}.$$
- Strong scaling parallel efficiency
$$E_s = \frac{\left[T_{tot}^{(ref)} \times \#cores^{(ref)}\right]}{[T_{tot} \times \#cores]}$$

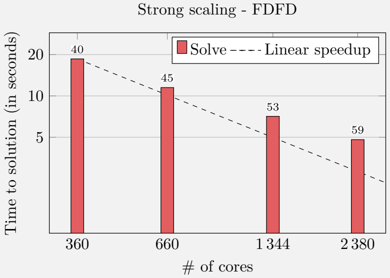
Numerical results

Strong scalability

GO_3D_OBS at 3.75 Hz:

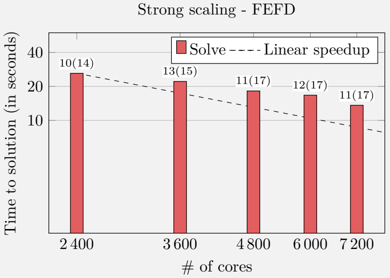
FD — 67.5 million dofs

#cores	#it	T_f(s)	T_s(s)	T_{tot}(s)	E_s
360	40	21.9	18.6	40.5	1
660	45	10.8	11.5	22.3	0.991
1344	53	4.4	7.1	11.5	0.943
2380	59	2.5	4.8	7.3	0.839



FE — 597.7 million dofs

#cores	#it	T_f(s)	T_s(s)	T_{tot}(s)	E_s
2400	10(14)	62.3	26.1	88.4	1
3600	13(15)	38.4	22.1	60.5	0.974
4800	11(17)	28.4	18.2	46.6	0.948
6000	12(17)	19.4	16.7	36.1	0.980
7200	11(17)	18.1	13.6	31.7	0.930



Numerical results

Comparison with a time-domain solver

Mimicking an inverse problem...
Test case: **GO_3D_OBS** at 3.75 Hz, 130 right-hand sides.

Finite-Difference Time-Domain			Finite-Difference Frequency-Domain							
			MUMPS					ORAS		
#c	$T_s^{(130)}$(s)	T_{hc}(hr)	#cores	T_f(s)	T_s^1(s)	T_s^{130}(s)	T_{hc}(hr)	#cores	T_s^{130}(s)	T_{hc}(hr)
12480	264	915	1920	1000	3.9	28.3	548	1344	256.8	96

- **Finite-Difference Time-Domain solver**: classical $\mathcal{O}(\Delta t^2, \Delta t^8)$ staggered-grid stencil using a grid interval of 100 m
- **MUMPS solver**: block low-rank version with compression threshold $\varepsilon_{BLR} = 10^{-5}$

Conclusion: the time-harmonic solver can be used as **forward engine for FWI** for the 3D visco-acoustic case.

Conclusions and openings: solvers for Helmholtz

Complexity* increases drastically with the frequency requiring clever solution strategies...

Specific remarks: geophysical applications

- We have: an **efficient, accurate and versatile** forward engine for 3D frequency domain FWI.
- For a similar accuracy, the **FDFD method outperforms the FEFD** in terms of computational efficiency.
- Two large objectives: (i) use it as **forward engine for FWI** to perform 3D visco-acoustic case studies (ii) Extension to **visco-elastic physics**.

Openings

- **Theoretical**: behaviour of a few methods is not completely understood $\rightsquigarrow$ new mathematical tools are needed. (e.g. spectral/microlocal analysis, optimisation).
- **Computational**: Can we avoid repeated solves? $\rightsquigarrow$ use surrogate models, operator learning for inverse problem.

* Problems as large as 74 million dof can be solved efficiently by a direct method (BLR MUMPS).

GeoScienceWorld

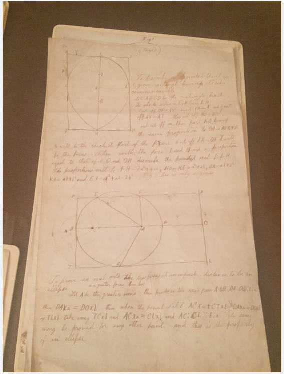
From: **Is 3D frequency-domain FWI of full-azimuth/long-offset OBN data feasible? The Gorgon data FWI case study**

The Leading Edge. 2023;42(3):173-183. doi:10.1190/tle42030173.1

What about Maxwell? (part 2)

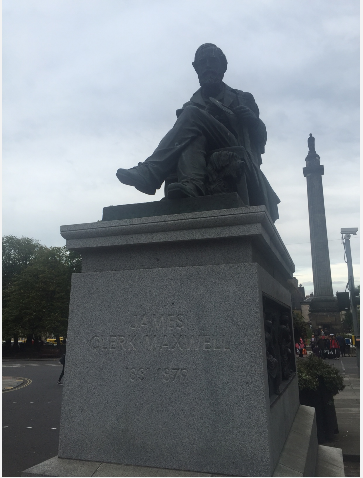
James Clerk Maxwell (1831-1879), Scottish mathematician

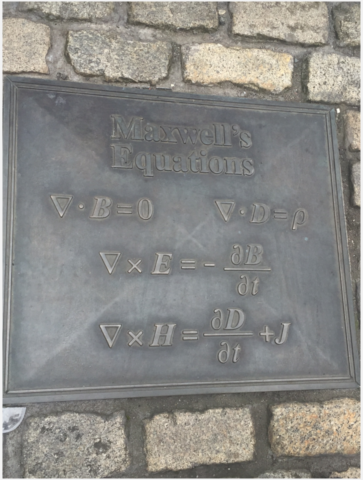
Maxwell's room at the Royal Society of Edinburgh: painting, hologram and manuscripts



James Clerk Maxwell (1831-1879), Scottish mathematician

Statue of Maxwell and his dog and plaque with his equations on George Street, Edinburgh





Interesting applications: low frequency time-harmonic Maxwell problem

Maxwell in mixed form [Li, Greif and Schötzau, 2012]

$$
\begin{aligned}
\nabla \times (\mu^{-1} \nabla \times \mathbf{E}) - \omega^2 \varepsilon \mathbf{E} + \varepsilon \nabla \mathrm{p} &= \mathbf{f} && \text{in } \Omega \\
\nabla \cdot (\varepsilon \mathbf{E}) &= 0 && \text{in } \Omega \\
\mathbf{E} \times \mathbf{n} &= \mathbf{0} && \text{on } \partial\Omega \\
\mathrm{p} &= 0 && \text{on } \partial\Omega
\end{aligned}
$$

- **E** is the electric field.
- if $\omega \ll 1 \rightsquigarrow$ problem close to **singular**.
- add an artificial variable p.

Discretisation

Nédélec elements for **E** and **nodal elements** for p

$$
\begin{pmatrix} \mathrm{K} - \omega^2 \mathrm{M} & \mathrm{B}^{\mathrm{T}} \\ \mathrm{B} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ 0 \end{pmatrix}
$$

Interesting applications: low frequency time-harmonic Maxwell problem

Maxwell in mixed form [Li, Greif and Schötzau, 2012]

$$
\begin{aligned}
\nabla \times (\mu^{-1} \nabla \times \mathbf{E}) - \omega^2 \varepsilon \mathbf{E} + \varepsilon \nabla p = \mathbf{f} \quad & \text{in } \Omega \\
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\mathbf{E} \times \mathbf{n} = \mathbf{0} \quad & \text{on } \partial\Omega \\
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\end{aligned}
$$

- **E** is the electric field.
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- add an artificial variable p.

Discretisation : saddle point system

Nédélec elements for **E** and **nodal elements** for p

$$
\begin{pmatrix} K - \omega^2 M & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ 0 \end{pmatrix}
$$

$\mathcal{K}$ is **symmetric** but **indefinite**

- $K \in \mathbb{R}^{n \times n}$ corresponds to $\nabla \times (\mu^{-1} \nabla \times)$ and has a **large kernel** of dimension m
- $M \in \mathbb{R}^{n \times n}$ is the ε-weighted **mass matrix**
- $B \in \mathbb{R}^{m \times n}$ is a full row rank matrix corresponding to the **divergence constraint**

Interesting applications: low frequency time-harmonic Maxwell problem

Maxwell in mixed form [Li, Greif and Schötzau, 2012]

$$
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Discretisation and solution

Nédélec elements for **E** and **nodal elements** for p

$$
\begin{pmatrix} \mathrm{K} - \omega^2 \mathrm{M} & \mathrm{B}^T \\ \mathrm{B} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ 0 \end{pmatrix}
$$

A **block preconditioner**

$$
\mathcal{P}_{\mathrm{M,L}} = \begin{pmatrix} \mathcal{P}_{\mathrm{M}} & 0 \\ 0 & \mathrm{L} \end{pmatrix}, \; \mathcal{P}_{\mathrm{M}} = \mathrm{K} + \gamma \mathrm{M}, \; \gamma = 1 - \omega^2 > 0
$$

and L- nodal ε**-weighted Laplace operator**.

Interesting applications: low frequency time-harmonic Maxwell problem

Maxwell in mixed form [Li, Greif and Schötzau, 2012]

$$\begin{aligned} \nabla \times (\mu^{-1}\nabla \times \mathbf{E}) - \omega^2 \varepsilon \mathbf{E} + \varepsilon \nabla p &= \mathbf{f} && \text{in } \Omega \\ \nabla \cdot (\varepsilon \mathbf{E}) &= 0 && \text{in } \Omega \\ \mathbf{E} \times \mathbf{n} &= \mathbf{0} && \text{on } \partial\Omega \\ p &= 0 && \text{on } \partial\Omega \end{aligned}$$

- **E** is the electric field.
- if $\omega \ll 1 \rightsquigarrow$ problem close to **singular**.
- add an artificial variable p.

Discretisation and solution

Nédélec elements for **E** and **nodal elements** for p

$$\begin{pmatrix} K - \omega^2 M & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ 0 \end{pmatrix}$$

A **block preconditioner**

$$\mathcal{P}_{M,L} = \begin{pmatrix} \mathcal{P}_M & 0 \\ 0 & L \end{pmatrix}, \quad \mathcal{P}_M = K + \gamma M, \quad \gamma = 1 - \omega^2 > 0$$

and L- nodal ε**-weighted Laplace operator**.

Main challenge [Hiptmair and Xu, 2007]

Solving efficiently with $\mathcal{P}_M$ (discretisation of a **positive Maxwell** problem ($\gamma > 0$, e.g. $\gamma = (\Delta t)^{-1}$)

$$\begin{aligned} \nabla \times (\mu^{-1}\nabla \times \mathbf{E}) + \gamma \varepsilon \mathbf{E} &= \mathbf{f} && \text{in } \Omega \\ \mathbf{E} \times \mathbf{n} &= \mathbf{0} && \text{on } \partial\Omega \end{aligned}$$

AMS preconditioner - One of the major breakthroughs in 2008 - DOE report!

The fictitious space lemma (FSL) [Nepomnyaschikh, 1991]

Hypotheses

Hilbert spaces H and H_D and **symmetric positive bilinear forms**

- $a\colon H \times H \to \mathbb{R}$ with $A\colon H \to H$ such that

$$(Au, v) = a(u, v) \qquad \forall u, v \in H$$

- $b\colon H_D \times H_D \to \mathbb{R}$ with $B\colon H_D \to H_D$ such that

$$(Bu_D, v_D)_D = b(u_D, v_D) \qquad \forall u_D, v_D \in H_D$$

A **linear surjective** operator $\mathcal{R}\colon H_D \to H$:

- **Continuity**: $\exists c_R > 0$ s.t.

$$a(\mathcal{R}u_D, \mathcal{R}u_D) \leq c_R\, b(u_D, u_D) \quad \forall u_D \in H_D$$

- **Stable decomposition**: $\exists c_T > 0$ s.t. $\forall u \in H$ $\exists u_D \in H_D$ with $\mathcal{R}u_D = u$ and

$$c_T\, b(u_D, u_D) \leq a(u, u)$$

The fictitious space lemma (FSL) [Nepomnyaschikh, 1991]

Hypotheses

Hilbert spaces H and H_D and **symmetric positive bilinear forms**

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$$c_T\, b(u_D, u_D) \leq a(u, u)$$

Conclusions

Let the adjoint operator $\mathcal{R}^* : H \to H_D$ be

$$(\mathcal{R}u_D,\ u) = (u_D,\ \mathcal{R}^* u)_D,\ \forall u_D \in H_D,\ u \in H$$

We have the following **spectral estimate**:

$$\boxed{c_T a(u, u) \leq a\left(\mathcal{R}B^{-1}\mathcal{R}^* Au,\ u\right) \leq c_R\, a(u, u)\, \forall u}$$

Thus the eigenvalues of the **preconditioned operator** are bounded from below by c_T and from above by c_R $\rightsquigarrow$ **condition number estimate**

$$\boxed{\kappa_2(\mathcal{R}B^{-1}\mathcal{R}^* A) \leq c_T^{-1} c_R}$$

The Near Kernel (NK) Coarse space

Q: How do we take into account the kernel of K?
A: Use it to construct a NK CS.

NK Coarse space

- Let $G \subset \mathbb{R}^{\#\mathcal{N}}$ be the NK of A (e.g. the **gradient of** H^1 **functions** on Ω)
- Let $G_i = R_i G$, the **restriction of** G **on** Ω_i
- Let $b_i(\mathbf{U}_i, \mathbf{V}_i) := (R_i A R_i^T \mathbf{U}_i, \mathbf{V}_i)$ local forms
- Let $V_G \subset \mathbb{R}^{\#\mathcal{N}}$ be the vector space spanned by $(R_i^T D_i G_i)_{1 \le i \le N}$ so that $G \subset V_G$.
- Let $Z \in \mathbb{R}^{\#\mathcal{N}_G \times \#\mathcal{N}}$ be a rectangular matrix whose columns are a basis of $V_0 := V_G$.
- E the **coarse space matrix**: $E = Z^T A Z$

Apply the fictitious space lemma (FSL)

- $H_D := \mathbb{R}^{\#\mathcal{N}_G} \times \prod_{i=1}^N \mathbb{R}^{\#\mathcal{N}_i}$
- $\mathcal{U} = (\mathbf{U}_0, (\mathbf{U}_i)_{i=1}^N), \mathcal{V} = (\mathbf{V}_0, (\mathbf{V}_i)_{i=1}^N) \in H_D$
- $b(\mathcal{U}, \mathcal{V}) := (E\mathbf{U}_0, \mathbf{V}_0) + \sum_{i=1}^N b_i(\mathbf{U}_i, \mathbf{V}_i)$
- Linear **surjective operator** $\mathcal{R}_{AS} : H_D \longrightarrow H$

$$\mathcal{R}_{AS}(\mathcal{U}) := Z\mathbf{U}_0 + (I - P_0) \sum_{i=1}^{N} R_i^T \mathbf{U}_i$$

where P_0 is the A-orthogonal projection on V_0.

Then the AS preconditioner verifies

$$\boxed{\kappa_2(\underbrace{\mathcal{R}_{AS} B^{-1} \mathcal{R}_{AS}^*}_{M_{AS}^{-1}} A) \le (1 + k_1 \tau_0) k_0}$$

For some constants $k_0, k_1, \tau_0 > 0$ (**τ_0 can be large because of the heterogeneity**)

The NK-GenEO Coarse space

Idea: enlarge the coarse space using GenEO. Want to work in the orthogonal of the near-kernel G_i

NK-GenEO Coarse space

- Let ξ_{0i} denote the b_i-orthogonal projection from $\mathbb{R}^{\#\mathcal{N}_i}$ on G_i parallel to $G_i^{\perp_{B_i}}$ where
- Find $(\mathbf{V}_{jk}, \lambda_{jk}) \in \mathbb{R}^{\#\mathcal{N}_j} \setminus \{0\} \times \mathbb{R}$ such that

$$(I - \xi_{0j}^T) D_j R_j A R_j^T D_j (I - \xi_{0j}) \mathbf{V}_{jk} = \lambda_{jk} \widetilde{A}_j \mathbf{V}_{jk}$$

- Let V_{geneo}^{τ} be the vector space spanned by the collection vector spaces $((R_j^T D_j (I - \xi_{0j}) \mathbf{V}_{jk})_{\lambda_{jk} > \delta})_{1 \le j \le N}$
- Define the **coarse space** $V_0 := V_G + V_{geneo}^{\tau}$
- Let Z the basis of V_0 and E the **coarse space matrix**: $E = Z^T A Z$

Apply fictitious space lemma (FSL)

- $H_D := \mathbb{R}^{\#\mathcal{N}_G} \times \prod_{i=1}^N \mathbb{R}^{\#\mathcal{N}_i}$
- $\mathcal{U} = (\mathbf{U}_0, (\mathbf{U}_i)_{i=1}^N), \mathcal{V} = (\mathbf{V}_0, (\mathbf{V}_i)_{i=1}^N) \in H_D$
- $b(\mathcal{U}, \mathcal{V}) := (E\mathbf{U}_0, \mathbf{V}_0) + \sum_{i=1}^N b_i(\mathbf{U}_i, \mathbf{V}_i)$
- Linear **surjective operator** $\mathcal{R}_{AS,2} : H_D \longrightarrow H$

$$\mathcal{R}_{AS}(\mathcal{U}) := Z\mathbf{U}_0 + (I - P_0) \sum_{i=1}^N R_i^T \mathbf{U}_i$$

where P_0 is the A-orthogonal projection on V_0.

Then the AS preconditioner verifies

$$\boxed{\kappa_2(\underbrace{\mathcal{R}_{AS,2} B^{-1} \mathcal{R}_{AS,2}^*}_{M_{AS,2}^{-1}} A) \le (1 + k_1 \delta) k_0}$$

(δ is user defined)

Numerical results

All numerical tests were performed with the free open-source domain specific language Freefem. For each test configuration we compare the iteration counts of the following methods:

- **AMS**: the auxiliary-space Maxwell solver (**Hiptmair and Xu**) and available via PETSc;
- **AS**: the one-level additive Schwarz preconditioner;
- **AS-SNK**: the two-level Schwarz preconditioner + CS consisting of the split near-kernel (SNK);
- **AS-SNK-GenEO**: the two-level Schwarz preconditioner + CS consisting of SNK plus $V^{\tau}_{\mathrm{GenEO}}$;
- **AS-NK**: the two-level Schwarz preconditioner + CS consisting of the “global” near-kernel (NK).
- **AS-NK-GenEO**:: the two-level Schwarz preconditioner +CS consisting of NK plus $V^{\tau}_{\mathrm{GenEO}}$.

Two aspects taken into account: **geometry** and **heterogeneity**.

Bootland, Dolean, Nataf, Tournier: A robust and adaptive GenEO-type DD for H(curl) problems in general non-convex three-dimensional geometries [...], arXiv, 2023.

Numerical results - homogeneous holes across and along

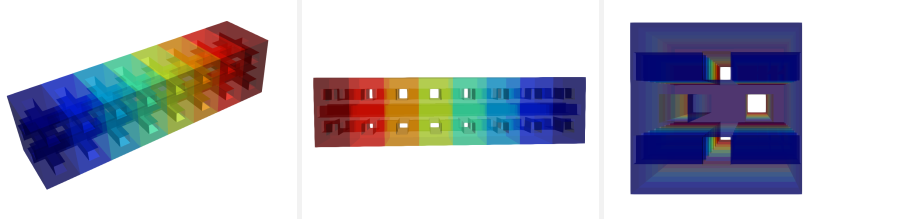


Table 1: A weak scalability study for the (non-convex) homogeneous beam problem with holes

N	8	16	32	64	128	256
#dofs	113K	226K	451K	901K	1800K	3600K
NK size	18K	36K	72K	144K	288K	576K
SNK size	24K	49K	99K	198K	397K	794K
GenEO size	18	42	90	186	378	762
AMS	43	67	113	321	588	1302
AS	37	61	106	173	294	557
AS-SNK	36	62	109	202	383	554
AS-SNK-GenEO	23	24	25	26	27	27
AS-NK	36	62	111	203	386	588
AS-NK-GenEO	24	25	25	28	30	37

Numerical results - homogeneous holes across and along

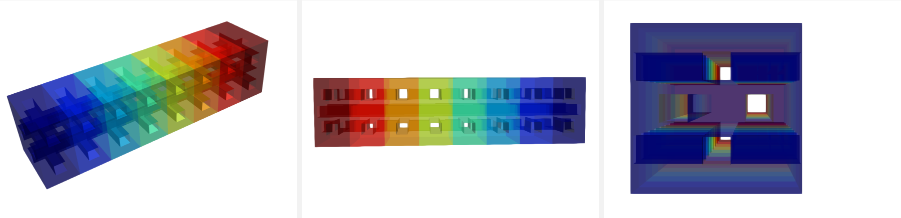


Table 1: Varying the parameter γ for the (non-convex) homogeneous beam problem with holes, $N = 256$

γ	10^{-5}	10^{-4}	10^{-3}	10^{-2}	10^{-1}	1	10	10^2
GenEO size	762	762	762	762	762	762	0	0
AMS	2057	2193	1302	303	86	33	14	6
AS	618	579	557	463	150	46	15	7
AS-SNK	772	761	554	444	144	45	17	9
AS-SNK-GenEO	28	27	27	26	23	20	17	9
AS-NK	776	765	588	444	144	45	17	10
AS-NK-GenEO	51	49	37	25	24	20	17	10

Numerical results - heterogeneous case: parameters varying in the location of the holes

Table 2: Heterogeneous ε and $N = 256$ subdomains.

$\varepsilon_{\text{holes}}$	10^{-4}	10^{-3}	10^{-2}	10^{-1}	1	10	10^2	10^3	10^4
GenEO size	0	0	0	0	0	0	0	0	0
AMS	12	12	12	12	12	12	13	12	12
AS	232	232	232	232	231	231	226	180	135
AS-SNK	18	18	18	18	18	17	17	16	15
AS-SNK-GenEO	18	18	18	18	18	17	17	16	15
AS-NK	42	42	42	42	42	41	38	33	24
AS-NK-GenEO	42	42	42	42	42	41	38	33	24

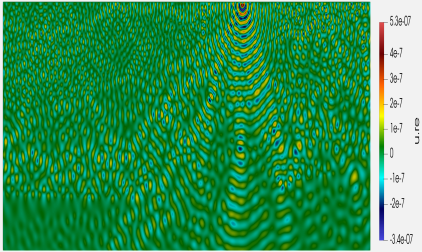
Table 3: Heterogeneous μ and $N = 256$ subdomains.

μ_{holes}	10^{-4}	10^{-3}	10^{-2}	10^{-1}	1	10	10^2	10^3	10^4
GenEO size	0	0	0	0	0	0	762	1016	15808
AMS	18	18	16	13	12	12	20	32	43
AS	216	216	216	219	231	241	247	299	448
AS-SNK	18	18	18	18	18	23	45	119	287
AS-SNK-GenEO	18	18	18	18	18	23	26	24	25
AS-NK	39	39	39	39	42	44	53	132	299
AS-NK-GenEO	39	39	39	39	42	44	45	45	43

Conclusions and discussion

Challenges for time-harmonic wave problems

- **Theoretical**: behaviour of a few methods is not completely understood ⇝ new mathematical tools are needed.
- **Practical**: exploitation of specific features not covered by theory ⇝ application specific tuning is necessary.
- **Computational**: interplay between precision and performance: **do not to artificially increase complexity!**



Thanks for your attention!