

# Using Spectral Coarse Spaces of the GenEO Type for Efficient Solutions of the Helmholtz Equation

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Preconditioning, Atlanta, 10 June 2024

## How to solve Helmholtz equation efficiently

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# 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

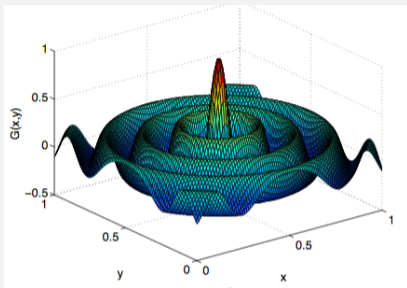
$$-\Delta u - n(x)^2 \omega^2 u = f,$$

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]

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

- For a bounded error  $h \sim \omega^{-1-1/2p}$  [Du, Wu, SINUM, 2015].

## 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).

## Efficient solution of the discretised problem

We want: solution of the discretised PDEs in **optimal time** using solvers with **good parallel properties** and **robust w.r.t heterogeneities**

### 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  $\omega$ : its size  $n$  grows like  $N^d \sim \omega^{(1+1/p)d}$  where  $N \sim 1/h$ .

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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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... But conventional iterative methods fail. [Ernst, Gander (2012)], [Gander, Zhang (2019)]

**Idea:** use domain decomposition! How large is truly large to justify the use of **domain decomposition**?

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## The main message (from geophysicists)

- Problems in FWI do not need to be over-resolved. (Too much precision not necessary!)
- Use direct solvers whenever possible!



Amestoy, Brossier, Buttari, L'Excellent, Mary, Métivier, Miniussi, Operto: [Fast 3D frequency-domain full-waveform inversion \[...\]](#), Geophysics, 2016



# One and two-level methods

“If the only tool you have is a hammer, you tend to see every problem as a nail.” (Abraham Maslow)

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

## The one-level preconditioner

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

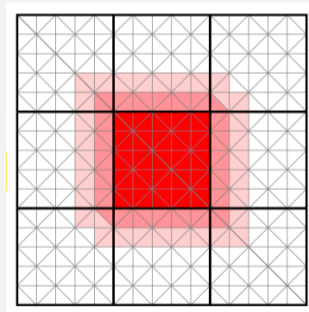
$R_j$   $\Omega \rightarrow \Omega_j$  restriction operator  
 $R_j^T$   $\Omega_j \rightarrow \Omega$  prolongation operator

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

$B_j$  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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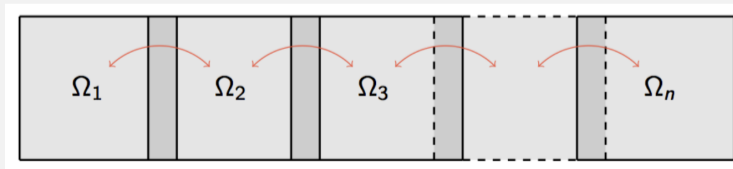
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One level is not enough (only neighbouring subdomains communicate)



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The **two-level (additive)** preconditioner

$$M_{AS,2}^{-1} = \sum_{j=1}^N R_j^T B_j^{-1} R_j + M_0^{-1}, \text{ where}$$

$R_j$      $\Omega \rightarrow \Omega_j$     **restriction operator**  
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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]

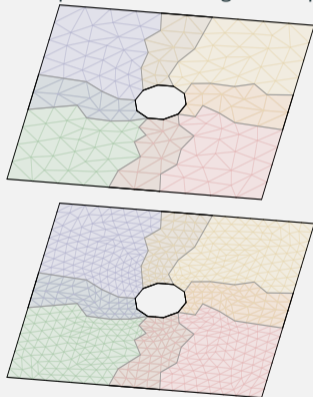
## The grid coarse space (Grid CS)

- is based on a **geometrical** coarse mesh of diameter  $H_{\text{coarse}}$
- $R_0^T$  interpolation matrix from the fine to the coarse grid
- $Z = R_0^T$  matrix spanning the coarse space
- $E = Z^T B Z$  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  $H_{\text{coarse}} \sim k^{-\alpha}$ ,  $0 < \alpha \leq 1$ .
- $|\xi| \sim k^2$  and  $\delta \sim H_{\text{coarse}}$ , then weighted GMRES will converge with the number of iterations **independent of the wavenumber**.

Is the grid CS optimal for heterogeneous problems?



## Spectral coarse spaces for indefinite Helmholtz

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## A more general BVP

$$\begin{aligned} -\nabla \cdot (A(\mathbf{x})\nabla u) - k^2 u &= f && \text{in } \Omega, \\ u &= 0 && \text{on } \partial\Omega, \end{aligned}$$

with  $A$  an SPD matrix-valued function,  
 $a_{\min}|\xi|^2 \leq A(\mathbf{x})\xi \cdot \xi \leq a_{\max}|\xi|^2, \mathbf{x} \in \Omega, \xi \in \mathbb{R}^d.$

The FEM solution  $u_h \in V^h$  satisfies the weak formulation  $b(u_h, v_h) = F(v_h)$

$$b(u, v) = \int_{\Omega} \left( A(\mathbf{x})\nabla u \cdot \nabla v - k^2 uv \right) d\mathbf{x}$$

Discretised symmetric but indefinite linear system

$$\mathbf{B}\mathbf{u} = \mathbf{f}$$

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## Domain decomposition

- **Overlapping partition**  $\{\Omega_j\}_{1 \leq j \leq N}$  of  $\Omega$ , with  $\Omega_j$
- $H$  the maximal diameter of the subdomains.

Define  $\tilde{V}^j = \{v|_{\Omega_j} : v \in V_h\}$ ,

$V^j = \{v \in \tilde{V}^j : \text{supp}(v) \subset \Omega_j\}$ , and for  $u, v \in \tilde{V}^j$

$$b_{\Omega_j}(u, v) := \int_{\Omega_j} (A(\mathbf{x})\nabla u \cdot \nabla v - k^2 uv) \, dx.$$

## One-level additive Schwarz preconditioner

$$M_{AS,1}^{-1} = \sum_{j=1}^N R_j^T (R_j B R_j^T)^{-1} R_j.$$

# Spectral Coarse Space - GenEO type - how to achieve robustness

A **spectral coarse space** can be constructed.

Spillane, Dolean, Hauret, Nataf, Pechstein, Scheichl. **Abstract robust coarse spaces for systems of PDEs via generalized eigenproblems in the overlaps**, Numer. Math., 2014.

## Bilinear forms

$$b_{\Omega_j}(u, v) = \int_{\Omega_j} (A \nabla u \cdot \nabla v - k^2 uv) \, dx, \quad a_{\Omega_j}(u, v) = \int_{\Omega_j} (A \nabla u \cdot \nabla v) \, dx.$$

### $\Delta$ - GenEO

- Consider a nearby generalised eigenvalue problem  $a_{\Omega_j}$  (e.g. Laplace).
- In each of  $\Omega_j$ , solve the **eigenproblem**

$$a_{\Omega_j}(u, v) = \lambda a_{\Omega_j}(\Xi_j(u), \Xi_j(v)), \quad \forall v \in V_j.$$

- At the discrete level

$$\tilde{L}_j \mathbf{u}_j^l = \lambda^l D_j L_j D_j \mathbf{u}_j^l.$$

Bootland, Dolean, Graham, Ma, Scheichl. **Overlapping Schwarz methods with GenEO coarse spaces for indefinite and nonself-adjoint problems**, IMA, 2023.

### $H_k$ -GenEO

- Using the complete problem definition,  $b_{\Omega_j}$  in combination with a  $k$  - weighted scalar product.
- In each of  $\Omega_j$ , solve the **eigenproblem**

$$b_{\Omega_j}(u, v) = \lambda (\Xi_j(u), \Xi_j(v))_{1,k,\Omega_j}, \quad \forall v \in V_j.$$

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Bootland, Dolean. **Can DtN and GenEO Coarse Spaces Be Sufficiently Robust for Heterogeneous Helmholtz Problems?**, MCA, 2022.



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## Definition of the coarse space

GenEO coarse spaces:  $m_i$  (dominant) eigenfunctions corresponding to  $\lambda_1^i \leq \lambda_2^i \leq \dots \leq \lambda_{m_i}^i$ .  
The coarse information is defined as the thin and long matrix

$$Z = \left[ \left( R_i^T D_i \mathbf{u}_i^l \right)_{l=1, \dots, m_i} \right]_{i=1, \dots, N}$$

# Spectral Coarse Space - GenEO type

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- At the discrete level

$$\tilde{L}_i \mathbf{u}_i^l = \lambda^l D_i L_i D_i \mathbf{u}_i^l.$$

## Key advantages

- **Spectral nearby SPD problem:** can apply spectral results!
- Use of the **a-weighted norms**.
- Robustness for mild heterogeneities and low frequencies.

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## Key advantages

- **Genuine indefinite problem:** spectral theory for SPD problem does not work!
- Use of the **k-weighted norms**.
- Robustness achieved via a **k-dependent coarse space**  $\rightsquigarrow$  high wave-numbers.

# Main theoretical results

Work on indefinite Helmholtz with homogeneous Dirichlet BVP.

GenEO coarse spaces:  $m_i$  (dominant) eigenfunctions corresponding to  $\lambda_1^i \leq \lambda_2^i \leq \dots \leq \lambda_{m_i}^i$ .

Notations:  $\tau := \min_{i=1}^N \lambda_{m_i+1}^i$ .  $C_{\text{stab}} > 0$  stability constant for the BVP, **H- subdomains diameter**

## $\Delta$ -GenEO robustness

Initial bounds (IMA, 2023 paper)

$$H \lesssim \kappa^{-2} \quad \text{and} \quad (C_{\text{stab}} + 1)^2 \kappa^8 \lesssim \tau.$$

The bounds can be improved:

$$H \lesssim \kappa^{-1} \quad \text{and} \quad (1 + C_{\text{stab}})^2 \kappa^4 \lesssim \tau.$$

An A-weighted norm:  $\|u\|_a^2 = \int_{\Omega} A |\nabla u|^2, dx$ .

## $\mathcal{H}_k$ -GenEO robustness

Necessary conditions for robustness are:

$$H \lesssim \kappa^{-1} \quad \text{and} \quad (1 + C_{\text{stab}})^2 \kappa^2 \lesssim \tau.$$

A k-weighted norm:  $\|u\|_{1,k}^2 = \|u\|_a^2 + k^2 \|u\|^2$ .

**Key ingredient:**  $\lambda_{m_i+1}^i > 0$ . (include all the negative modes in the CS)  $\rightsquigarrow$  the size of the coarse space increases with k!

## GMRES convergence

Under the assumptions on H and  $\tau$ , weighted GMRES applied to the preconditioned problem yields a robust convergence (iteration count independent of problem parameters).



## Remarks and theoretical ingredients

Constraints on  $H$  and  $\tau$  (generally overly pessimistic): robustness is achieved with sufficiently small domains and many modes (increasing drastically with  $k!$ ). In practice, things are better!

### Notations

- Bilinear form

$$b_{\Omega}(u, v) = \int_{\Omega} A \nabla u \nabla v - k^2 uv \, dx$$

- Extension operators:  $E_i : V_i \rightarrow V^h$ .
- Projectors

$$b_{\Omega_i}(T_i u, v) = b(u, E_i v), \forall v \in V_i$$

- Two-level Schwarz preconditioner:

$$T = \sum_i E_i T_i.$$

### Technical steps of the proof

- $T_i$  are well defined and stable.

$$\|T_i u\|_{1,k,\Omega_i} \leq 2 \|u\|_{1,k,\Omega_i}$$

- Stable decomposition.
- $T_0$  is well defined and stable

$$\|u - T_0 u\|_{1,k} \leq 2 \|u\|_{1,k}$$

- Technical estimates

$$c_1 \|u\|_{1,k}^2 \leq (Tu, u)_{1,k}, \quad \|Tu\|_{1,k}^2 \leq c_2 \|u\|_{1,k}^2$$

- Apply Elman theory (GMRES convergence)

## Two-level DD preconditioner

Solve  $\mathbf{B}\mathbf{u} = \mathbf{b}$ , i.e.  $M_{AS,2}^{-1}\mathbf{B}\mathbf{u} = M_2^{-1}\mathbf{b}$  by GMRES. DD preconditioner based on  $N$  domains of diameter  $\sim H$ .

$$M_{AS,2}^{-1} = \sum_{j=1}^N R_j^T B_j^{-1} R_j + Z(Z^* B Z)^{-1} Z^*$$

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  $DtN_{\Omega_j}(u_{\Gamma_j}^l) = \lambda^l u_{\Gamma_j}^l$ ,  $Z$  is formed from **local harmonic extensions** ( $\mathcal{H}$ ) of modes, **weighted** ( $D_j$ ) and **extended globally**  $R_j^T D_j \mathcal{H} u_{\Gamma_j}^l$
- **$\Delta$ -GenEO** ( $\mathcal{H}_k$ -GenEO): solve  $L_j u_j^l = \lambda^l D_j L_j D_j u_j^l$  ( $\tilde{B}_j u_j^l = \lambda^l D_j B_{j,k} D_j u_j^l$ ),  $Z$  is formed from **weighted** ( $D_j$ ) and **extended globally** modes  $R_j^T D_j u_{\Gamma_j}^l$

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## Advantages and available results

- ⊕ **Grid CS**: Theoretical/numerical results absorptive problem, robustness for  $H \sim k^{-\alpha}$ ,  $0 < \alpha \leq 1$ .
- ⊕  **$\Delta$ -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**.



## Numerical Results

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## Numerical Results: $\Delta$ -GenEO vs. Hk-GenEO

### Problem definition:

$$\begin{aligned} -\nabla \cdot (A(x)\nabla u) - k^2 u &= f && \text{in } \Omega, \\ u &= 0 && \text{on } \partial\Omega, \end{aligned}$$

### Homogeneous Problem

- Helmholtz:  $A = I$ , varying  $k$ .
- Theory ensures robustness for **small enough domains** with **enough modes**.
- Hk-GenEO performs better with **higher frequencies**.

Preconditioned GMRES iteration counts. A uniform decomposition into  $\sqrt{N} \times \sqrt{N}$  square subdomains is used.

	$\Delta$ - GenEO				Hk - GenEO			
$k \setminus N$	16	25	49	100	16	25	49	100
10	16	16	17	16	15	15	17	16
100	27	25	24	21	17	18	19	19
1000	98	106	123	90	17	18	22	17
10 000	407	468	814	DNC	68	54	42	46

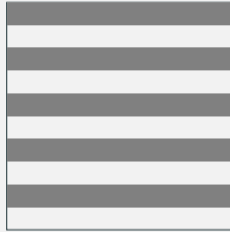


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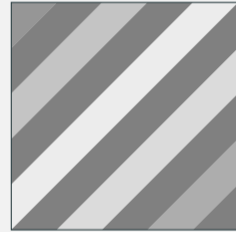
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(a) Increasing layers



(b) Alternating layers



(c) Diagonal alternating layers

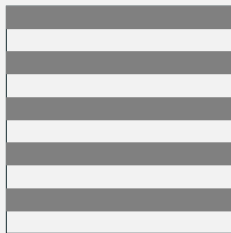
## Heterogeneous Problem

- Piecewise constant heterogeneity, varying  $k$ .
- For the darkest shade,  $a(\mathbf{x}) = a_{\min}$ , for the lightest shade  $a(\mathbf{x}) = a_{\max}$ .

# Numerical Results: $\Delta$ -GenEO vs. Hk-GenEO



(a) Increasing layers



(b) Alternating layers



(c) Diagonal alternating layers

$k \setminus N$	$\Delta$ - GenEO				Hk - GenEO			
	16	25	49	100	16	25	49	100
10	25	26	25	26	25	26	25	26
100	26	26	26	26	25	26	26	26
1000	43	42	46	45	25	32	27	28
10 000	138	145	179	205	35	49	49	75

(a) Increasing layers

$k \setminus N$	$\Delta$ - GenEO				Hk - GenEO			
	16	25	49	100	16	25	49	100
10	20	19	20	20	20	19	20	20
100	21	20	21	21	20	19	21	20
1000	72	73	76	82	22	22	22	22
10 000	361	213	653	362	41	49	51	33

(b) Alternating layers

$k \setminus N$	$\Delta$ - GenEO				Hk - GenEO			
	16	25	49	100	16	25	49	100
10	21	20	21	22	20	20	21	21
100	21	21	22	22	21	20	22	22
1000	74	89	81	75	24	26	39	31
10 000	258	304	496	720	53	47	53	61

## Conclusion

- Hk-GenEO is **robust** w.r.t. **heterogeneities, wave number, decomposition**.
- Hk-GenEO outperforms  $\Delta$ -GenEO model problems.

k \ N	$\Delta$ - GenEO				Hk - GenEO			
	16	25	49	100	16	25	49	100
10	25	26	25	26	25	26	25	26
100	26	26	26	26	25	26	26	26
1000	43	42	46	45	25	32	27	28
10 000	<b>138</b>	<b>145</b>	<b>179</b>	<b>205</b>	35	49	49	75

(a) Increasing layers

k \ N	$\Delta$ - GenEO				Hk - GenEO			
	16	25	49	100	16	25	49	100
10	20	19	20	20	20	19	20	20
100	21	20	21	21	20	19	21	20
1000	72	73	76	82	22	22	22	22
10 000	<b>361</b>	<b>213</b>	<b>653</b>	<b>362</b>	41	49	51	33

(b) Alternating layers

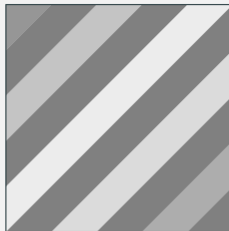
k \ N	$\Delta$ - GenEO				Hk - GenEO			
	16	25	49	100	16	25	49	100
10	21	20	21	22	20	20	21	21
100	21	21	22	22	21	20	22	22
1000	74	89	81	75	24	26	39	31
10 000	<b>258</b>	<b>304</b>	<b>496</b>	<b>720</b>	53	47	53	61

(c) Diagonal alternating layers

# Numerical comparison Dirichlet problem: $\Delta$ -GenEO vs. $\mathcal{H}$ -GenEO modes

## Heterogeneous indefinite Helmholtz

- Piecewise constant heterogeneity  $a(\mathbf{x})$ .
- Theory ( $\Delta$ -GenEO) ensures robustness for **small frequencies, small enough domains** with **enough modes**.



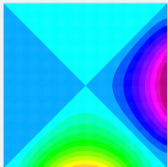
For the darkest shade  $a(\mathbf{x}) = 1$ ,  
for the lightest shade  
 $a(\mathbf{x}) = a_{\max}$

$\Delta$ -GenEO

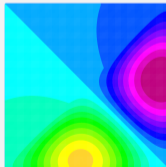
$\mathcal{H}$ -GenEO  
 $\kappa = 1000$

$\mathcal{H}$ -GenEO  
 $\kappa = 10000$

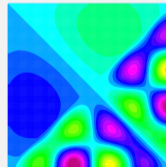
Diagonal layers



$\lambda = 0.057$



$\lambda = -0.014$

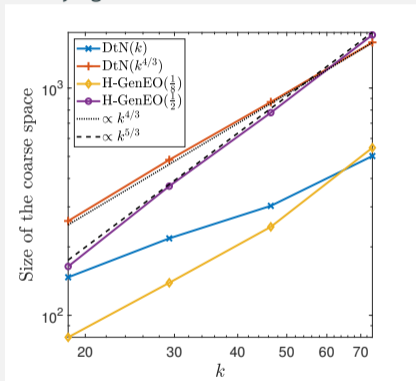


$\lambda = -0.052$

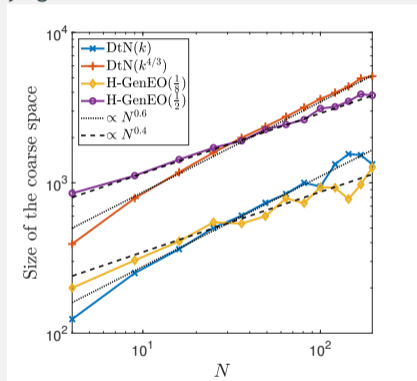


# Numerical comparison. DtN vs. $\mathcal{H}$ -GenEO: size<sup>1</sup> of the coarse space

Varying the wave number  $k$  for  $N = 25$

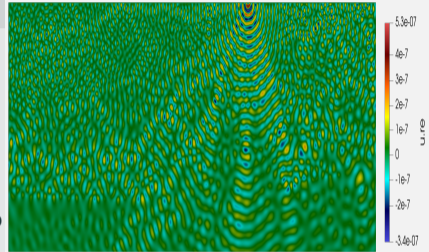


Varying the number of subdomains  $N$  for  $k = 73.8$



## Challenges for time-harmonic wave problems

- **Theoretical:** behaviour of a few methods is not completely understood  $\rightsquigarrow$  new mathematical tools are needed.
- **Practical:** exploitation of specific features not covered by theory  $\rightsquigarrow$  application specific tuning is necessary.
- **Computational:** interplay between precision and performance: we need explicit bounds in the wavenumber to assess the complexity of the coarse spaces!



Thanks for your attention