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# Iterative Trefftz method for three-dimensional electromagnetic waves simulation

Sébastien Pernet<sup>1</sup>, Margot Sirdey<sup>1,2</sup>, Sébastien Tordeux<sup>2</sup>

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WAVES 2022

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## Adimensional Maxwell problem

**Studied problem:**

$$\begin{cases} \nabla \times \mathbf{H} &= ik\varepsilon_r \mathbf{E} \\ \nabla \times \mathbf{E} &= -ik\mu_r \mathbf{H}, \text{ on } \Omega, \end{cases}$$

where  $\Omega \subset \mathbb{R}^3$  is a three-dimensional domain,  $\varepsilon_r$  and  $\mu_r$  are the relative permittivity and permeability.

**Objective:** computation on very large domains

→ up to 200 wavelengths =  $200\lambda = 64 \times 10^6$  elements in the  $\lambda/2$ -mesh.



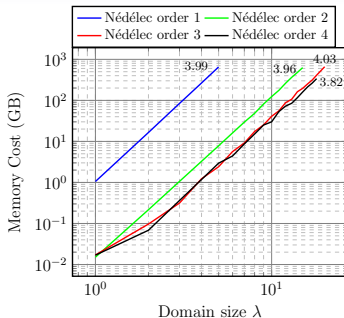
Large domain size with respect to the wavelength  $\Leftrightarrow L \gg \lambda$

$\Rightarrow$  numerical dispersion problem

Frigate Surcouf at sea near Toulon. Date: 13 April 2004. Author: Franck Dubey. Source: netmarine.net.

## Memory limits of a classic solver<sup>i</sup>

- Use of **second order Maxwell problem** leads to a continuous formulation **reducing the number of degrees of freedom**
- Finite Element method **handles spurious modes**



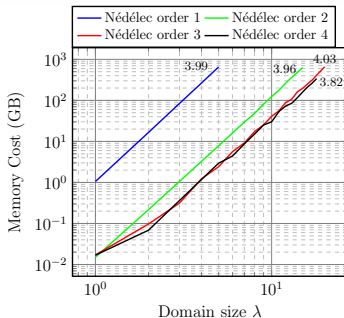
Memory used by the Nédélec solver in function of the size of the domain, **memory =  $\lambda^4$** .

	Memory	Sockets	Domain size	Power	Cost	Hours.Sockets
Laptop	32 GB	1	10 $\lambda$	200 W	0.034 €/h	0.25
// Computing	1 TB	16	24 $\lambda$	3.2 KW	0.544 €/h	19.9
HPC	320 TB	5000	100 $\lambda$	1 MW	170 €/h	> 25000
HPC	<b>5120 TB</b>	<b>80000</b>	<b>200<math>\lambda</math></b>	<b>16 MW</b>	<b>2720 €/h</b>	<b>&gt; 800000</b>

<sup>i</sup>F. Ihlenburg and I. Babuska, *Finite element solution of the Helmholtz equation with high wave number part II: the hp version of the FEM*, *SIAM Journal on Numerical Analysis*, 34 (1), pp. 315–358 (1997).

## Memory limits of a classic solver<sup>i</sup>

Efficient optimisation cannot overcome the **memory issue** → iterative solvers ?



Memory used by the Nédélec solver in function of the size of the domain, **memory** =  $\lambda^4$ .

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## No convergence with iterative solvers

**GMRES iterative solver** example on

high order Nédélec Finite Element method (FE)

and

high order Discontinuous Galerkin method (DG)

from first order Maxwell problem and the impedance boundary condition

$$\gamma_t \mathbf{E} + Z_{\partial\Omega} \mathbf{n}_{\partial\Omega} \times \gamma_t \mathbf{H} = \mathbf{g} \quad \text{on } \partial\Omega \quad \text{with} \quad Z_{\partial\Omega} = \frac{1 - R_{\partial\Omega}}{1 + R_{\partial\Omega}}.$$

## No convergence with iterative solvers

GMRES iterative solver example on

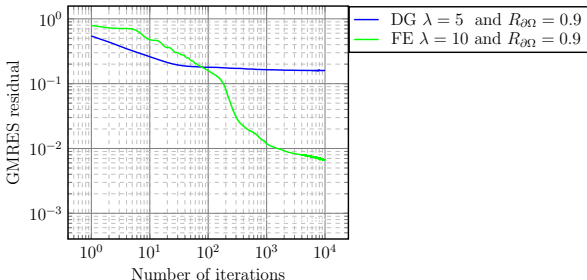
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Convergence for GMRES Nédélec FE method and for GMRES DG method.

→ Need to develop **low memory cost methods** based on **domain decomposition**.

## Trefftz method construction steps

### Trefftz method advantages<sup>ii</sup>

- Non dispersive basis functions
- Adapted to domain decomposition

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<sup>ii</sup>R. Hiptmair, A. Moiola and I. Perugia, A survey of Trefftz methods for the Helmholtz equation, In Building bridges: connections and challenges in modern approaches to numerical partial differential equations, pp. 237–279. Springer (2016).



## Trefftz method construction steps

Trefftz method advantages<sup>ii</sup>

- Non dispersive basis functions
  - Adapted to domain decomposition
1. Virtual work principle on an element  $K$

$$W_K = -ik_0 \int_K \varepsilon_r \mathbf{E}^K \cdot \overline{\mathbf{E}'^K} + \mu_r \mathbf{H}^K \cdot \overline{\mathbf{H}'^K} dK.$$

2. The solution and the basis functions satisfy Maxwell on each element  $K$

$$\left\{ \begin{array}{l} W_K = - \int_K \underbrace{\nabla \times \mathbf{H}^K}_{ik_0 \varepsilon_r \mathbf{E}^K} \cdot \overline{\mathbf{E}'^K} - \underbrace{\nabla \times \mathbf{E}^K}_{-ik_0 \mu_r \mathbf{H}^K} \cdot \overline{\mathbf{H}'^K} dK, \\ W_K = \int_K \mathbf{E}^K \cdot \underbrace{\nabla \times \overline{\mathbf{H}'^K}}_{ik_0 \varepsilon_r \mathbf{E}'^K} - \mathbf{H}^K \cdot \underbrace{\nabla \times \overline{\mathbf{E}'^K}}_{-ik_0 \mu_r \mathbf{H}'^K} dK. \end{array} \right.$$

3. Thanks to the general Stokes formula, a variational formulation is imposed on boundaries: reciprocity formula,

$$\sum_K \int_{\partial K} \left( \mathbf{n}_K \times \gamma_t \mathbf{H}^K \right) \cdot \gamma_t \overline{\mathbf{E}'^K} + \gamma_t \mathbf{E}^K \cdot \left( \mathbf{n}_K \times \gamma_t \overline{\mathbf{H}'^K} \right) = 0.$$

<sup>ii</sup>R. Hiptmair, A. Moiola and I. Perugia, A survey of Trefftz methods for the Helmholtz equation, In Building bridges: connections and challenges in modern approaches to numerical partial differential equations, pp. 237–279. Springer (2016).

## Trefftz variational formulation

4. Find  $\mathbf{x} = (\mathbf{E}, \mathbf{H}) \in \mathbb{X}$ , such that for all  $\mathbf{x}' = (\mathbf{E}', \mathbf{H}') \in \mathbb{X}$ ,

$$\mathbf{a}(\mathbf{x}, \mathbf{x}') = \ell(\mathbf{x}'),$$

with  $\mathbb{X}$  a **discontinuous space of local solutions of Maxwell system**, and

$$\mathbf{a}(\mathbf{x}, \mathbf{x}') = \sum_K \int_{\partial K} \widehat{\gamma_{\times}^K \mathbf{H}^K} \cdot \gamma_t \overline{\mathbf{E}'^K} + \widehat{\gamma_t \mathbf{E}^K} \cdot \gamma_{\times}^K \overline{\mathbf{H}'^K}, \quad \text{with } \gamma_{\times} \mathbf{H}^K = \mathbf{n}_K \times \gamma_t \mathbf{H}^K.$$

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5. Clever choices of **numerical fluxes**  $\widehat{\gamma_t \mathbf{E}^F}$  and  $\widehat{\gamma_{\times} \mathbf{H}^F}$  ensure a **strict coercivity**

A numerical flux is defined on a face  $F$   
either an **interior face** or a **boundary face**.

### Equivalency between

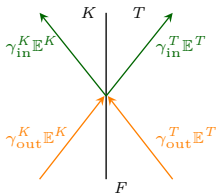
- Upwind schemes,
- UWVF methods,
- Riemann solvers.

## Trefftz variational formulation

- Upwind schemes

Incoming and outgoing traces

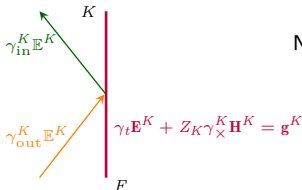
$$\gamma_{\text{in}}^K \mathbb{E}^K := \gamma_t \mathbf{E}^K + Z_K \gamma_{\times}^K \mathbf{H}^K \quad \text{and} \quad \gamma_{\text{out}}^K \mathbb{E}^K := \gamma_t \mathbf{E}^K - Z_K \gamma_{\times}^K \mathbf{H}^K.$$



Numerical fluxes on interior face

$$\widehat{\gamma_t \mathbf{E}^F} = \frac{Z_T}{Z_K + Z_T} \gamma_{\text{out}}^K \mathbb{E}^K + \frac{Z_K}{Z_K + Z_T} \gamma_{\text{out}}^T \mathbb{E}^T,$$

$$\widehat{\gamma_{\times}^K \mathbf{H}^F} = -\frac{1}{Z_K + Z_T} \gamma_{\text{out}}^K \mathbb{E}^K + \frac{1}{Z_K + Z_T} \gamma_{\text{out}}^T \mathbb{E}^T.$$



Numerical fluxes on boundary face

$$\widehat{\gamma_t \mathbf{E}^F} = \frac{Z_{\partial\Omega}}{Z_K + Z_{\partial\Omega}} \gamma_{\text{out}}^K \mathbb{E}^K + \frac{Z_K}{Z_K + Z_{\partial\Omega}} \mathbf{g}^K,$$

$$\widehat{\gamma_{\times}^K \mathbf{H}^F} = -\frac{1}{Z_{\partial\Omega} + Z_K} \gamma_{\text{out}}^K \mathbb{E}^K + \frac{1}{Z_{\partial\Omega} + Z_K} \mathbf{g}^K.$$

## Trefftz variational formulation

- **Riemann solvers**<sup>iii</sup>

Homogeneous numerical fluxes

$$\widehat{\gamma_t \mathbf{E}^F} = \{\{\gamma_t \mathbf{E}\}\}_F - \frac{\llbracket \gamma_{\times} \mathbf{H} \rrbracket_F}{2}, \quad \text{and} \quad \widehat{\gamma_{\times} \mathbf{H}^F} = \{\{\gamma_{\times} \mathbf{H}\}\}_F + \frac{\llbracket \gamma_t \mathbf{E} \rrbracket_F}{2}.$$

4. Find  $\mathbf{x} = (\mathbf{E}, \mathbf{H}) \in \mathbb{X}$ , such that for all  $\mathbf{x}' = (\mathbf{E}', \mathbf{H}') \in \mathbb{X}$ ,

$$\mathbf{a}(\mathbf{x}, \mathbf{x}') = \sum_K \int_{\partial K} \widehat{\gamma_{\times}^K \mathbf{H}^K} \cdot \gamma_t \overline{\mathbf{E}'^K} + \widehat{\gamma_t \mathbf{E}^K} \cdot \gamma_{\times}^K \overline{\mathbf{H}'^K} = \ell(\mathbf{x}'),$$

with  $\mathbb{X}$  a **discontinuous space of local solutions of Maxwell system**.

5. Clever choices of **numerical fluxes**  $\widehat{\gamma_t \mathbf{E}^F}$  and  $\widehat{\gamma_{\times} \mathbf{H}^F}$  ensure a **strict coercivity**.
6. **Consistency**: accuracy of the best approximation is ensured by the choice of  $\mathbb{X}$ .
7. Trefftz method is **convergent** and provides **convergence theory for the iterative method**<sup>iv</sup>.

⇒ **How to construct  $\mathbb{X}$  ?**

<sup>iii</sup>S. Pernet, N. Serdiuk, M. Sirdey, et S. Tordeux, (2021). Discontinuous Galerkin Method based on Riemann fluxes for the time domain Maxwell System. Research report, INRIA Bordeaux-Sud-Ouest.

<sup>iv</sup>A. Buffa, P. Monk, Error estimates for the ultra weak variational formulation of the Helmholtz equation, Mathematical Modelling and Numerical Analysis 42 (6) (2008) 925940.

## Trefftz variational formulation

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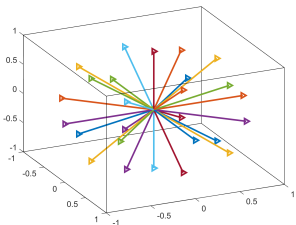
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## Basis functions space

An electromagnetic plane wave  $\mathbf{E} = \vec{p} e^{ik\vec{d}\cdot\vec{x}}$  is defined by :

- a direction of propagation  $\vec{d} = (d_x, d_y, d_z)$ ,
- a polarization  $\vec{p} = (p_x, p_y, p_z)$  orthogonal to  $\vec{d}$ .

### 3D discrete space



A plane waves basis in a cube, composed of normalized basis functions  $\mathbf{w}^j$ , for  $j = 1, N$ .

- On an element  $K$ , the numerical wave  $\mathbf{x}^K := (\mathbf{E}^K, \mathbf{H}^K)$  is

$$\mathbf{E}^K = \sum_{j=1}^N u_j \underbrace{\vec{p}_j e^{ik\vec{d}_j\cdot\vec{x}}}_{\mathbf{w}^j}$$

$$\mathbf{H}^K = \sum_{j=1}^N u_j \left( \vec{p}_j \times \vec{d}_j \right) e^{ik\vec{d}_j\cdot\vec{x}}$$

- The number of plane waves  $N$  is the number of degrees of freedom for each element  $K$ .
- What is the optimal number of plane waves ?

## Non exhaustive references about plane waves basis and alternatives

### What is the optimal number of plane waves ?

- Moiola, A. (2011). Trefftz-discontinuous Galerkin methods for time-harmonic wave problems (Doctoral dissertation, ETH Zurich). (Page 156).
- Moiola, A., Hiptmair, R., Perugia, I. (2011). Vekua theory for the Helmholtz operator. *Zeitschrift für angewandte Mathematik und Physik*, 62(5), 779-807.

### In this presentation: Basis reduction strategy → Conditioning improvement

- T. Luostari, T. Huttunen, P. Monk, (2013). Improvements for the ultra weak variational formulation, *Int. J. Numer. Meth. Engng* 94, 598624.
- S. Congreve, J. Gedicke, I. Perugia, (2019). Numerical investigation of the conditioning for plane wave discontinuous Galerkin methods, Vol. 126 of *Lecture Notes in Computational Science and Engineering*, Springer.
- H. Barucq, A. Bendali, J. Diaz, S. Tordeux, (2021). Local strategies for improving the conditioning of the plane-wave Ultra-Weak Variational Formulation. *Journal of Computational Physics*, 441, 110449.

### Alternatives could be used for the basis functions space

- **Evanescence modes**
  - E. Parolin, D. Huybrechs, A. MOIOLA, (2022). Stable approximation of Helmholtz solutions by evanescent plane waves. *arXiv preprint arXiv:2202.05658*.
- **Quasi-Trefftz methods**
  - L. M. Imbert-Gérard, A. Moiola, P. Stocker, (2020). A space-time quasi-Trefftz DG method for the wave equation with piecewise-smooth coefficients. *arXiv preprint arXiv:2011.04617*.
  - H. S. Fure, S. Pernet, M. Sirdey, S. Tordeux, (2020). A discontinuous Galerkin Trefftz type method for solving the two dimensional Maxwell equations. *SN Partial Differ. Equ. Appl.* 1, 23.



## General matrix shape

$$\mathbf{A}[\mathbf{x}] = \mathbf{F},$$

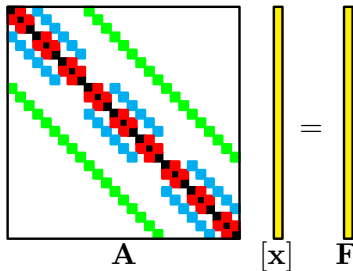
where

$$\mathbf{A}_{i,j} := \mathbf{a}(\mathbf{w}^j, \mathbf{w}^i)$$

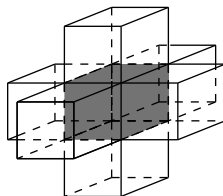
$$\mathbf{F}_i := \mathbf{l}(\mathbf{w}^i) \quad \text{for } i, j = 1, N_{\text{dof}}.$$

$$N_{\text{dof}} := N \times N_{\text{elem}}$$

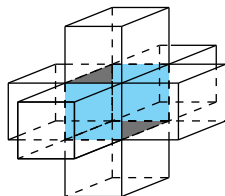
$$\text{size}(\mathbf{A}) = N^2 \times 7 \times N_{\text{elem}}$$



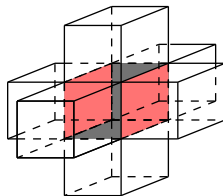
Element assembling of  $\mathbf{A}$  for  $N_{\text{elem}} = 27 = 3^3$  cubes.



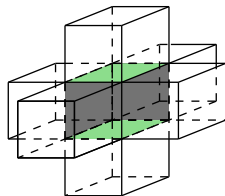
Self-interaction



Front and back interactions

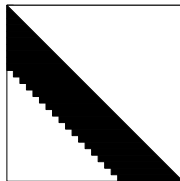
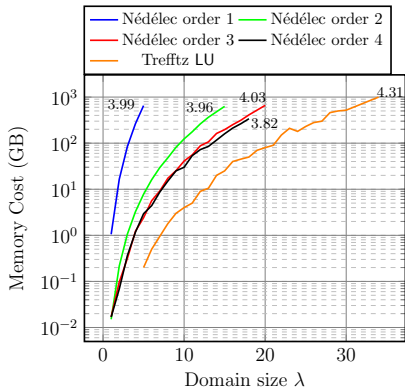


Left and right interactions

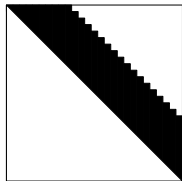


Bottom and top interactions

## Memory limit of the direct solver



L



U

Domain size	$5\lambda$	$10\lambda$	$20\lambda$	$100\lambda$	$200\lambda$
$N_{\text{elem}}$	1000	8000	64000	$8 \times 10^6$	$64 \times 10^6$
LU memory	4.3 GB	69 GB	1.1 TB	690 TB	11040 TB

Table: LU factorization memory in function of the domain size.

## GMRES method alternative

**Coercivity property**  $\operatorname{Re}(a(\mathbf{x}, \mathbf{x}')) > 0 \rightarrow$  suitable framework for GMRES.

$$[\mathbf{x}]^{N_{\text{kry}}} = \text{GMRES}(\mathbf{A}, \mathbf{F}, N_{\text{kry}})$$

General Minimal RESidual (GMRES) approximates the solution  $\mathbf{x}^{N_{\text{kry}}} \in \mathbb{K}^{N_{\text{kry}}}$  of

$$\text{Find } \mathbf{x}^{N_{\text{kry}}} \in \mathbb{K}^{N_{\text{kry}}}, \mathbf{a}(\mathbf{x}^{N_{\text{kry}}}, \mathbf{x}') = \mathbf{l}(\mathbf{x}'), \forall \mathbf{x}' \in \mathbb{K}^{N_{\text{kry}}}$$

$$\iff \text{Find } [\mathbf{x}^{N_{\text{kry}}}] \in [\mathbb{K}^{N_{\text{kry}}}], \quad [\mathbf{x}']^* \mathbf{A} [\mathbf{x}^{N_{\text{kry}}}] = [\mathbf{x}']^* \mathbf{F}, \quad \forall [\mathbf{x}'] \in [\mathbb{K}^{N_{\text{kry}}}],$$

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where the **Krylov space** of dimension  $N_{\text{kry}}$  is

$$[\mathbb{K}^{N_{\text{kry}}}] := \text{span} \left[ \underbrace{\left( \begin{array}{c} \vdots \\ \mathbf{F} \\ \vdots \end{array} \right), \left( \begin{array}{c} \vdots \\ \mathbf{A}\mathbf{F} \\ \vdots \end{array} \right), \dots, \left( \begin{array}{c} \vdots \\ \mathbf{A}^{N_{\text{kry}}-1}\mathbf{F} \\ \vdots \end{array} \right)}_{N_{\text{kry}}} \right] \Bigg\} N_{\text{dof}},$$

$\implies \text{size}(\text{Krylov}) = N_{\text{kry}} \times N_{\text{dof}}$ , where  $N_{\text{dof}}$  is the dimension of  $\mathbf{F}$ .

## Trefftz GMRES method

- **GMRES convergence depends on the spectrum of the matrix  $\mathbf{A}$ .**

Classic theorem for the residual norm of a GMRES solver is given by<sup>v</sup>

$$\|[\mathbf{x}]^{m+1} - [\mathbf{x}]^m\| = \|r^{m+1}\| \leq \|\mathbf{P}\| \|\mathbf{P}^{-1}\| \|r^0\| \varepsilon^m,$$

with

$$\varepsilon^m = \min_{\substack{p \in \mathcal{P}^m \\ p(0)=1}} \max_{\lambda_i \in \rho(\mathbf{A})} |p(\lambda_i)| \quad \text{and} \quad \mathbf{P} \text{ the eigenvectors matrix.}$$

**More accurate** studies do exist<sup>vi</sup>

But classic theorem is enough when  $\mathbf{A}$  has good properties

- The consideration of huge cases depends on the **memory cost** of the method

$$\text{size(Krylov)} + \text{size}(\mathbf{A}) = N_{\text{kry}} \times N \times N_{\text{elem}} + N^2 \times 7 \times N_{\text{elem}}$$

**We propose strategies to**

1. **Remove the spectrum of  $\mathbf{A}$  from 0.**
2. **Reduce the memory cost** of the Trefftz GMRES method.

<sup>v</sup>Saad, Youcef and Schultz, Martin H, GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM, 7, 3, 856–869, 1986

<sup>vi</sup>J. Liesen, P. Tichý, (2012). The field of values bound on ideal GMRES. Preprint arXiv:1211.5969.

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- **GMRES convergence depends on the spectrum of the matrix  $\mathbf{A}$ .**

Classic theorem for the residual norm of a GMRES solver is given by<sup>v</sup>

$$\|[\mathbf{x}]^{m+1} - [\mathbf{x}]^m\| = \|r^{m+1}\| \leq \| |\mathbf{P}| \| |\mathbf{P}^{-1}| \| r^0 \| \varepsilon^m,$$

with

$$\varepsilon^m = \min_{\substack{p \in \mathcal{P}^m \\ p(0)=1}} \max_{\lambda_i \in \rho(\mathbf{A})} |p(\lambda_i)| \quad \text{and} \quad \mathbf{P} \text{ the eigenvectors matrix.}$$

**More accurate** studies do exist<sup>vi</sup>

But classic theorem is enough when  $\mathbf{A}$  has good properties

- **The consideration of huge cases depends on the memory cost of the method**

$$\text{size(Krylov)} + \text{size}(\mathbf{A}) = N_{\text{kry}} \times N \times N_{\text{elem}} + N^2 \times 7 \times N_{\text{elem}}$$

**We propose strategies to**

1. **Remove the spectrum of  $\mathbf{A}$  from 0.**
2. **Reduce the memory cost of the Trefftz GMRES method.**

<sup>v</sup>Saad, Youcef and Schultz, Martin H, GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM, 7, 3, 856–869, 1986

<sup>vi</sup>J. Liesen, P. Tichý, (2012). The field of values bound on ideal GMRES. Preprint arXiv:1211.5969.

## GMRES method with a restart strategy

GMRES converges in theory in  $N_{\text{dof}}$  iterations, ie  $N_{\text{kry}} = N_{\text{dof}}$ .

- $N_{\text{elem}}$  the number of elements
- $N = 52$  the number of plane waves
- $N_{\text{dof}} = N \times N_{\text{elem}}$  the number of degrees of freedom

$$\rightarrow \text{size(Krylov)} = N_{\text{kry}} \times N_{\text{dof}} = 10^6 \times 52 \times 10^6 = 43264 \text{ TB.}$$

Problems when  $N_{\text{dof}}$  becomes large, ie when  $N_{\text{elem}}$  becomes large

- Huge memory cost to store  $\mathbb{K}^{N_{\text{kry}}}$
- Rounding errors accumulated at each step

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Problems when  $N_{\text{dof}}$  becomes large, ie when  $N_{\text{elem}}$  becomes large

- Huge memory cost to store  $\mathbb{K}^{N_{\text{kry}}}$
- Rounding errors accumulated at each step

Idea: truncate Krylov space  $\mathbb{K}^{N_{\text{kry}}}$  into smaller spaces of size  $N_{\text{kry}}^{\text{restart}} < N_{\text{kry}}$

$$[\mathbf{x}]^k = [\mathbf{x}]^{k-1} + \text{GMRES}(\mathbf{A}, \mathbf{F} - \mathbf{A}[\mathbf{x}]^{k-1}), \quad [\mathbf{x}]^0 = 0.$$

Example with  $N_{\text{kry}}^{\text{restart}} = 50$ :

$$\text{size(Krylov)} = N_{\text{kry}}^{\text{restart}} \times N_{\text{dof}} = 50 \times 52 \times 10^6 = 41.6 \text{ GB}$$

→ Strategy with restart reduces the memory cost



## Memory cost with matrix storage

**Memory cost** to run GMRES method **with matrix storage** is

$$\text{size(Krylov)} + \text{size(A)} = 50 \times N \times N_{\text{elem}} + N^2 \times 7 \times N_{\text{elem}}$$

$$\frac{\text{size(A)}}{\text{size(Krylov)}} \simeq 7$$

**With matrix storage: the blocking structure is  $N_{\text{elem}}$**

## Memory cost with matrix storage

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With matrix storage: the blocking structure is  $N_{\text{elem}}$

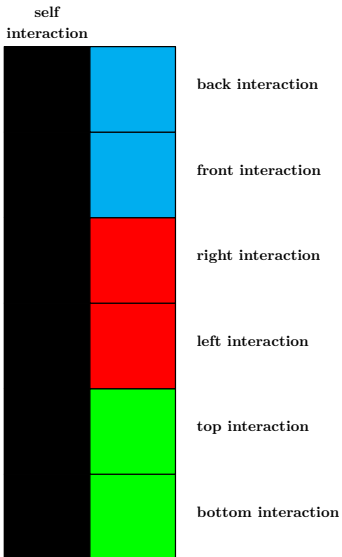
- $N_{\text{kry}}^{\text{restart}} = 50$  the dimension of the Krylov space
- $N_{\text{elem}}$  the number of elements
- $N = 52$  the number of plane waves
- $N_{\text{dof}} = N \times N_{\text{elem}}$  the number of degrees of freedom

Domain size	$5\lambda$	$10\lambda$	$20\lambda$	$100\lambda$	$200\lambda$
$N_{\text{elem}}$	1000	8000	64000	$8 \times 10^6$	$64 \times 10^6$
<b>With matrix storage</b>	344 MB	2.75 GB	22.04 GB	2.75 TB	<b>2204 TB</b>

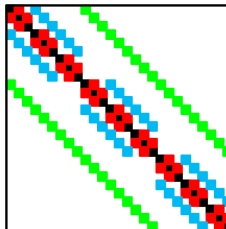
Table: Memory cost for the storage of the matrix **A** in function of the domain size.

**Solution: run GMRES method without matrix storage**

# Memory cost for matrix storage $7 \times N^2$



Cartesian structure



A

A is seeing as actions.

## Memory cost without matrix storage

Memory cost to run GMRES method ~~with matrix storage~~ without matrix storage is

$$\text{size(Krylov)} + \text{size(A)} = 50 \times N \times N_{\text{elem}} + \cancel{N^2 \times 7 \times N_{\text{elem}}}$$

$$\text{size(Krylov)} + \text{size(interactions)} = 50 \times N \times N_{\text{elem}} + N^2 \times 7$$

Without matrix storage: only **interactions** between elements are stored

## Memory cost without matrix storage

Memory cost to run GMRES method ~~with matrix storage~~ **without matrix storage** is

$$\text{size(Krylov)} + \text{size(A)} = 50 \times N \times N_{\text{elem}} + N^2 \times 7 \times N_{\text{elem}}$$

$$\text{size(Krylov)} + \text{size(interactions)} = 50 \times N \times N_{\text{elem}} + N^2 \times 7$$

**Without matrix storage: only interactions** between elements are stored

- $N_{\text{kry}}^{\text{restart}} = 50$  the dimension of the Krylov space
- $N_{\text{elem}}$  the number of elements
- $N = 52$  the number of plane waves
- $N_{\text{dof}} = N \times N_{\text{elem}}$  the number of degrees of freedom

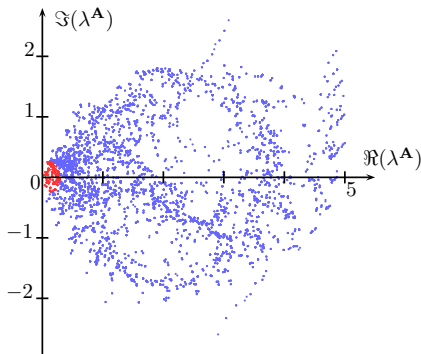
Domain size	$5\lambda$	$10\lambda$	$20\lambda$	$100\lambda$	$200\lambda$
$N_{\text{elem}}$	1000	8000	64000	$8 \times 10^6$	$64 \times 10^6$
<b>With matrix storage</b>	344 MB	2.75 GB	22.04 GB	2.75 TB	<b>2204 TB</b>
<b>Without matrix storage</b>	41.9 MB	0.332 GB	2.66 GB	332 GB	<b>2.66 TB</b>
$\frac{\text{size(interactions)}}{\text{size(Krylov)}}$	$7.3\text{E}^{-3}$	$9.1\text{E}^{-4}$	$1.1\text{E}^{-4}$	$9.1\text{E}^{-7}$	$1.1\text{E}^{-7}$

Table: Comparison of a GMRES method with or without matrix storage.

## Cessenat-Després preconditioner

The GMRES method convergence depends on the **spectrum of  $A$**  and on the **eigenvalues close to 0**.

**Idea:** use a **preconditioned GMRES** method solving  $A^\# A[x] = A^\# F$ .



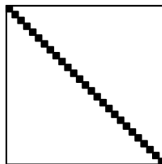
Real and complex parts of the spectrum  $\lambda^A$  of matrix  $A$ , for a  $6\lambda$  domain size.

$$A = M + N$$

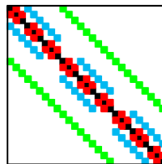
$$M_{\ell,k}^{i,j} = (\mathbf{w}_k^i, \mathbf{w}_\ell^i)_{L_t^2(\partial\mathcal{T})} \delta_{i,j}$$

Cessenat-Després decomposition <sup>a</sup>

M



N



<sup>a</sup>O. Cessenat and B. Despres, (1998). Application of an ultra weak variational formulation of elliptic PDEs to the two-dimensional Helmholtz problem. SIAM journal on numerical analysis, 35(1), 255-299.

## Cessenat-Després preconditioner

The GMRES method convergence depends on the **spectrum of  $A$**  and on the **eigenvalues close to 0**.

**Idea:** use a **preconditioned GMRES** method solving  $A^\# A[x] = A^\# F$ .

$$A^\#(M + N)[x] = A^\# F$$

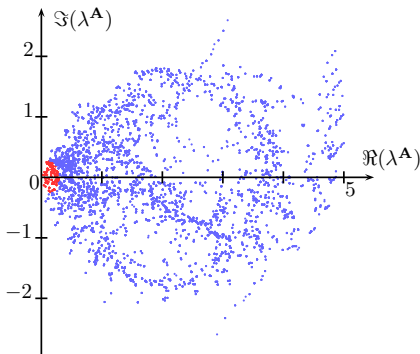
$$A^\# M[x]^{n+1} = -A^\# N[x]^n + A^\# F$$

→ a **preconditioner** can be  $A^\# = M^{-1}$

$M$  is a scalar product

→ **symetric preconditioner**

$$\tilde{A} = M^{-\frac{1}{2}} A M^{-\frac{1}{2}} = \text{Id} + M^{-\frac{1}{2}} N M^{-\frac{1}{2}}$$



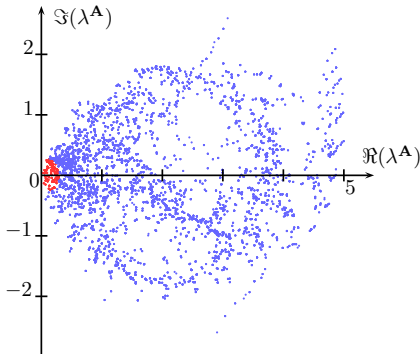
Real and complex parts of the spectrum  $\lambda^A$  of matrix  $A$ , for a  $6\lambda$  domain size.

## Cessenat-Després preconditioner

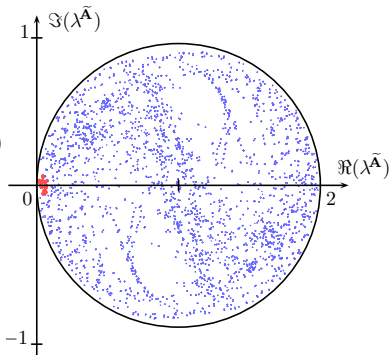
The GMRES method convergence depends on the **spectrum of  $A$**  and on the **eigenvalues close to 0**.

$$\tilde{A} = \text{Id} + M^{-\frac{1}{2}} N M^{-\frac{1}{2}}$$

**is contractant**



Real and complex parts of the spectrum  $\lambda^A$  of matrix  $A$ , for a  $6\lambda$  domain size.



Real and complex parts of the spectrum  $\lambda^{\tilde{A}}$  of matrix  $\tilde{A}$ , for a  $6\lambda$  domain size.



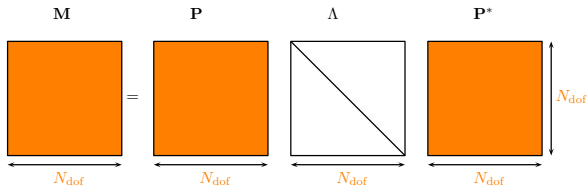
## Basis reduction strategy

**M** is symmetric positive definite

$$M_{\ell,k}^{i,j} = (\mathbf{w}_k^i, \mathbf{w}_\ell^i)_{L_t^2(\partial\mathcal{T})} \delta_{i,j}$$

for  $i, j = 1, N_{\text{elem}}$

and  $\ell, k = 1, N$ .



**P** is the orthogonal eigenvector matrix.

$\Lambda$  is the diagonal eigenvalue matrix satisfying

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{N_{\text{dof}}} \quad \text{with } \lambda_i = \Lambda_{i,i}.$$

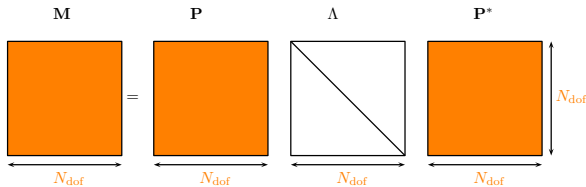
## Basis reduction strategy

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for  $i, j = 1, N_{\text{elem}}$

and  $\ell, k = 1, N$ .



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**Λ** is the diagonal eigenvalue matrix satisfying

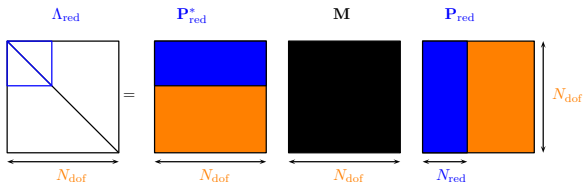
$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{N_{\text{dof}}} \quad \text{with } \lambda_i = \Lambda_{i,i}.$$

$$\begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_{N_{\text{red}}} \\ \vdots \\ \lambda_{N_{\text{dof}}-1} \\ \lambda_{N_{\text{dof}}} \end{pmatrix}$$

Filtering

$$\frac{\lambda_i}{\lambda_1} < \varepsilon$$

$$\begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_{N_{\text{red}}} \end{pmatrix}$$



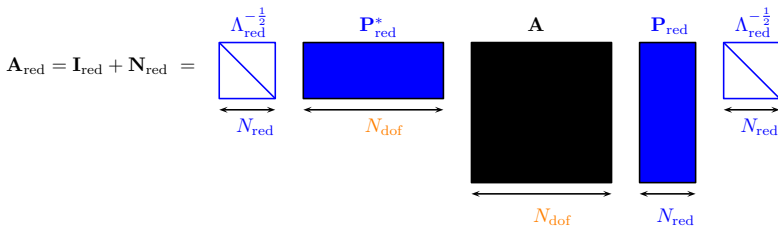
## Normalized reduced basis

The unknown has a new representation

$$\mathbf{x} = \sum_{i=1}^N [x]_i \mathbf{w}^i = \sum_{i=1}^N [y]_i \tilde{\mathbf{w}}^i \simeq \sum_{i=1}^{N_{\text{red}}} [y]_i \tilde{\mathbf{w}}^i, \quad \mathbf{Y}_{\text{red}} = [y]_{i=1, N_{\text{red}}}.$$

This approximation **does not lose information** since  $\frac{\lambda_i}{\lambda_1} < \varepsilon$ , with  $\varepsilon$  well chosen.

The **reduced basis** can be **normalized** and the new matrix is



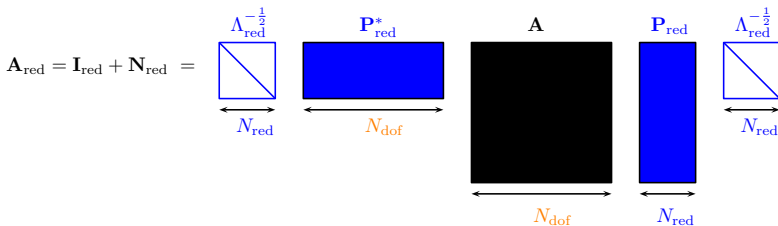
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$$\mathbf{x} = \sum_{i=1}^N [x]_i \mathbf{w}^i = \sum_{i=1}^N [y]_i \tilde{\mathbf{w}}^i \simeq \sum_{i=1}^{N_{\text{red}}} [y]_i \tilde{\mathbf{w}}^i, \quad \mathbf{Y}_{\text{red}} = [y]_{i=1, N_{\text{red}}}.$$

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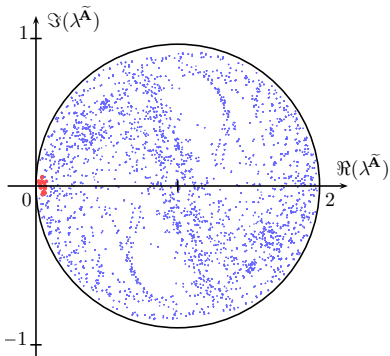


Computation of  $\mathbf{M}^{-1}$  is trivial  $\rightarrow$  **memory gain**

$$[\mathbf{x}^{n+1}] = -\mathbf{N}_{\text{red}}[\mathbf{x}^n] + \mathbf{F}_{\text{red}}, \quad \text{with } \mathbf{N}_{\text{red}} := \Lambda_{\text{red}}^{-\frac{1}{2}} \mathbf{P}_{\text{red}}^* \mathbf{N} \mathbf{P}_{\text{red}} \Lambda_{\text{red}}^{-\frac{1}{2}} \quad \text{and} \quad [\mathbf{x}^0] = 0.$$

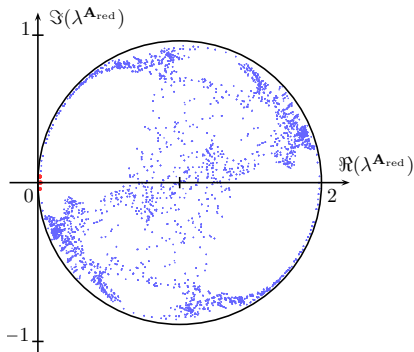
## Basis reduction improves matrix conditioning

Unreduced preconditioned matrix  $\tilde{\mathbf{A}}$



Real and complex parts of the spectrum  $\lambda^{\tilde{\mathbf{A}}}$  of matrix  $\tilde{\mathbf{A}}$ , for a  $6\lambda$  domain size.

Reduced preconditioned matrix  $\mathbf{A}_{\text{red}}$



Real and complex parts of the spectrum  $\lambda^{\mathbf{A}_{\text{red}}}$  of  $\mathbf{A}_{\text{red}}$ , for a  $6\lambda$  domain size and  $\epsilon = 10^{-5}$ .

## Basis reduction improves memory burden

$N_{\text{red}}$  depends on the size of an element  $K$  and of the threshold  $\varepsilon$ .

Size of $K$ \ $\varepsilon$	$10^{-13}$	$10^{-11}$	$10^{-9}$	$10^{-7}$	$10^{-5}$	$10^{-4}$	$10^{-3}$	$10^{-2}$
$0.25\lambda$	154	126	96	70	48	48	30	24
$0.5\lambda$	190	186	174	132	96	84	70	48
$1\lambda$	196	196	196	190	180	174	148	114

**Table:** Values of  $N_{\text{red}}$  when reducing the basis of size  $N = 196$  according to  $\varepsilon$  and the size of an element  $K$  in wavelength.

**$0.25\lambda$  case,**  $N_{\text{kry}}^{\text{restart}} = 500$ .

$10^{-15}$	$\varepsilon$	$10^{-13}$	$10^{-11}$	$10^{-9}$	$10^{-7}$	$10^{-5}$	$10^{-4}$	$10^{-3}$	$10^{-2}$
<b><math>N = 196</math></b>	$N_{\text{red}}$	154	126	96	70	48	36	30	16
<b>1.57 GB</b>	Memory cost (GB)	1.23	1.01	0.76	0.56	0.38	0.28	0.24	0.13

**Table:** Memory cost in GigaBytes (GB) for the storage of the non-reduced matrix  $\mathbf{A}$  and of the reduced matrix  $\mathbf{A}_{\text{red}}$  according to  $N_{\text{red}}$ , for a  $10\lambda$  domain size.

More reduction → less noise in the solution → improvement of the conditioning  
 Too much reduction → numerical solution deteriorates

## How far can we reduce the plane wave basis ?

$\varepsilon$	$10^{-7}$	$10^{-5}$	$10^{-4}$	$10^{-3}$	$10^{-2}$
Trefftz error	N/A	$3.4 \times 10^{-2}$	$9.8 \times 10^{-2}$	0.15	0.74
Memory cost (GB)	0.56	0.38	0.28	0.24	0.13
Time (hours)	55	27	11.3	7.23	0.58

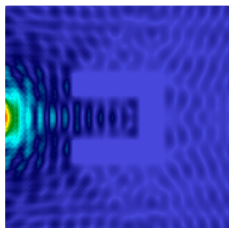
Table: Trefftz error  $\frac{\sqrt{\|[\mathbf{x}_\varepsilon - \mathbf{x}_{\text{ref}}]^* \mathbf{M} [\mathbf{x}_\varepsilon - \mathbf{x}_{\text{ref}}]\|_z}}{\sqrt{\|[\mathbf{x}_{\text{ref}}]^* \mathbf{M} [\mathbf{x}_{\text{ref}}]\|_z}}$ , computation time and memory cost for a  $10^{-8}$  GMRES residual for  $[\mathbf{x}_\varepsilon]$  according to each  $\varepsilon$ .

GMRES residual =  $10^{-8}$  but poor approximation when  $\varepsilon$  is not well chosen.

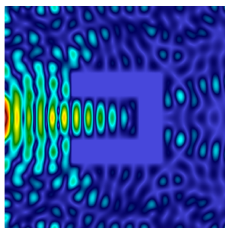
Too much reduction  
 $N_{\text{red}} = 16 \quad \varepsilon = 10^{-2}$

A "optimal" trade-off  
 $N_{\text{red}} = 36 \quad \varepsilon = 10^{-4}$

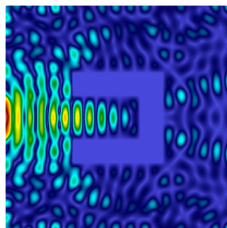
Solution of reference  
 $N_{\text{red}} = 70 \quad \varepsilon = 10^{-7}$



Electromagnetic Field Magnitude  
 0.0e+00    4    6    8    1.1e+01



Electromagnetic Field Magnitude  
 0.0e+00    4    6    8    1.1e+01



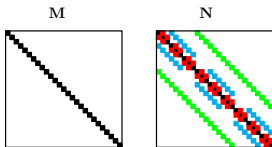
Electromagnetic Field Magnitude  
 0.0e+00    4    6    8    1.1e+01

## Global left preconditioner

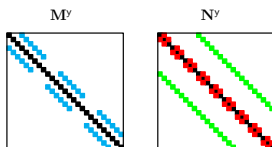
$A[x] = (M^{x/y/z} + N^{x/y/z}) [x] = F$ , lead to **iterative** formulas

$$M^{x/y/z}[x^{n+1}] = F - N^{x/y/z}[x^n].$$

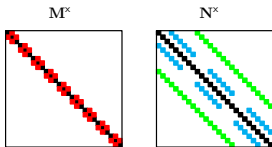
Cessenat-Després decomposition



Decomposition in y direction



Decomposition in x direction



Decomposition in z direction

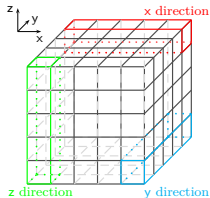
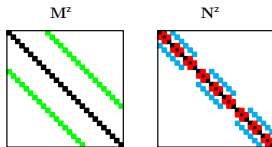


Figure: Global one-dimensional subdomains in a cube.

Figure: Matrices structures for the Cessenat-Després decomposition and the decompositions in x, y or z direction.



## Better conditioning with cyclic decomposition

By **applying successively** each of these 1D preconditioners, we get a global preconditioner associating  $[\mathbf{x}^n]$  to  $[\mathbf{x}^{n+1}]$  thanks to the iterative scheme

$$\left\{ \begin{array}{l} \mathbf{M}^x[\mathbf{x}_0^{n+1}] = \mathbf{F} - \mathbf{N}^x[\mathbf{x}^n], \\ \mathbf{M}^y[\mathbf{x}_1^{n+1}] = \mathbf{F} - \mathbf{N}^y[\mathbf{x}_0^{n+1}], \\ \mathbf{M}^z[\mathbf{x}^{n+1}] = \mathbf{F} - \mathbf{N}^z[\mathbf{x}_1^{n+1}]. \end{array} \right.$$

## Better conditioning with cyclic decomposition

### Preconditioned reduced GMRES problem

$$\mathbf{P}_{\text{red}}^{\text{xyz}} \mathbf{A}_{\text{red}} [\mathbf{x}]_{\text{red}} = \mathbf{P}_{\text{red}}^{\text{xyz}} \mathbf{F}_{\text{red}},$$

where  $\mathbf{P}_{\text{red}}^{\text{xyz}}$  is the reduced (and consequently symetrized) version of

$$\mathbf{P}^{\text{xyz}} := (\mathbf{M}^z)^{-1} \mathbf{N}^z (\mathbf{M}^y)^{-1} \mathbf{N}^y (\mathbf{M}^x)^{-1}.$$

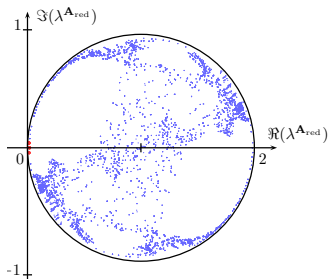


Figure: Real and complex parts of the spectrum  $\lambda^{\mathbf{A}_{\text{red}}}$  of  $\mathbf{A}_{\text{red}}$ .

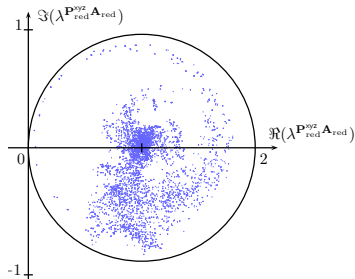
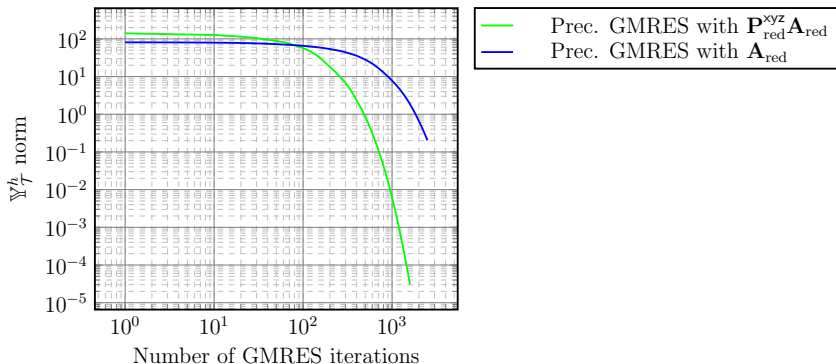


Figure: Real and complex parts of the spectrum  $\lambda^{\mathbf{P}_{\text{red}}^{\text{xyz}} \mathbf{A}_{\text{red}}}$  of  $\mathbf{P}_{\text{red}}^{\text{xyz}} \mathbf{A}_{\text{red}}$ .

## Faster convergence with the left global preconditioner



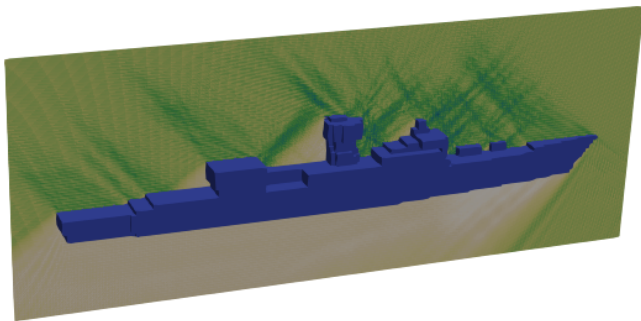
**Figure:** Comparison of the convergence rate of the preconditioned GMRES UWVF using either  $\mathbf{A}_{red}$  or  $\mathbf{P}_{red}^{xyz}\mathbf{A}_{red}$ , with  $\mathbb{Y}_7^h$  the UWVF norm.

## Heterogeneous visualization

**Interpretation: complex nearby electromagnetic field and shadow under the boat.**

**Boat size =  $24 \times 61 \times 154$  meters.**

**Cartesian mesh =  $96 \times 244 \times 616$  elements.**



Three-dimensional electromagnetic wave striking the top of a boat, for  $\lambda = 1$  meter,  $\lambda/4$  mesh.

#elem	$N_{\text{red}}$	$N$	#dof <sub>red</sub>	#dof
$> 14.4 \times 10^6$	46	52	$> 0.663 \times 10^9$	$> 0.75 \times 10^9$

GMRES iterations	Memory cost	Total duration	GMRES residual
800	<b>389 GB</b>	28.6 hours	$3.8 \times 10^{-2}$

Table: Numerical data and results associated to the boat case.

**Thank you for your attention !**

References, preprint:

- Fure, H.S., Pernet, S., Sirdey, M. et al. A discontinuous Galerkin Trefftz type method for solving the two dimensional Maxwell equations. SN Partial Differ. Equ. Appl. 1, 23 (2020).
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