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Sébastien Pernet, Margot Sirdey, Sébastien Tordeux. Trefftz iterative method for three-dimensional electromagnetic waves propagation. JCJC, Nov 2022, Sophia Antipolis, France. hal-03945447

**HAL Id: hal-03945447**

**<https://hal.science/hal-03945447v1>**

Submitted on 19 Jan 2023

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# Iterative Trefftz method for three-dimensional electromagnetic waves simulation

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JCJC 2022

INRIA Sophia-Antipolis, France, 29<sup>th</sup>, November, 2022



## Adimensioned Maxwell problem

$$\begin{cases} \nabla \times \mathbf{H} & = ik\varepsilon_r \mathbf{E} \\ \nabla \times \mathbf{E} & = -ik\mu_r \mathbf{H} \end{cases} \text{ in } \Omega \subset \mathbb{R}^3,$$

where  $\varepsilon_r$  and  $\mu_r$  are the relative permittivity and permeability.

**Goal:** achieve numerical computations on very large domains

$$200\lambda \implies 416 \times 10^6 \text{ dof } (\lambda\text{-mesh}) \text{ or } 3 \times 10^9 \text{ dof } (\frac{\lambda}{2}\text{-mesh})$$



The frigate Surcouf at sea near Toulon.  
Author: Franck Dubey. Source:  
netmarine.net.

Size of the computational domain large with respect to the wavelength  $\Leftrightarrow L \gg \lambda$

### Numerical pollution problem<sup>a</sup>

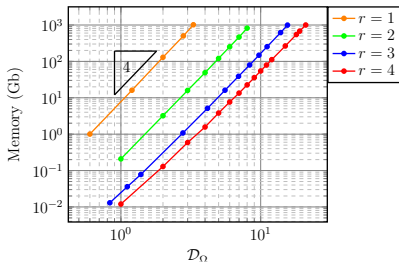
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<sup>a</sup>F. Ihlenburg and I. Babuska, *Finite element solution of the Helmholtz equation with high wave number part II: the hp version of the FEM*, *SIAM Journal on Numerical Analysis*, 34 (1), pp. 315–358 (1997).

## Memory limit of a classic solver

$$\mathbf{A}[\mathbf{E}] = \mathbf{F}$$

- Second order Maxwell system and continuous finite elements leads to **less degrees of freedom**.
- The Finite Element method deals correctly with **the geometry and evanescent modes**.



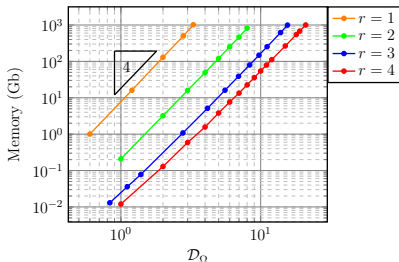
Memory cost of the Nédélec solver for different domain sizes  $\mathcal{D}_\Omega$  and approximation orders  $r$ , **memory =  $(\mathcal{D}_\Omega)^4$** .

	Memory	Sockets	$\mathcal{D}_\Omega$	Power	Cost
Laptop	32 Gb	1	$10\lambda$	200 W	0.034 €/h
// Computation	1 Tb	16	$24\lambda$	3.2 KW	0.544 €/h
HPC	320 Tb	5000	$100\lambda$	1 MW	170 €/h
HPC+	<b>5120 Tb</b>	<b>80000</b>	<b><math>200\lambda</math></b>	<b>16 MW</b>	<b>2720 €/h</b>

## Memory limit of a classic solver

$$\mathbf{A}[\mathbb{E}] = \mathbf{F}$$

- Even efficient optimizations cannot overcome the **memory issue**.
- An iterative method ?



Memory cost of the Nédélec solver for different domain sizes  $\mathcal{D}_\Omega$  and approximation orders  $r$ , **memory** =  $(\mathcal{D}_\Omega)^4$ .

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HPC	320 Tb	5000	$100\lambda$	1 MW	170 €/h
HPC+	<b>5120 Tb</b>	<b>80000</b>	<b><math>200\lambda</math></b>	<b>16 MW</b>	<b>2720 €/h</b>

## Example of GMRES solver with classic methods

Let  $\Omega := [0, \mathcal{D}_\Omega]^3$ . We solve

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

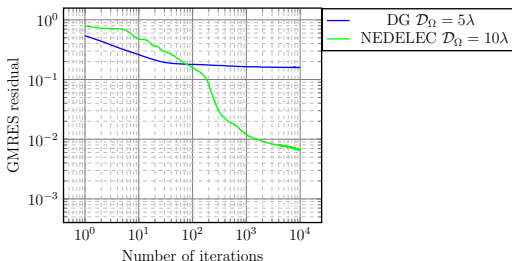
equipped with the **impedance boundary condition**

$$\gamma_t \mathbf{E} + Z_{\partial\Omega} \mathbf{n}_{\partial\Omega} \times \gamma_t \mathbf{H} = \mathbf{g} \quad \text{on } \partial\Omega, \quad \text{with} \quad \gamma_t \mathbf{E} = \mathbf{E} - (\mathbf{E} \cdot \mathbf{n})\mathbf{n}.$$

**GMRES solver is not convergent**

High order Nedelec Finite element on hexahedra (NEDELEC)

High order Dicontinuous Galerkin on tetrahedra (DG)



## Is the Trefftz method an alternative ?

### Particularity of Trefftz methods: basis functions are local solutions of the problem.

- O. Cessenat, and B. Després. "Application of an ultra weak variational formulation of elliptic PDEs to the two-dimensional Helmholtz problem." SIAM journal on numerical analysis. 1998.
- P. Monk, and D. Q. Wang. A least-squares method for the Helmholtz equation. Computer methods in applied mechanics and engineering. 1999.
- A. Moiola. Trefftz-discontinuous Galerkin methods for time-harmonic wave problems. Diss. ETH Zurich. 2011.
- R. Hiptmair, A. Moiola, and I. Perugia. "A survey of Trefftz methods for the Helmholtz equation." Building bridges: connections and challenges in modern approaches to numerical partial differential equations. Springer, Cham, 2016.
- H. Barucq, A. Bendali, M. Fares, V. Mattesi, and S. Tordeux. A symmetric Trefftz-DG formulation based on a local boundary element method for the solution of the Helmholtz equation. J.C.P. 2017.

## General problematic

Are Trefftz methods an efficient alternative to study large computational domains ?

### Addressed issues in this presentation

1. Is the **Trefftz direct** method an alternative ?

- Choice of the variational formulation
- Limits of a LU factorisation

2. Is it possible to define a **Trefftz iterative** method ?

- Ultra-Weak Variational Formulation (UWVF)
- Krylov-type solver

3. Is it possible to **optimize** this method to reach one **billion degrees of freedom** ?

- Use of a reduced space
- Use of preconditioners



## General problematic

Are Trefftz methods an efficient alternative to study large computational domains ?

Code developed from scratch

FORTRAN code, **GoTEM3**, linked to the GMRES of CERFACS<sup>©</sup> <sup>a</sup>

- **Go** → **Giga**octet (**Gig**abyte in french),
- **T** → **Tre**fftz method,
- **EM** → **E**lectro**M**agnetic waves,
- **3** → **3D**

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<sup>a</sup>V. Frayssé, L. Giraud, S. Gratton, and J. Langou (2005). Algorithm 842: A set of GMRES routines for real and complex arithmetics on high performance computers. ACM Transactions on Mathematical Software (TOMS), 31(2), 228-238.

## Steps to define a Trefftz method

1. The solution and the test functions satisfy the Maxwell problem in every element  $T$

$$\nabla \times \mathbf{H}^T = ik_0 \varepsilon_r \mathbf{E}^T \quad \text{and} \quad \nabla \times \mathbf{E}^T = -ik_0 \mu_r \mathbf{H}^T.$$

2. **Virtual work** principle in an element  $T$ :  $W_T = -ik_0 \int_T \varepsilon_r \mathbf{E}^T \cdot \overline{\mathbf{E}'^T} + \mu_r \mathbf{H}^T \cdot \overline{\mathbf{H}'^T}$ , can be written as

$$\begin{aligned} W_T &= - \int_T \underbrace{\nabla \times \mathbf{H}^T}_{ik_0 \varepsilon_r \mathbf{E}^T} \cdot \overline{\mathbf{E}'^T} - \underbrace{\nabla \times \mathbf{E}^T}_{-ik_0 \mu_r \mathbf{H}^T} \cdot \overline{\mathbf{H}'^T}, \\ W_T &= \int_T \mathbf{E}^T \cdot \underbrace{\overline{\nabla \times \mathbf{H}'^T}}_{ik_0 \varepsilon_r \mathbf{E}'^T} - \mathbf{H}^T \cdot \underbrace{\overline{\nabla \times \mathbf{E}'^T}}_{-ik_0 \mu_r \mathbf{H}'^T}. \end{aligned}$$

3. **Stokes formula** leads to the **reciprocity formula**, defined on **boundaries**

$$\sum_T \int_{\partial T} \left( \mathbf{n}_T \times \gamma_t \mathbf{H}^T \right) \cdot \overline{\gamma_t \mathbf{E}'^T} + \gamma_t \mathbf{E}^T \cdot \left( \mathbf{n}_T \times \overline{\gamma_t \mathbf{H}'^T} \right) = 0.$$

4. Find  $\mathbb{E} := (\mathbf{E}, \mathbf{H}) \in \mathbb{X}$ , such that  $\forall \mathbb{E}' := (\mathbf{E}', \mathbf{H}') \in \mathbb{X}$ , we have  $\mathbf{a}(\mathbb{E}, \mathbb{E}') = \ell(\mathbb{E}')$ , with  $\mathbb{X}$  a **discontinuous space of local Maxwell solutions** and

$$\mathbf{a}(\mathbb{E}, \mathbb{E}') = \sum_T \int_{\partial T} \widehat{\gamma_X^T \mathbf{H}^T} \cdot \gamma_t \overline{\mathbf{E}'^T} + \widehat{\gamma_t \mathbf{E}^T} \cdot \gamma_X^T \overline{\mathbf{H}'^T}, \quad \text{with } \gamma_X^T \mathbf{H}^T := \mathbf{n}_T \times \gamma_t \mathbf{H}^T.$$

## Numerical traces choices

Clever choices of the numerical traces  $\widehat{\gamma}_t \mathbf{E}^T$  and  $\widehat{\gamma}_x^T \mathbf{H}^T$  ensure the **coercivity**.

Numerical traces are defined on interior and boundary faces  $F$ .

**Consistence:** coefficients are chosen so that the exact solution satisfies

$$\begin{aligned} \widehat{(\gamma_t \mathbf{E})}|_F &= \gamma_t \mathbf{E}^T = \gamma_t \mathbf{E}^K = \gamma_t \mathbf{E}, \\ \widehat{(\gamma_x^K \mathbf{H})}|_F &= \gamma_x^T \mathbf{H}^T = -\gamma_x^K \mathbf{H}^K = \gamma_x^T \mathbf{H}. \end{aligned}$$

### Equivalent approaches to compute numerical traces

- Riemann solver,
- Upwind fluxes,
- UWVF method.

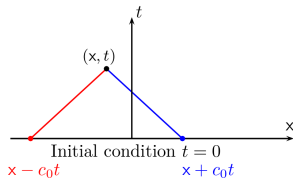


Illustration for a Riemann solver.

## Upwind numerical traces

The incoming and outgoing traces

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

Coefficients are chosen so that the exact solution satisfies

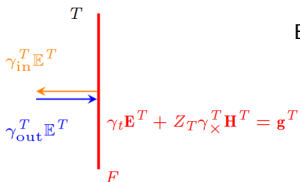
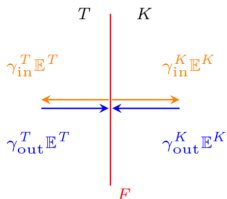
$$\begin{aligned} \widehat{(\gamma_t \mathbf{E})}_{|F} &= \gamma_t \mathbf{E}^T = \gamma_t \mathbf{E}^K = \gamma_t \mathbf{E}, \\ \widehat{(\gamma_{\times}^K \mathbf{H})}_{|F} &= \gamma_{\times}^T \mathbf{H}^T = -\gamma_{\times}^K \mathbf{H}^K = \gamma_{\times}^T \mathbf{H}. \end{aligned}$$

Interior numerical traces

$$\begin{aligned} \widehat{(\gamma_t \mathbf{E})}_{|F} &= \alpha^T \gamma_{\text{out}}^T \mathbf{E}^T + \alpha^K \gamma_{\text{out}}^K \mathbf{E}^K, \\ \widehat{(\gamma_{\times}^T \mathbf{H})}_{|F} &= \beta^T \gamma_{\text{out}}^T \mathbf{E}^T + \beta^K \gamma_{\text{out}}^K \mathbf{E}^K. \end{aligned}$$

Boundary numerical traces

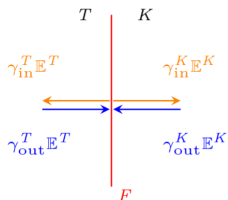
$$\begin{aligned} \widehat{(\gamma_t \mathbf{E})}_{|F} &= \alpha^T \gamma_{\text{out}}^T \mathbf{E}^T + \alpha^K \mathbf{g}^T, \\ \widehat{(\gamma_{\times}^T \mathbf{H})}_{|F} &= \beta^T \gamma_{\text{out}}^T \mathbf{E}^T + \beta^K \mathbf{g}^T. \end{aligned}$$



## Upwind numerical traces

The incoming and outgoing traces

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



Coefficients are chosen so that the exact solution satisfies

$$\begin{aligned} \widehat{(\gamma_t \mathbf{E})}_{|F} &= \gamma_t \mathbf{E}^T = \gamma_t \mathbf{E}^K = \gamma_t \mathbf{E}, \\ \widehat{(\gamma_{\times}^T \mathbf{H})}_{|F} &= \gamma_{\times}^T \mathbf{H}^T = -\gamma_{\times}^K \mathbf{H}^K = \gamma_{\times}^T \mathbf{H}. \end{aligned}$$

Interior numerical traces

$$\begin{aligned} \widehat{(\gamma_t \mathbf{E})}_{|F} &= \frac{Z_K}{Z_T + Z_K} \gamma_{\text{out}}^T \mathbf{E}^T + \frac{Z_T}{Z_T + Z_K} \gamma_{\text{out}}^K \mathbf{E}^K, \\ \widehat{(\gamma_{\times}^T \mathbf{H})}_{|F} &= -\frac{1}{Z_T + Z_K} \gamma_{\text{out}}^T \mathbf{E}^T + \frac{1}{Z_T + Z_K} \gamma_{\text{out}}^K \mathbf{E}^K. \end{aligned}$$

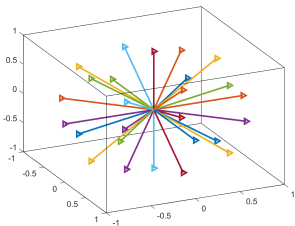
Boundary numerical traces

$$\begin{aligned} \widehat{(\gamma_t \mathbf{E})}_{|F} &= \frac{Z_{\partial\Omega}}{Z_T + Z_{\partial\Omega}} \gamma_{\text{out}}^T \mathbf{E}^T + \frac{Z_T}{Z_T + Z_{\partial\Omega}} \mathbf{g}^T, \\ \widehat{(\gamma_{\times}^T \mathbf{H})}_{|F} &= -\frac{1}{Z_{\partial\Omega} + Z_T} \gamma_{\text{out}}^T \mathbf{E}^T + \frac{1}{Z_{\partial\Omega} + Z_T} \mathbf{g}^T. \end{aligned}$$

## Plane wave Galerkin space

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

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



26 plane wave directions and  
52 polarisations.

- In each element  $T$ , the approximated solution  $\mathbb{E}^T := (\mathbf{E}^T, \mathbf{H}^T)$  is

$$\left\{ \begin{array}{l} \mathbf{E}^K = \sum_{j=1}^N u_j \underbrace{\vec{p}_j^T e^{ik\vec{d}_j \cdot \vec{x}}}_{w_j}, \\ \mathbf{H}^K = \sum_{j=1}^N u_j \left( \vec{p}_j^T \times \vec{d}_j^T \right) e^{ik\vec{d}_j \cdot \vec{x}}. \end{array} \right.$$

- What is the optimal number  $N$  of plane waves ?

$N$  small leads to a bad approximation.

$N$  large leads to rounding errors.

## Some references about the optimal choice of basis functions

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

- A. [Moiola](#). Trefftz-discontinuous Galerkin methods for time-harmonic wave problems. Diss. ETH Zurich. 2011.
- A. [Moiola](#), R. [Hiptmair](#), I. [Perugia](#). Vekua theory for the Helmholtz operator. Zeit. für ang. Math. und Phys. 2011.

### Strategies to minimize the effect of numerical pollution

- T. [Luostari](#), T. [Huttunen](#), P. [Monk](#). Improvements for the ultra weak variational formulation, Int. J. Numer. Meth. Engng 94. 2013.
- S. [Congreve](#), J. [Gedicke](#), I. [Perugia](#). Numerical investigation of the conditioning for plane wave discontinuous Galerkin methods, Vol. 126 of Lecture Notes in Comp. Sc. and Eng., Springer. 2019.
- H. [Barucq](#), A. [Bendali](#), J. [Diaz](#), S. [Tordeux](#). Local strategies for improving the conditioning of the plane-wave Ultra-Weak Variational Formulation. J.C.P. 2021.

### Some alternatives exist (evanescent modes or Quasi-Trefftz methods)

- E. [Parolin](#), D. [Huybrechs](#), A. [Moiola](#). Stable approximation of Helmholtz solutions by evanescent plane waves. 2022.
- L.-M. [Imbert-Gérard](#), and P. [Monk](#). "Numerical simulation of wave propagation in inhomogeneous media using generalized plane waves." ESAIM: Mathematical Modelling and Numerical Analysis 51.4 2017.
- H. S. [Fure](#), S. [Pernet](#), M. [Sirdey](#), S. [Tordeux](#). A discontinuous Galerkin Trefftz type method for solving the two dimensional Maxwell equations. SN Partial Differ. Equ. Appl. 2020.

## The Trefftz matrix for a structured mesh

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

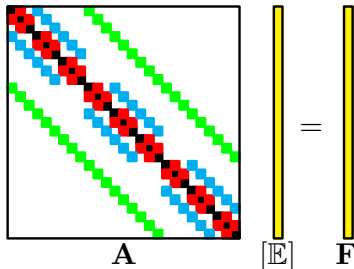
where

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

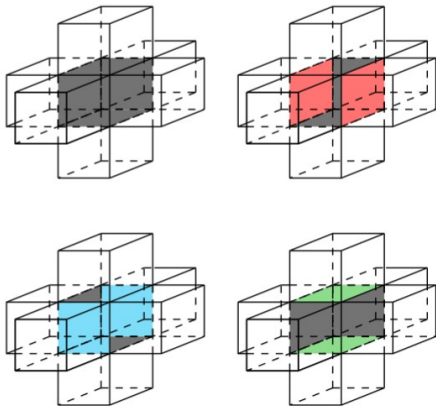
$$\mathbf{F}_i := \mathbf{l}(\mathbf{w}^i) \quad \text{for } i, j = 1, N_{\text{dof}}.$$

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

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

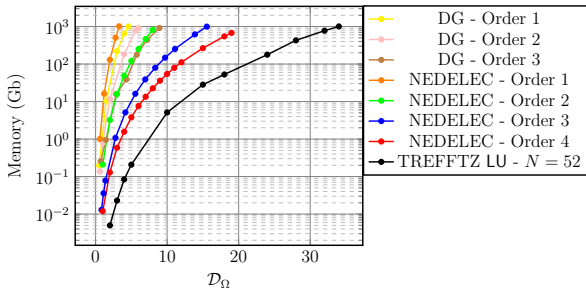


The matrix  $\mathbf{A}$  for  $N_{\text{elem}} = 27 = 3^3$  cubes.

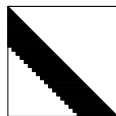




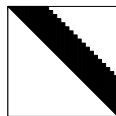
## Memory limit of the Trefftz direct solver



### LU Factorisation



L



U

$\mathcal{D}_\Omega$	$5\lambda$	$10\lambda$	$20\lambda$	$100\lambda$	$200\lambda$
$N_{\text{elem}}$	25	1000	8000	$1 \times 10^6$	$8 \times 10^6$
$N_{\text{dof}}$	1300	$52 \times 10^3$	$416 \times 10^6$	$52 \times 10^6$	$416 \times 10^6$
LU Memory	312 Mb	5 Gb	80 Gb	50 Tb	800 Tb

**Table:** Memory cost of the LU factorisation with respect to the domain size  $\mathcal{D}_\Omega$ , for  $N = 52$  and for  $h = 1$ .

## Cessenat-Després decomposition

Singular regular decomposition

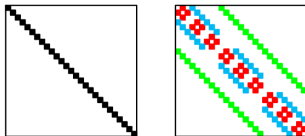
$$\mathbf{A} = \mathbf{M} + \mathbf{N},$$

with two conditions

1.  $\mathbf{M}$  easily invertible,
2.  $\rho(\mathbf{M}^{-1}\mathbf{N}) < 1$ .

Picard fixed point algorithm:  $\mathbf{M}[\mathbb{E}_{n+1}] = \mathbf{F} - \mathbf{N}[\mathbb{E}_n]$ .

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



The two conditions are theoretically satisfied.

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<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 decomposition

Singular regular decomposition

$$\mathbf{A} = \mathbf{M} + \mathbf{N},$$

with two conditions

1.  $\mathbf{M}$  easily invertible,
2.  $\rho(\mathbf{M}^{-1}\mathbf{N}) < 1$ .

**Picard solver based on Jacobi decomposition:**

$$\mathbf{M}[\mathbf{E}_{n+1}^{\text{jac}}] = -\mathbf{N}[\mathbf{E}_n^{\text{jac}}] + \mathbf{F}.$$

Randomly divergent due to rounding errors.

$\mathcal{D}_\Omega$	$10\lambda$	$30\lambda$	$50\lambda$	$80\lambda$	$100\lambda$
$\rho(\mathbf{M}^{-1}\mathbf{N})$	$1 - 0.0097$	$1 - 0.0033$	$1 - 0.0024$	$1 + 0.00064$	$1 - 0.00043$

**Table:** The largest eigenvalue of  $\mathbf{M}^{-1}\mathbf{N}$  computed with respect to the size  $\mathcal{D}_\Omega$  of the domain.

## Krylov methods

**Coercivity:**  $\text{Re}(a(\mathbb{E}, \mathbb{E}')) > 0 \rightarrow$  Good framework for GMRES/Krylov Galerkin method.

$$[\mathbb{E}_{N_{\text{kry}}}] = \text{KG}(\mathbf{A}, \mathbf{F}, N_{\text{kry}})$$

We approximate the solution  $\mathbb{E}_{N_{\text{kry}}} \in \mathbb{K}^{N_{\text{kry}}}$  of

(Krylov Galerkin) Find  $[\mathbb{E}_{N_{\text{kry}}}] \in [\mathbb{K}^{N_{\text{kry}}}]$ ,  $[\mathbb{E}']^* \mathbf{A} [\mathbb{E}_{N_{\text{kry}}}] = [\mathbb{E}']^* \mathbf{F}$ ,  $\forall [\mathbb{E}'] \in [\mathbb{K}^{N_{\text{kry}}}]$ ,

(GMRES) Find  $[\mathbb{E}_{N_{\text{kry}}}] \in [\mathbb{K}^{N_{\text{kry}}}]$ ,  $[\mathbb{E}']^* \mathbf{A}^* \mathbf{A} [\mathbb{E}_{N_{\text{kry}}}] = [\mathbb{E}']^* \mathbf{A}^* \mathbf{F}$ ,  $\forall [\mathbb{E}'] \in [\mathbb{K}^{N_{\text{kry}}}]$ ,

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

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

$\implies \text{size}(\text{Krylov}) = N_{\text{kry}} \times N_{\text{dof}}$ , with  $\dim(\mathbf{F}) = N_{\text{dof}}$ .

## Krylov method issues

- The convergence rate of the **GMRES** method is slow down by **the smallest eigenvalues of  $\mathbf{A}$** . GMRES Convergence Theorem<sup>i</sup>

$$\|\mathbf{E} - \mathbf{E}_n\| \leq C \varepsilon_n \|\mathbf{F}\|,$$

with

$$\varepsilon_n = \inf_{\deg(p) \leq n-1} \sup_{\lambda \in \Lambda} \left| \frac{1}{\lambda} - p(\lambda) \right|.$$

**Better estimates** also exist <sup>ii</sup>.

- Need to reduce **memory** for large domains

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

### Our objectives

1. **Move away from zero** the eigenvalues.
2. **Reduce memory** cost.

---

<sup>i</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>ii</sup>J. Liesen, P. Tichý, (2012). The field of values bound on ideal GMRES.

## Restart strategies for Krylov methods

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

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

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

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

- High memory cost to store  $\mathbb{K}^{N_{\text{kry}}}$ .
- Accumulation of rounding errors at each iteration.

Idea: **Truncate** the Krylov space  $\mathbb{K}^{N_{\text{kry}}}$  with  $N_{\text{kry}}^{\text{restart}} < N_{\text{kry}}$

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

Example with  $N_{\text{kry}}^{\text{restart}} = 20$ :

$$\text{size(Krylov)} = N_{\text{kry}}^{\text{restart}} \times N_{\text{dof}} = 20 \times 52 \times 10^6 = 16 \text{ Gb.}$$

$\rightarrow$  restart strategy reduces the memory cost.

## Matrix free strategy

The **memory cost** of GoTEM3 with **matrix storage** is

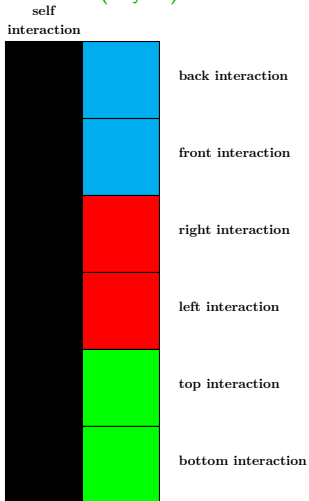
$$\text{size(Krylov)} + \text{size(A)} = 20 \times N \times N_{\text{elem}} + N^2 \times 7 \times N_{\text{elem}}$$
$$\frac{\text{size(A)}}{\text{size(Krylov)}} \simeq 7 \rightarrow \text{when assembling : the most costly structure is A.}$$

## Matrix free strategy

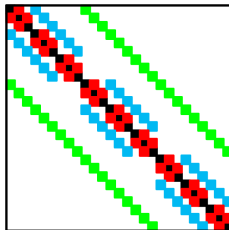
The **memory cost** of GoTEM3 with matrix storage is

$$\text{size}(\text{Krylov}) + \text{size}(\mathbf{A}) = 20 \times N \times N_{\text{elem}} + N^2 \times 7 \times N_{\text{elem}}$$

$$\frac{\text{size}(\mathbf{A})}{\text{size}(\text{Krylov})} \simeq 7 \rightarrow \text{when assembling : the most costly structure is } \mathbf{A}.$$



Structured mesh



$\mathbf{A}$

$U \mapsto \mathbf{A}U$  is an element by element product.



## Matrix free strategy

The memory cost **without** with **matrix free strategy** is

$$\text{size(Krylov)} + \text{size(A)} = 20 \times N \times N_{\text{elem}} + N^2 \times 7 \times N_{\text{elem}}$$

$$\text{size(Krylov)} + \text{size(interactions)} = 20 \times N \times N_{\text{elem}} + N^2 \times 7$$

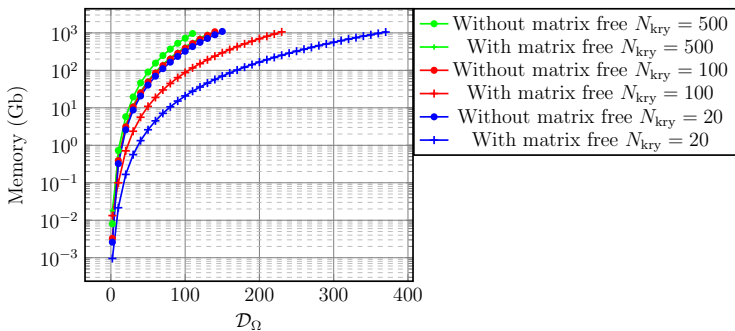
with matrix free: only the **interactions** between elements are stored

- $N_{\text{kry}} = 20$  the dimension of the Krylov space
- $N_{\text{elem}}$  the number of basis functions
- $N = 52$  the number plane waves per element
- $N_{\text{dof}} = N \times N_{\text{elem}}$  the number of degrees of freedom

$\mathcal{D}_\Omega$	$5\lambda$	$10\lambda$	$20\lambda$	$100\lambda$	$200\lambda$
$N_{\text{elem}}$	25	1000	8000	$1 \times 10^6$	$8 \times 10^6$
$N_{\text{dof}}$	1300	$52 \times 10^3$	$416 \times 10^3$	$52 \times 10^6$	$416 \times 10^6$
<b>Without matrix free</b>	7.9 Mb	0.31 Gb	2.5 Gb	0.31 Tb	<b>2.5 Tb</b>
<b>With matrix free</b>	0.71 Kb	16 Mb	0.13 Gb	16 Gb	<b>0.13 Tb</b>

Table: Comparison with or without matrix free strategy.

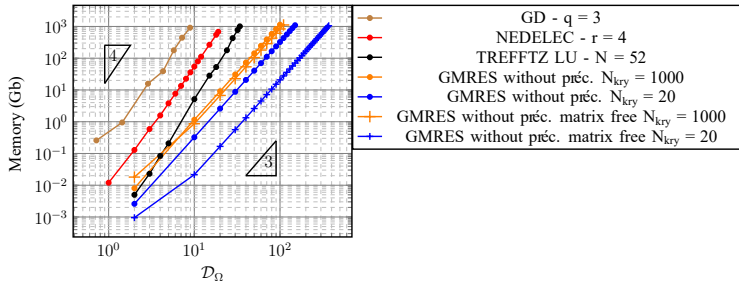
## Reduction of the memory cost with the matrix free strategy



Comparison of the GMRES method memory costs with or without matrix free strategy, for different  $N_{\text{kry}}$ .

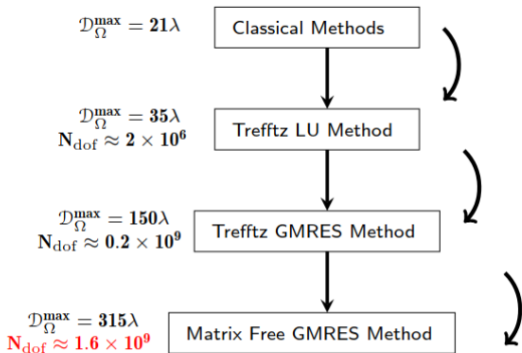
Restart ↘ ⇒ Matrix free effect ↗

## Comparison of memory costs



**GoTEM3** :  $D_\Omega^{\text{max}} = 315\lambda \iff N_{\text{elem}} = 30 \times 10^6 \iff N_{\text{dof}} = 1.6 \times 10^9$

## Larger computational scenes



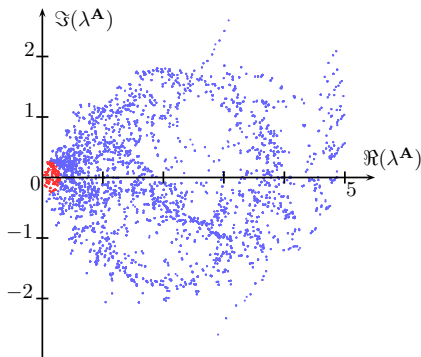
$$\mathcal{D}_{\Omega}^{\max} = 315\lambda \text{ for 1Tb}$$
$$\approx 1.6 \times 10^9 \text{ degrees of freedom}$$

## Cessenat-Després preconditioning

The convergence of the GMRES method depends on the **spectrum of  $A$** .

Objective: **move away from 0** eigenvalues and avoid rounding errors.

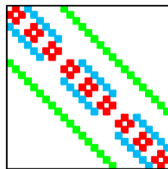
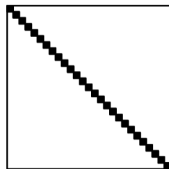
Idea: use **Preconditioned GMRES** which solves  $A\#A[E] = A\#F$ .



Real and imaginary parts of the eigenvalues  $\lambda^A$  of the matrix  $A$ , for a domain with size  $\mathcal{D}_\Omega = 6\lambda$ .

$$A = M + N$$

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



<sup>a</sup>O. Cessenat and B. Després, (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 preconditioning

The convergence of the GMRES method depends on the **spectrum of  $A$** .

Objective: **move away from 0** eigenvalues and avoid rounding errors.

**Idea:** use a **preconditioned GMRES** which solves  $A^\# A[E] = A^\# F$ .

Cessenat-Després iteration

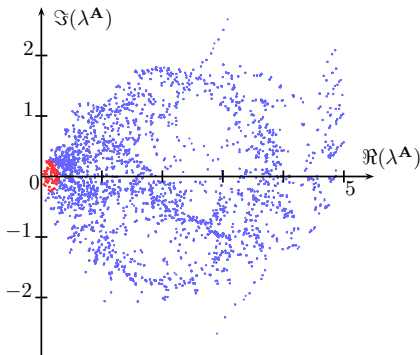
$$M[E]^{n+1} = -N[E]^n + F$$

Define  $A^\# = M^{-1}$  with  $M$  block diagonal.

**Symmetric preconditioning**

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

Computation of  $M^{-\frac{1}{2}}$  is trivial.



Real and imaginary parts of the eigenvalues  $\lambda^A$  of the matrix  $A$ , for a domain with size  $\mathcal{D}_\Omega = 6\lambda$ .

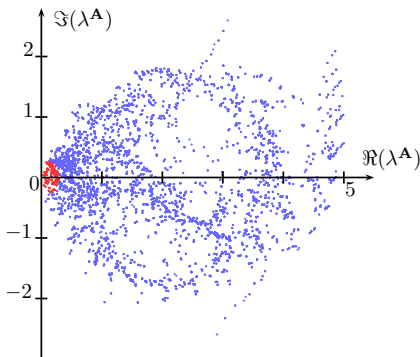
## Cessenat-Després preconditioning

The convergence of the GMRES method depends on the **spectrum of  $\mathbf{A}$** .

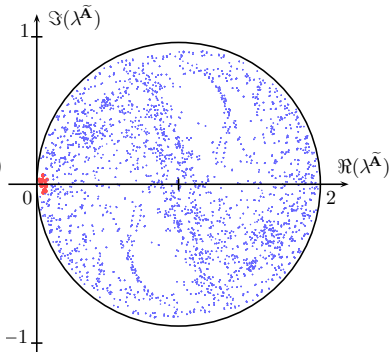
Objective: **move away from 0** eigenvalues and avoid rounding errors.

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

**is contractant**



Real and imaginary parts of the eigenvalues  $\lambda^{\mathbf{A}}$  of the matrix  $\mathbf{A}$ , for a domain with size  $\mathcal{D}_{\Omega} = 6\lambda$ .



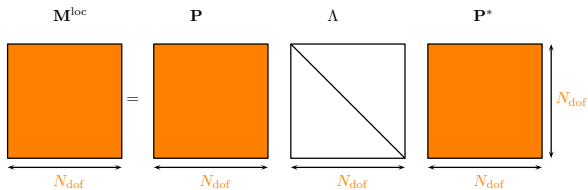
Real and imaginary parts of the eigenvalues  $\lambda^{\tilde{\mathbf{A}}}$  of the matrix  $\tilde{\mathbf{A}}$ , for a domain with size  $\mathcal{D}_{\Omega} = 6\lambda$ .

## Basis reduction strategy

$\mathbf{M}^{\text{loc}}$  is a **symmetric positive definite** matrix

$$\mathbf{M}_{\ell,k}^{\text{loc}} = (\gamma_{\text{out}} \mathbf{w}_k, \gamma_{\text{out}} \mathbf{w}_\ell)$$

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



$\mathbf{P}$  is the eigenvector matrix.

$\Lambda$  is the eigenvalue matrix.

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

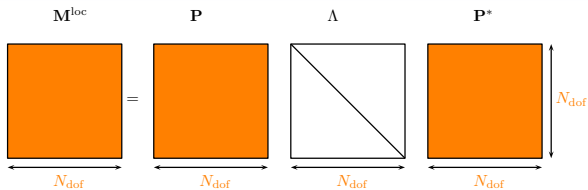


## Basis reduction strategy

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$$M_{\ell,k}^{\text{loc}} = (\gamma_{\text{out}} \mathbf{w}_k, \gamma_{\text{out}} \mathbf{w}_\ell)$$

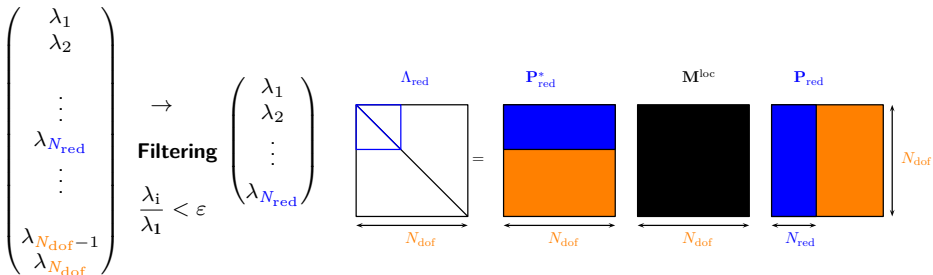
for  $\ell, k = 1, N$ .



$P$  is the eigenvector matrix.

$\Lambda$  is the eigenvalue matrix.

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



## Normalized Reduced Basis

The unknown of the problem is represented as

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

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

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

$$\mathbf{A}_{\text{red}} = \mathbf{I}_{\text{red}} + \mathbf{N}_{\text{red}} =$$

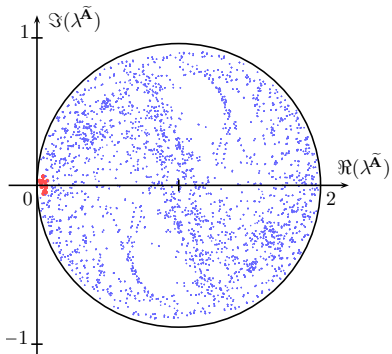
The diagram illustrates the structure of the reduced matrix  $\mathbf{A}_{\text{red}} = \mathbf{I}_{\text{red}} + \mathbf{N}_{\text{red}}$ . It consists of five components arranged horizontally:

- A square matrix  $\Lambda_{\text{red}}^{-\frac{1}{2}}$  with a diagonal line, having a width of  $N_{\text{red}}$ .
- A blue rectangular matrix  $\mathbf{P}_{\text{red}}^*$  with a width of  $N_{\text{dof}}$ .
- A black square matrix  $\mathbf{A}$  with a width of  $N_{\text{dof}}$ .
- A blue rectangular matrix  $\mathbf{P}_{\text{red}}$  with a width of  $N_{\text{red}}$ .
- A square matrix  $\Lambda_{\text{red}}^{-\frac{1}{2}}$  with a diagonal line, having a width of  $N_{\text{red}}$ .

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

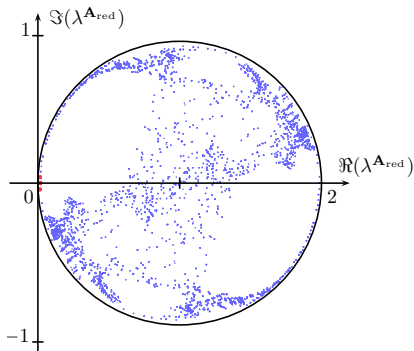
## Improvement of the conditioning with basis reduction

Non reduced preconditioned matrix  $\tilde{\mathbf{A}}$



Real and imaginary parts of the eigenvalues  $\lambda^{\tilde{\mathbf{A}}}$  of  $\tilde{\mathbf{A}}$ , for  $\mathcal{D}_\Omega = 6\lambda$ .

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



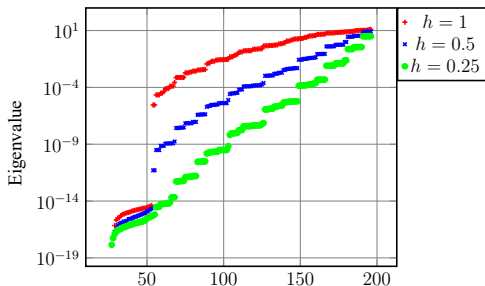
Real and imaginary parts of the eigenvalues  $\lambda^{\mathbf{A}_{\text{red}}}$  of  $\mathbf{A}_{\text{red}}$ , for  $\mathcal{D}_\Omega = 6\lambda$  and  $\varepsilon = 10^{-5}$ .

## Eigenvalues of $M^{\text{loc}}$

$N_{\text{red}}$  depends on the size of each element  $T$  and the threshold value  $\varepsilon$ .

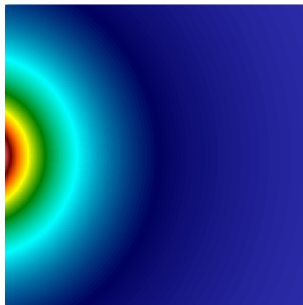
$h \backslash \varepsilon$	$10^{-16}$	$10^{-15}$	$10^{-13}$	$10^{-11}$	$10^{-9}$	$10^{-7}$	$10^{-5}$	$10^{-4}$	$10^{-3}$	$10^{-2}$
0.25	180	175	154	126	96	70	48	36	30	16
0.5	196	196	190	186	174	132	96	84	70	48
1	196	196	196	196	196	190	180	174	148	114

**Table:** Values of  $N_{\text{red}}$  with respect to  $\varepsilon$  and  $h$ , when performing basis reduction for  $N = 196$  plane waves per element.



## The quality of the solution depends on $\varepsilon$

Field generated by a dipolar source located on the left of the domain for different values of  $\varepsilon$  with  $N = 196$ ,  $\mathcal{D}_\Omega = 5\lambda$ ,  $h = 0.25\lambda$ .



Electromagnetic Field Magnitude

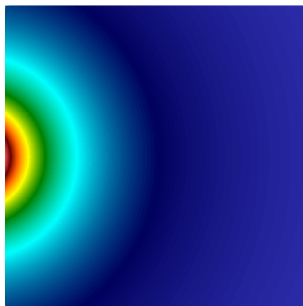
2.7e-01 2 4 6 8.5e+00



Electromagnetic field magnitude for  $\varepsilon = 10^{-16}$ , ie  $N_{\text{red}} = 180$ .

## The quality of the solution depends on $\varepsilon$

Field generated by a dipolar source located on the left of the domain for different values of  $\varepsilon$  with  $N = 196$ ,  $\mathcal{D}_\Omega = 5\lambda$ ,  $h = 0.25\lambda$ .



Electromagnetic Field Magnitude

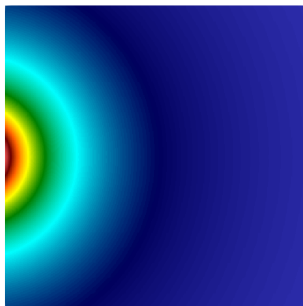
2.7e-01 2 4 6 8.5e+00



Electromagnetic field magnitude for  $\varepsilon = 10^{-9}$ , ie  $N_{\text{red}} = 96$ .

## The quality of the solution depends on $\varepsilon$

Field generated by a dipolar source located on the left of the domain for different values of  $\varepsilon$  with  $N = 196$ ,  $\mathcal{D}_\Omega = 5\lambda$ ,  $h = 0.25\lambda$ .



Electromagnetic Field Magnitude

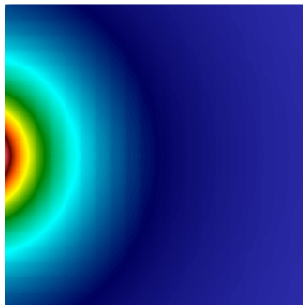
2.7e-01 2 4 6 8.5e+00



Electromagnetic field magnitude for  $\varepsilon = 10^{-5}$ , ie  $N_{\text{red}} = 48$ .

## The quality of the solution depends on $\varepsilon$

Field generated by a dipolar source located on the left of the domain for different values of  $\varepsilon$  with  $N = 196$ ,  $\mathcal{D}_\Omega = 5\lambda$ ,  $h = 0.25\lambda$ .



Electromagnetic Field Magnitude

2.7e-01 2 4 6 8.5e+00

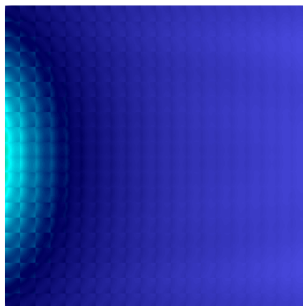


Electromagnetic field magnitude for  $\varepsilon = 10^{-4}$ , ie  $N_{\text{red}} = 36$ .



## The quality of the solution depends on $\varepsilon$

Field generated by a dipolar source located on the left of the domain for different values of  $\varepsilon$  with  $N = 196$ ,  $\mathcal{D}_\Omega = 5\lambda$ ,  $h = 0.25\lambda$ .



Electromagnetic Field Magnitude

2.7e-01 2 4 6 8.5e+00



Electromagnetic field magnitude for  $\varepsilon = 10^{-2}$ , ie  $N_{\text{red}} = 16$ .

## The quality of the solution depends on $\varepsilon$

Field generated by a dipolar source located at the left of the domain for different values of  $\varepsilon$  with  $N = 196$ ,  $\mathcal{D}_\Omega = 5\lambda$ ,  $h = 0.25\lambda$ .

$$e^\varepsilon := \frac{\|\mathbb{E}_{\text{red}}^\varepsilon - \mathbb{E}^{\text{ex}}\|_\infty}{\|\mathbb{E}^{\text{ex}}\|_\infty}, \quad \text{with } \|\mathbb{E}\|_\infty := \max_{i=1,27} \mathbb{E}(x_i).$$

$\varepsilon$	$10^{-16}$	$10^{-9}$	$10^{-5}$	$10^{-4}$	$10^{-2}$
$N_{\text{red}}$	180	96	48	36	16
$N_{\text{dof,red}}$	1440000	768000	384000	288000	128000
Time (s)	4121	1085	254.9	141.8	25.61
Memory (Gb)	0.15	0.08	0.04	0.03	0.01
$e^\varepsilon$	$6.35 \times 10^{-7}$	$4.83 \times 10^{-5}$	$6.33 \times 10^{-3}$	$2.39 \times 10^{-2}$	0.59

Table: Results for a GMRES residual  $= 10^{-12}$  ( $N_{\text{kry}} = 100$ ).

The larger is  $\varepsilon$   $\rightarrow$  the less rounding error  $\rightarrow$  improvement of the conditioning  
Too much reduction  $\rightarrow$  bad quality of the approximation

## The quality of the solution depends on $\varepsilon$

Improvement on the computation time : 94%

Improvement on the memory cost : 75%

$\varepsilon$	$10^{-16}$	$10^{-9}$	$10^{-5}$	$10^{-4}$	$10^{-2}$
$N_{\text{red}}$	180	96	48	36	16
$\#\text{dof}_{\text{red}}$	1440000	768000	384000	288000	128000
Time (s)	4121	1085	254.9	141.8	25.61
Memory (Gb)	0.15	0.08	0.04	0.03	0.01
$e^\varepsilon$	$6.35 \times 10^{-7}$	$4.83 \times 10^{-5}$	$6.33 \times 10^{-3}$	$2.39 \times 10^{-2}$	0.59

GMRES residual =  $10^{-12}$  but the approximation is too poor when  $\varepsilon$  is not correctly chosen.

Too much reduction

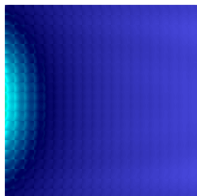
$N_{\text{red}} = 16, \varepsilon = 10^{-2}$

Optimal trade-off

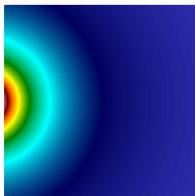
$N_{\text{red}} = 48, \varepsilon = 10^{-5}$

Reference solution

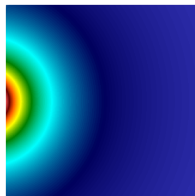
$N_{\text{red}} = 180, \varepsilon = 10^{-16}$



Electromagnetic Field Magnitude  
2.7e-01 2 4 6 8.5e+00



Electromagnetic Field Magnitude  
2.7e-01 2 4 6 8.5e+00



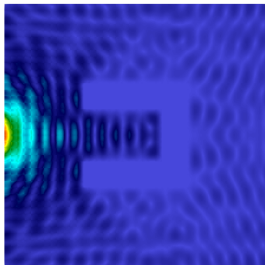
Electromagnetic Field Magnitude  
2.7e-01 2 4 6 8.5e+00

## Application to a case with a scatterer

$\varepsilon$	$10^{-7}$	$10^{-5}$	$10^{-4}$	$10^{-3}$	$10^{-2}$
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

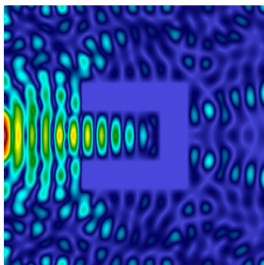
GMRES residual =  $10^{-8}$  but the approximation is too poor when  $\varepsilon$  is not correctly chosen.

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



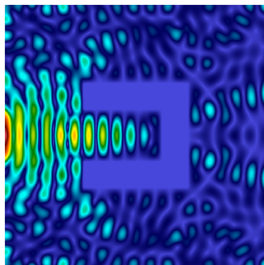
Electromagnetic Field Magnitude  
 0.0e+00 4 6 8 1.1e+01

Optimal trade-off  
 $N_{\text{red}} = 36$ ,  $\varepsilon = 10^{-4}$



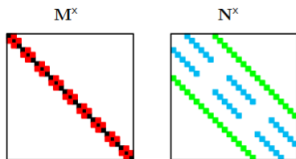
Electromagnetic Field Magnitude  
 0.0e+00 4 6 8 1.1e+01

Reference solution  
 $N_{\text{red}} = 70$ ,  $\varepsilon = 10^{-7}$

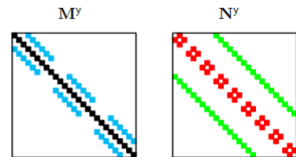


Electromagnetic Field Magnitude  
 0.0e+00 4 6 8 1.1e+01

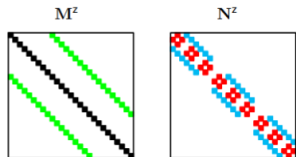
## Global preconditioner



Structures of  $M^x$  and  $N^x$ .



Structures of  $M^y$  and  $N^y$ .



Structures of  $M^z$  and  $N^z$ .

The new decomposition

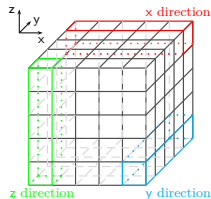
$$A = M^{x/y/z} + N^{x/y/z},$$

can be used as preconditioners

1.  $M^{x/y/z}$  easily invertible,
2.  $\rho\left((M^{x/y/z})^{-1}N^{x/y/z}\right) \ll 1$ ,

and leads to preconditioners:

$$[y] = (M^{x/y/z})^{-1}F.$$



1D subdomains.

## How to build a global preconditioner ?

By **successively applying** every preconditioner (x, y or z), we obtain a global preconditioner associating  $[\mathbf{y}]$  to  $[\mathbf{F}]$  with an iterative scheme

$$\begin{cases} \mathbf{M}^x[\mathbb{E}_0] &= \mathbf{F}, \\ \mathbf{M}^y[\mathbb{E}_1] &= \mathbf{F} - \mathbf{N}^y[\mathbb{E}_0], \\ \mathbf{M}^z[\mathbf{y}] &= \mathbf{F} - \mathbf{N}^z[\mathbb{E}_1]. \end{cases}$$

The **reduced preconditioned GMRES problem** is

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

where  $\mathbf{P}_{\text{red}}^{\text{xyz}}$  is the **reduced version** of

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

## Better conditioning with successive decompositions

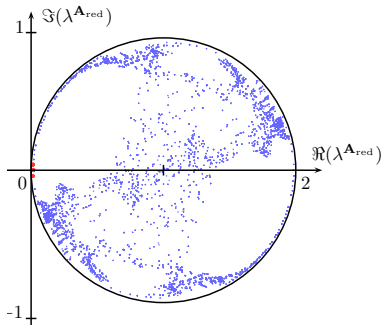


Figure: Real and imaginary parts of the eigenvalues  $\lambda^{\mathbf{A}_{\text{red}}}$  of  $\mathbf{A}_{\text{red}}$ .

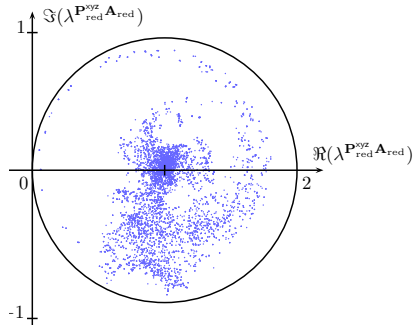


Figure: Real and imaginary parts of the eigenvalues  $\lambda^{\mathbf{P}_{\text{red}}^{\text{xyz}} \mathbf{A}_{\text{red}}}$  de  $\mathbf{P}_{\text{red}}^{\text{xyz}} \mathbf{A}_{\text{red}}$ .

## Convergence acceleration with the global preconditioner

Numerical case: electromagnetic dipole in a cup

$$\Omega = [0, 200] \times [0, 40] \times [0, 40], \quad h = 1, \quad R_{\partial\Omega} = 0.9, \quad N = 196, \quad N_{\text{red}} = 196, \quad \varepsilon = 10^{-9}, \\ N_{\text{kry}} = 25.$$

$$\text{GMRES residual} = \frac{\|\mathbf{A}[\mathbf{E}] - \mathbf{F}\|_2}{\|\mathbf{F}\|_2}.$$

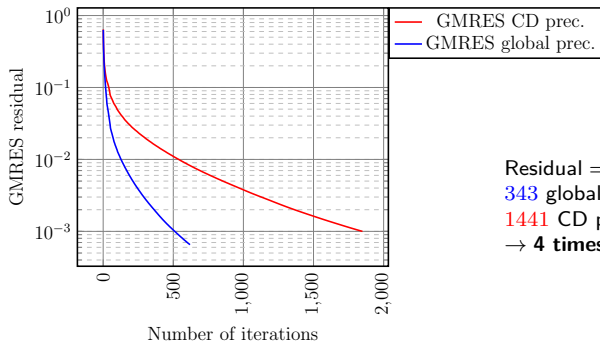


Figure: Comparison of the convergence rate between the GMRES method preconditioned with the Cessenat-Després or the global preconditioners.



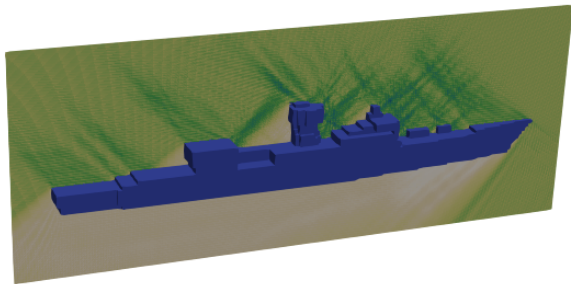
## A numerical case

Boat size =  $24 \times 61 \times 154 \lambda^3$ .

$R_{\partial\Omega} = 0$ .

Preconditioned GMRES with Cessenat-Després.

Interpretation : electromagnetic near field and shadow cone under the boat.



3D electromagnetic wave striking the boat from the top, for  $\lambda = 1$  meter and  $h = \lambda/4$ .

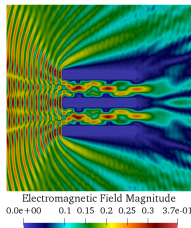
#elem	$N_{\text{red}}$	$N$	#dof <sub>red</sub>	#dof
$> 14.4 \times 10^6$	46	52	$> 0.663 \times 10^9$	$> 0.75 \times 10^9$

GMRES iterations	Memory cost	Computation time	GMRES residual
800	<b>389 Gb</b>	28.6 hours	$3.8 \times 10^{-2}$

## Iterative Trefftz solver GoTEM3

Maximal size for 1Tb :  $(315\lambda)^3$

$\approx 1.6 \times 10^9$  degrees of freedom



**Thank you for your attention !**

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- S. Pernet, N. Serdiuk, M. Sirdey, S. Tordeux. Discontinuous Galerkin Method based on Riemann fluxes for the time domain Maxwell System. [Research Report] RR-9431, INRIA Bordeaux - Sud-Ouest. 2021, pp.55. hal-03396721.
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