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Iterative Trefftz method for three-dimensional electromagnetic waves simulation

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¹MACI/LMA2S ONERA ²EPC INRIA Makutu

Oslo, Norway, June 6, 2022



Adimensional Maxwell problem

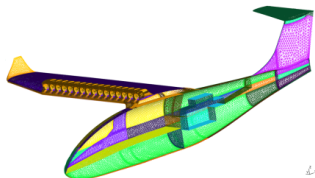
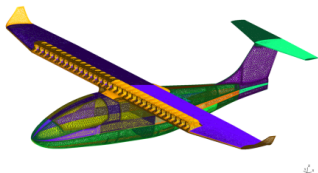
Studied problem:

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

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

Objective: computation on very large domains

→ **up to 200 wavelengths = $200\lambda = 8 \times 10^6$ elements in the mesh.**



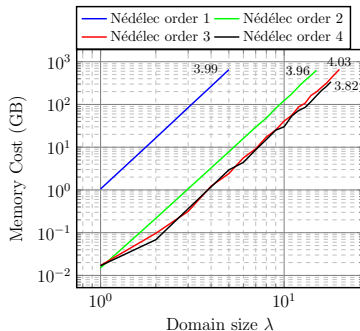
Ampere plane geometry (DEMR ONERA).

Memory limits of a classic solverⁱ

Numerical dispersion when large domain size with respect to the wavelength $\Leftrightarrow L \gg \lambda$

→ Efficient optimisation cannot overcome the **memory issue**.

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



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

Example of high order Nédélec finite elements

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

ⁱF. 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).

Trefftz method construction steps

Trefftz method advantagesⁱⁱ

- 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

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

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

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

ⁱⁱR. 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

1. Find $\mathbf{x} = (\mathbf{E}, \mathbf{H}) \in \mathbb{X}$ such as 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**.

2. Clever choices of **penalization forms combinations** ensure a **strict coercivity**
- Riemann solvers

$$\gamma_t \hat{\mathbf{E}} = \{ \{ \gamma_t \mathbf{E} \} \} - \frac{[[\gamma \times \mathbf{H}]]}{2},$$

$$\gamma \times \hat{\mathbf{H}} = \{ \{ \gamma_t \mathbf{H} \} \} + \frac{[[\gamma_t \mathbf{E}]]}{2},$$

- UWVF methods,
- Upwind schemes.

3. **Consistency**: accuracy of the best approximation is ensured by the choice of \mathbb{X} .
4. Trefftz method is **convergent** and provides **convergence theory for the iterative method** ⁱⁱⁱ.

⇒ **How to construct \mathbb{X} ?**

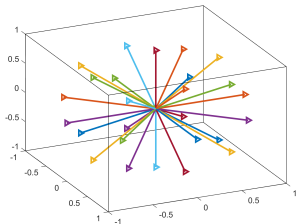
ⁱⁱⁱA. Buffa, P. Monk, Error estimates for the ultra weak variational formulation of the Helmholtz equation, Mathematical Modelling and Numerical Analysis 42 (6) (2008) 925940.

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 ? ⁱ ⁱⁱ
→ Basis reduction strategy

ⁱT. Luostari, T. Huttunen, P. Monk, Improvements for the ultra weak variational formulation, Int. J. Numer. Meth. Engng 94 (2013) 598624.

ⁱⁱS. Congreve, J. Gedicke, I. Perugia, Numerical investigation of the conditioning for plane wave discontinuous Galerkin methods, Vol. 126 of Lecture Notes in Computational Science and Engineering, Springer, 2019.

General matrix shape

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

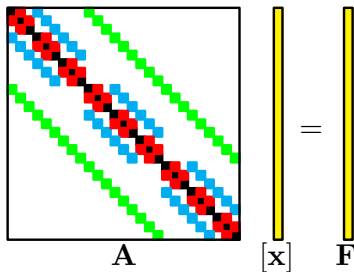
where

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

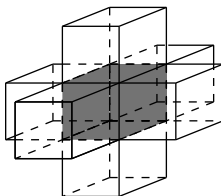
$$\mathbf{F}_i := \mathbf{l}(\mathbf{w}^i) \quad \text{for } i, j = 1, N_{\text{dof}}.$$

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

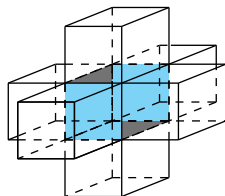
$$\text{size}(\mathbf{A}) = N^2 \times 7 \times N_{\text{elem}}$$



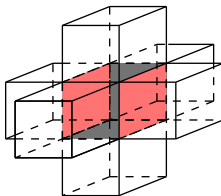
Element assembling of \mathbf{A} for $N_{\text{elem}} = 27 = 3^3$ cubes.



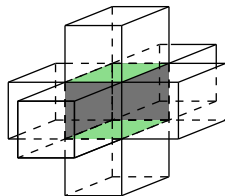
Self-interaction



Front and back interactions

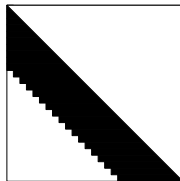
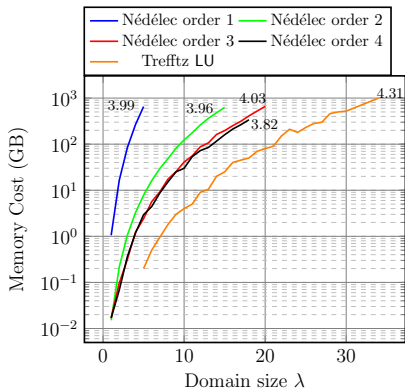


Left and right interactions

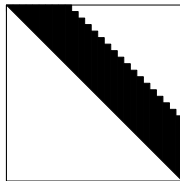


Bottom and top interactions

Memory limit of the direct solver



L



U

Domain size	5λ	10λ	20λ	100λ	200λ
Number of elements N_{elem}	512	1000	8000	10^6	8×10^6
LU memory	268 MB	4.3 GB	69 GB	43 TB	688 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

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

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

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

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

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

Trefftz GMRES method

- **GMRES convergence depends on the spectrum of the matrix A .**

The residual norm of a GMRES solver is given by^{iv}

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

with

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

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

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

We propose strategies to

1. **Remove the spectrum of A from 0.**
2. **Reduce the memory cost of the Trefftz GMRES method.**

^{iv}Saad, Youcef and Schultz, Martin H, GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM, 7, 3, 856–869, 1986

GMRES method with a restart strategy

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

- N_{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_{dof} becomes large, ie when N_{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

- $N_{\text{kry}}^{\text{restart}} = 50$ the dimension of the Krylov space
- N_{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

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

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

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

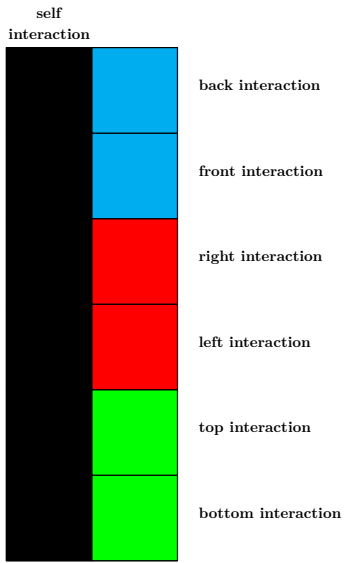
With matrix storage: the blocking structure is N_{elem}

Domain size	5λ	10λ	20λ	100λ	200λ
N_{elem}	512	1000	8000	10^6	8×10^6
With matrix storage	180 MB	344 MB	2.75 GB	344 GB	2.75 TB

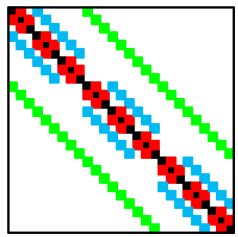
Table: Memory cost for the storage of the matrix **A** in function of the domain size.

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

- $N_{\text{kry}}^{\text{restart}} = 50$ the dimension of the Krylov space
- N_{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

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

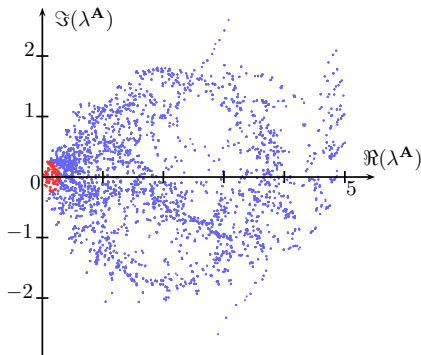
Domain size	5λ	10λ	20λ	100λ	200λ
N_{elem}	512	1000	8000	10^6	8×10^6
With matrix storage	180 MB	344 MB	2.75 GB	344 GB	2.75 TB
Without matrix storage	21.6 MB	41.9 MB	0.33 GB	41.6 GB	332 GB
$\frac{\text{size(interactions)}}{\text{size(Krylov)}}$	0.01	7×10^{-3}	9×10^{-4}	7×10^{-6}	9×10^{-7}

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 $A\#A[x] = A\#F$.

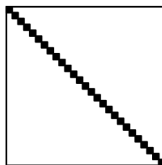


Real and complex parts of the spectrum λ^A of matrix A , for a 6λ domain size.

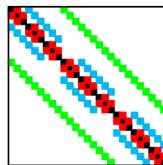
$$A = M - N$$

Cessenat-Després decomposition ^a

M



N



^aO. 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 preconditioner

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

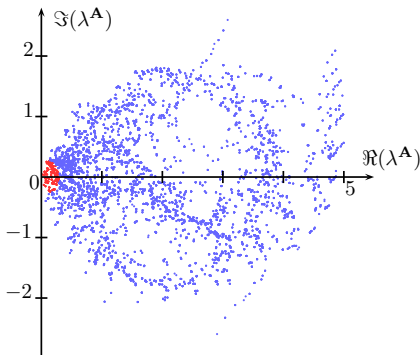
Idea: use a **preconditioned GMRES** method solving $A^\# A[x] = A^\# F$.

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

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

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

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

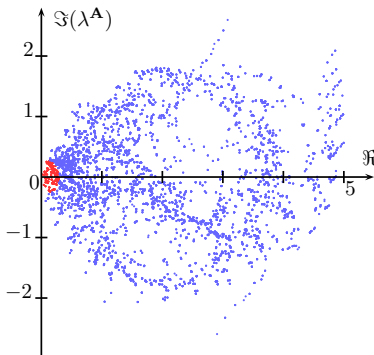


Real and complex parts of the spectrum λ^A of matrix A , for a 6λ domain size.

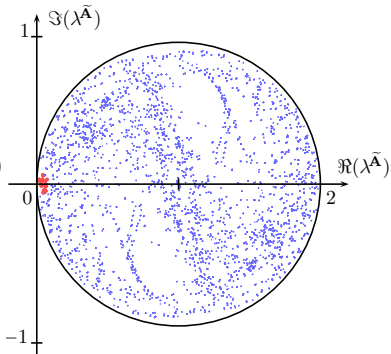
Cessenat-Després preconditioner

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

\tilde{A} is contractant



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



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

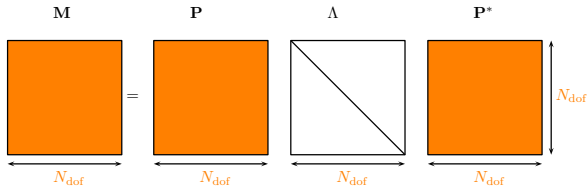
Basis reduction strategy

M is symmetric positive definite

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

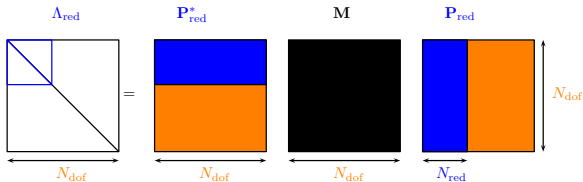
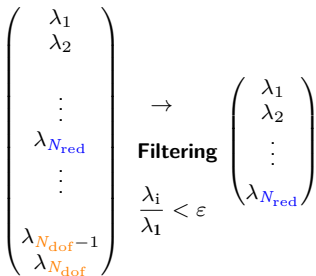
for $i, j = 1, N_{\text{elem}}$

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



P is the orthogonal eigenvector matrix.
Λ is the diagonal eigenvalue matrix satisfying

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



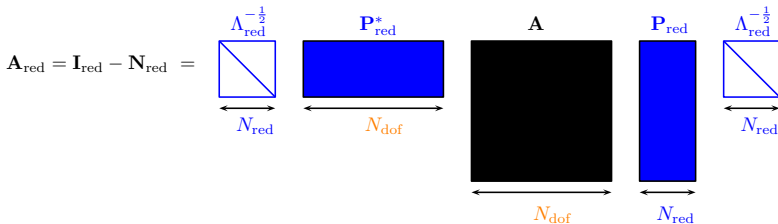
Normalized reduced basis

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 ε well chosen.

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

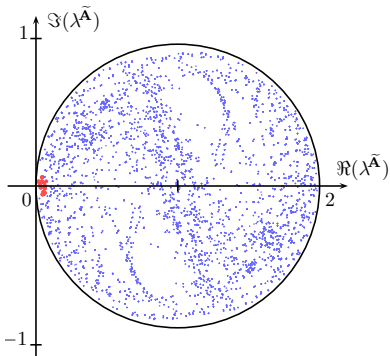


Computation of \mathbf{M}^{-1} is trivial \rightarrow **memory gain**

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

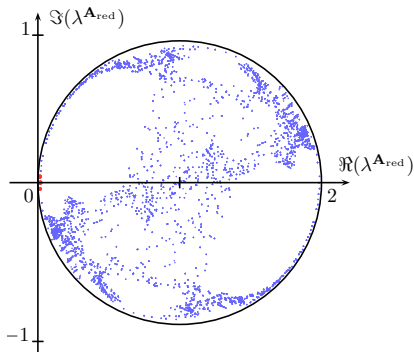
Basis reduction improves matrix conditioning

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



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

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



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

Basis reduction improves memory burden

N_{red} depends on the size of an element K and of the threshold $\lambda_1 \varepsilon$.

$\lambda_1 \varepsilon$ \ Size of K	10^{-13}	10^{-11}	10^{-9}	10^{-7}	10^{-5}	10^{-4}	10^{-3}	10^{-2}
0.25λ	154	126	96	70	48	48	30	24
0.5λ	190	186	174	132	96	84	70	48
1λ	196	196	196	190	180	174	148	114

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

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

10^{-15}	$\lambda_1 \varepsilon$	10^{-13}	10^{-11}	10^{-9}	10^{-7}	10^{-5}	10^{-4}	10^{-3}	10^{-2}
N = 196	N_{red}	154	126	96	70	48	36	30	16
1.57 GB	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}_{red} according to N_{red} , for a 10λ domain size.

GMRES does not converge without reduction → improvement of the conditioning

How far can we reduce the plane wave basis ?

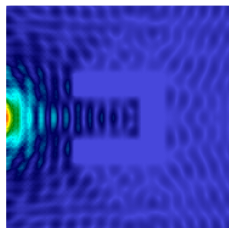
$\lambda_1 \varepsilon$	10^{-7}	10^{-5}	10^{-4}	10^{-3}	10^{-2}
Trefftz error	N/A	3.4×10^{-2}	9.8×10^{-2}	0.15	0.74
Memory cost (GB)	0.56	0.38	0.28	0.24	0.13
Time (hours)	55	27	11.3	7.23	0.58

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 $\lambda_1 \varepsilon$.

GMRES residual = 10^{-8} but poor approximation when $\lambda_1 \varepsilon$ is not well chosen.

Too much reduction

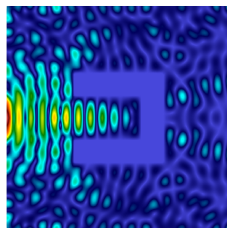
$$N_{\text{red}} = 16 \quad \lambda_1 \varepsilon = 10^{-2}$$



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

A better compromise

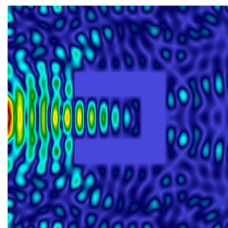
$$N_{\text{red}} = 36 \quad \lambda_1 \varepsilon = 10^{-4}$$



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

Solution of reference

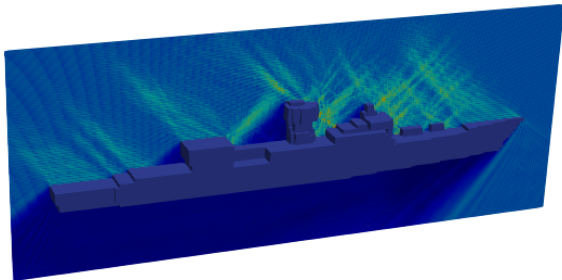
$$N_{\text{red}} = 70 \quad \lambda_1 \varepsilon = 10^{-7}$$



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

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.

#elem	N_{red}	N	$\#\text{dof}_{\text{red}}$	$\#\text{dof}$
$> 14.4 \times 10^6$	46	52	$> 663 \times 10^6$	$> 750 \times 10^6$

GMRES iterations	Memory cost	Total duration	GMRES residual
800	389 GB	28.6 hours	3.8×10^{-2}

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

Thank you for your attention !

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