Trefftz method for three-dimensional electromagnetic wave simulation

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Adimensional Maxwell problem

Studied problem :

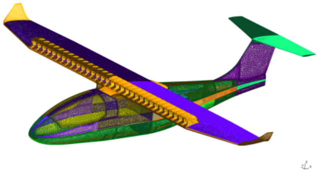
$$\begin{cases} \nabla \times \mathbf{H} & = & ik\mathbf{E} \\ \nabla \times \mathbf{E} & = & -ik\mathbf{H}, \text{ on } \Omega, \end{cases} \tag{1}$$

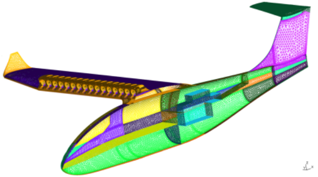
where $\Omega \subset \mathbb{R}^3$ is a connex domain.
For instance, let us consider an electric boundary condition :

$$\gamma_T \mathbf{E} = \mathbf{h} \text{ sur } \partial\Omega, \tag{2}$$

with $\mathbf{h} : \partial\Omega \to \mathbb{C}^3$ a tangent field and $\gamma_T \mathbf{E} = \mathbf{E} - (\mathbf{E} \cdot \mathbf{n}) \cdot \mathbf{n}$.

Objective : computation on very large domains.





Ampere plane geometry (DEMR ONERA).

Context

When does numerical dispersion appear ?

- Large size domain with respect to the wavelength $\Leftrightarrow L >> \lambda$.[a]

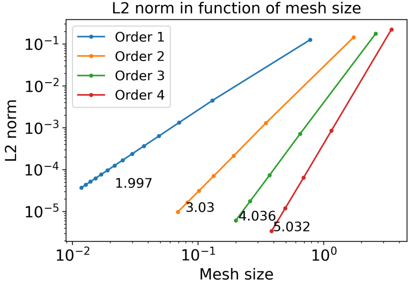
[a] F. Ihlenburg and I. Babuska., SIAM J. Numer. Anal., 1997

What are the existing numerical methods ?

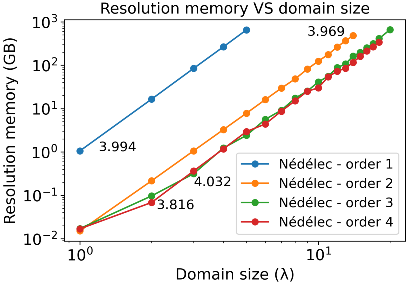
- High order finite elements method
- Discontinuous Galerkin method[a]

[a] M. Ainsworth. Journal of Computational Physics, 198:106–130, 2004.

Memory limits of a classic solver



Convergence of the Nédélec solver in function of the mesh size h.



Memory used by the Nédélec solver in function of the size of the domain.

Nédélec - order 4	Memory	Maximal domain size	Power	Cost
Laptop	32 GB	10λ	200 W	0.02 €/h
Parallel computing	1 TB	24λ	6.4 KW	0.64 €/h
HPC	100 TB	76λ	1 MW	500 €/h

$\rightarrow$ Efficient optimisation cannot overcome the **memory issue**.

$\rightarrow$ Need to develop **low memory cost methods** based on **domain decomposition**.

Trefftz method idea

When does numerical dispersion appear ?

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What are Trefftz method advantages ?

- Non dispersive basis functions[a]
- Adapted to domain decomposition

[a] R. Hiptmair, et al. A survey of trefftz methods. Springer, 2016.

Outline

Trefftz method particularities

1. **Virtual work** principle on an element K :

$$W_K = -ik \int_K \mathbf{E}^K \cdot \overline{\mathbf{E}'^K} + \mathbf{H}^{\mathbf{K}} \cdot \overline{\mathbf{H}'^{\mathbf{K}}} \mathrm{d}K. \tag{3}$$

2. **The solution and the test functions** satisfy Maxwell on each element K,

$$\begin{cases} W_K = -\displaystyle\int_K \underbrace{\nabla \times \mathbf{H}^K}_{ik\mathbf{E}^K} \cdot \overline{\mathbf{E}'^K} - \underbrace{\nabla \times \mathbf{E}^K}_{-ik\mathbf{H}^K} \cdot \overline{\mathbf{H}'^K} \mathrm{d}K, \\ W_K = \displaystyle\int_K \mathbf{E}^K \cdot \underbrace{\overline{\nabla \times \mathbf{H}'^K}}_{ik\mathbf{E}'^K} - \mathbf{H}^K \cdot \underbrace{\overline{\nabla \times \mathbf{E}'^K}}_{-ik\mathbf{H}'^K} \mathrm{d}K. \end{cases} \tag{4}$$

3. A variational formulation is imposed on an element **boundary**,

$$\sum_K \int_{\partial K} \left(\mathbf{n}_K \times \gamma_T \mathbf{H}^K\right) \cdot \gamma_T \overline{\mathbf{E}'^K} + \gamma_T \mathbf{E}^K \cdot \left(\mathbf{n}_K \times \gamma_T \overline{\mathbf{H}'^K}\right) = 0. \tag{5}$$

4. **Reciprocity formula** (5) is penalized by terms ensuring weakly
   - the continuity → Discontinuous Galerkin,
   - the boundary conditions.

Penalization forms

- **Ensure the continuity** of the solution between two elements K and V :

$$\int_{\Gamma_{int}} \underbrace{\left(\gamma_T \mathbf{E}^K - \gamma_T \mathbf{E}^V\right)}_{=0} \cdot \left(\gamma_T \overline{\mathbf{E}'^K} - \gamma_T \overline{\mathbf{E}'^V}\right) = 0, \tag{6}$$

$$\int_{\Gamma_{int}} \underbrace{\left(\gamma_T \mathbf{H}^K - \gamma_T \mathbf{H}^V\right)}_{=0} \cdot \left(\gamma_T \overline{\mathbf{H}'^K} - \gamma_T \overline{\mathbf{H}'^V}\right) = 0, \tag{7}$$

and other terms, with Γ_{int} the interior skeleton of the mesh.

- **Constrain boundary conditions**, on Γ_{ext} the exterior skeleton of the mesh :

$$\int_{\Gamma_{ext}} \underbrace{\left(\gamma_T \mathbf{E}^K - \mathbf{h}\right)}_{=0} \cdot \gamma_T \overline{\mathbf{E}'^K} = 0, \tag{8}$$

and other terms.

Variational formulation

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

$$a(\mathbb{E}, \mathbb{E}') = \ell(\mathbb{E}'),$$

with $\mathbb{X}$ **a discontinuous space of locally 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 provide **convergence theory for the iterative method** [i].

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

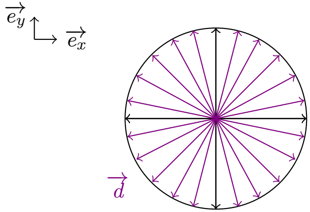
[i] A. Buffa, P. Monk, Error estimates for the ultra weak variational for- mulation of the Helmholtz equation, Mathematical Modelling and Nu- merical Analysis 42 (6) (2008) 925940.

Basis functions space

A scalar plane wave $\overrightarrow{\mathbf{E}} = \overrightarrow{p}\, e^{ik\overrightarrow{d}\cdot\overrightarrow{x}}$ is defined by :

- a direction of propagation $\overrightarrow{d} = (d_x, d_y, 0)$,
- a polarization $\overrightarrow{p} = (p_x, p_y, 0)$ orthogonal to $\overrightarrow{d}$.

2D discrete space



- The numerical wave is :

$$\overrightarrow{\mathbf{E}} = \sum_i u_i \overrightarrow{p}_i e^{ik\overrightarrow{d}_i\cdot\overrightarrow{x}},$$

$$\overrightarrow{\mathbf{H}} = \sum_i u_i \left(\overrightarrow{p}_i \times \overrightarrow{d}_i\right) e^{ik\overrightarrow{d}_i\cdot\overrightarrow{x}}.$$

- What is the optimal number of plane waves ? [i] [ii]

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

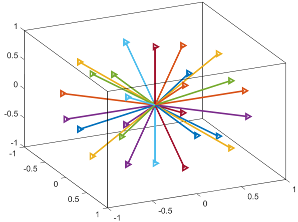
[ii] S. Congreve, J. Gedicke, I. Perugia, Numerical investigation of the conditioning for plane wave discontinuous Galerkin methods, Vol. 126 of Lecture Notes in Computational Science and Engineering, Springer, 2019.

Basis functions space

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

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

3D discrete space



A plane waves basis in a cube.

- The numerical wave is :

$$\overrightarrow{\mathbf{E}} = \sum_i u_i \overrightarrow{p}_i e^{ik\overrightarrow{d}_i\cdot\overrightarrow{x}},$$

$$\overrightarrow{\mathbf{H}} = \sum_i u_i \left(\overrightarrow{p}_i \times \overrightarrow{d}_i\right) e^{ik\overrightarrow{d}_i\cdot\overrightarrow{x}}.$$

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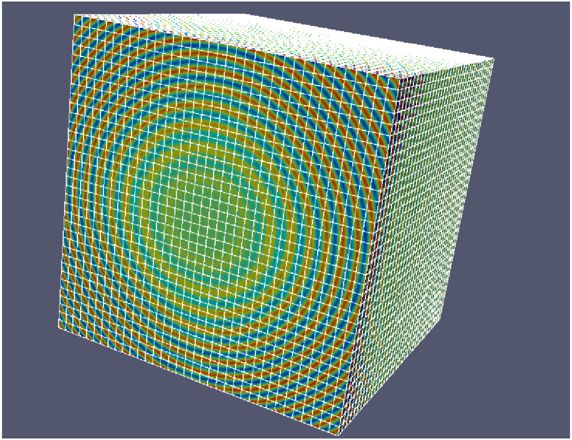
Outline

1. Direct Trefftz method
2. Numerical results
3. Iterative Trefftz method
4. Conclusion

Visualization example on a structured mesh

Domain size : $35\lambda \rightarrow 40000\lambda^3$

Field generated by an harmonic electric dipole situated on the left side of the domain, with 52 plane waves.

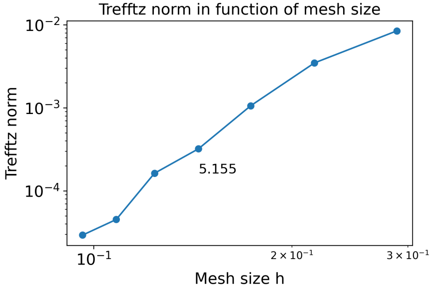


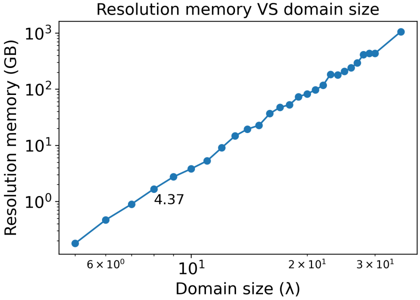
3D vizualisation of the electromagnetic field thanks to Previsio® software.

Memory limit of the direct solver

Trefftz norm definition

$$||\mathbb{E}||_z^2 = \sum_K \int_{\partial K} ||\gamma_t \mathbf{E}||^2 + ||\gamma_\times \mathbf{H}||^2 \qquad (9)$$





- **Up to** 1 **Tera** for a domain size $= \mathbf{35}\lambda$
- **Trefftz method improvment** ✓
  For 400 GB memory cost : $\mathbf{10}\lambda$ **more** than with Nédélec solver
  $\rightarrow$ Development of an **iterative Trefftz method**

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3. Iterative Trefftz method
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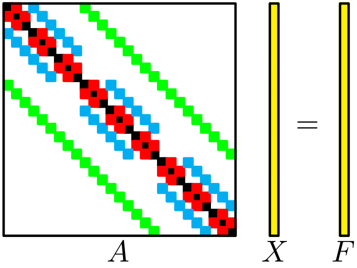
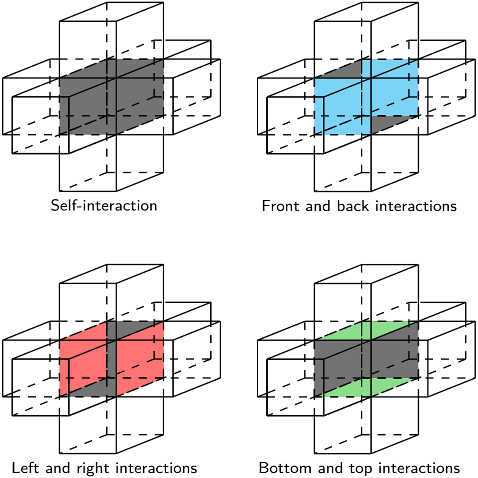
General matrix shape

General problem :

$$AX = F$$



Element assembling of A for $27 = 3^3$ cubes.



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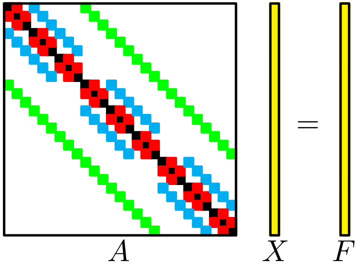
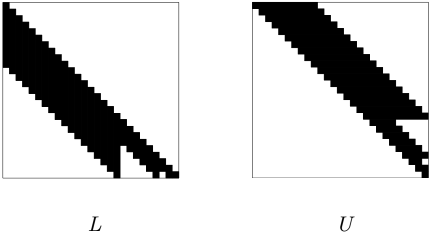


LU factorization :

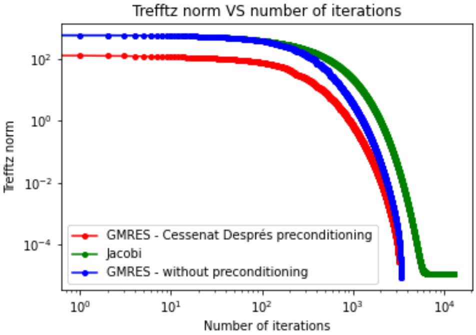


Element assembling of A for $27 = 3^3$ cubes.

Domain size	3λ	5λ	10λ	20λ	100λ
Number of elements	27	512	1000	8000	10^6
LU memory	10 MB	135 MB	4.3 GB	138 GB	432 TB

Iterative Trefftz methods

1. **Picard fixed points** ensure theoretical convergence[ii],
   → for a large number of elements **Jacobi method stagnates in practice**,
2. **GMRES** solver[iii] without preconditionning,
3. **GMRES** solver with Cessenat and Després preconditioning.



- Domain size : 20λ
- Number of elements : $20^3 = 8000$
- GMRES restart : 80
- Reflexion coefficient : 0.9

[ii] O. Cessenat and B. Després, *Application of the ultra-weak variational formulation of elliptic PDEs to the 2-dimensional Helmholtz problem*, SIAM J. Numer. Anal., 35 (1998), pp. 255-299.

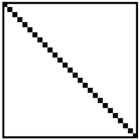
[iii] Y Saad, MH Schultz, *GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems*, SIAM Journal on scientific and statistical computing, 1986 - SIAM.

Domain decomposition

4 matrix decompositions : $A_i\ X = \left(M_i\ + N_i\right) X = F,$

lead to **iterative formulas** $M_i\ X^{n+1} = -N_i\ X^n + F,$ with $X^0 = 0.$

Decomposition 1 *(Cessenat and Després)*



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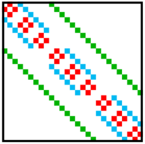
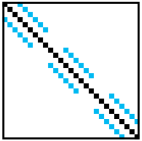


M_1 N_1

Decomposition 3 *(Front and back interactions)*



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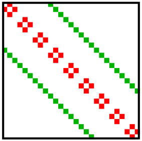
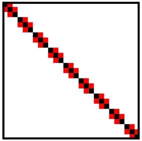


M_3 N_3

Decomposition 2 *(Left and right interactions)*



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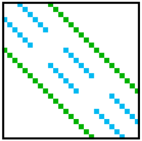
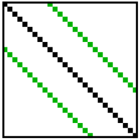


M_2 N_2

Decomposition 4 *(Bottom and top interactions)*



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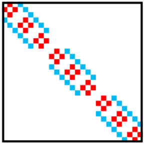

M_4 N_4

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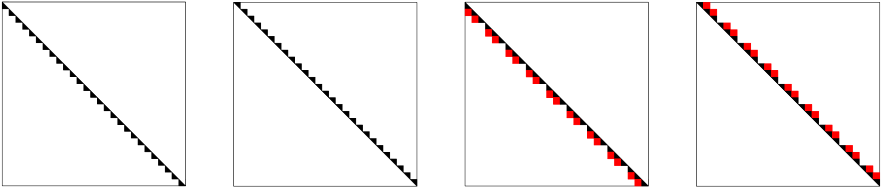
LU for M_1

LU for M_2, M_3, M_4



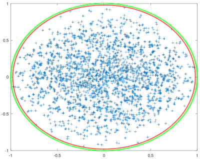
Domain size	3λ	5λ	10λ	20λ	100λ
Number of elements	27	512	1000	8000	10^6
LU memory for A	10 MB	135 MB	4.3 GB	138 GB	432 TB
LU memory for M_1	1 MB	5 MB	43 MB	340 MB	43 GB
LU memory for M_2, M_3, M_4	3 MB	15 MB	129 MB	1.02 GB	129 GB

$\rightarrow$ **Low memory cost with Trefftz decompositions**

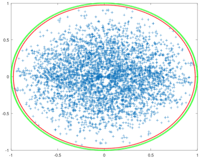
Domain decomposition

4 matrix decompositions : $A_i\ X = \left(M_i\ + N_i\right) X = F,$

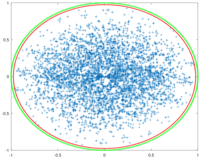
lead to **iterative formulas** $X^{n+1} = -\underbrace{\mathbf{M_i^{-1} N_i}}_{\mathbf{D_i}}\ X^n + M_i^{-1} F,$ with $X^0 = 0.$



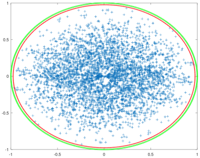
Eigenvalues of D_1



Eigenvalues of D_3



Eigenvalues of D_2



Eigenvalues of D_4

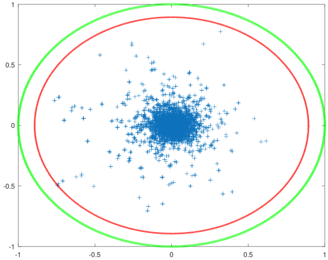
- D_i is **contractant** if its spectral radius $\rho(D_i) < 1$,
- Eigenvalues are close to **unit circle** $\Longrightarrow$ **poor conditioning**.

Domain decomposition

Cyclic decomposition 234 lead to the **iterative formula** :

$$X^{n+1} = -\underbrace{\mathbf{M}_4^{-1}\mathbf{N}_4\ \mathbf{M}_3^{-1}\mathbf{N}_3\ \mathbf{M}_2^{-1}\mathbf{N}_2}_{\mathbf{D}_{234}} X^n + M_4^{-1} N_4\ M_3^{-1} N_3\ M_2^{-1} F - M_4^{-1} N_4\ M_3^{-1} F + M_4^{-1} F$$

$$X^{n+1} = -\underbrace{\mathbf{D}_4\ \mathbf{D}_3\ \mathbf{D}_2}_{\mathbf{D}_{234}} X^n + D_4\ D_3\ M_2^{-1} F - D_4\ M_3^{-1} F + M_4^{-1} F$$

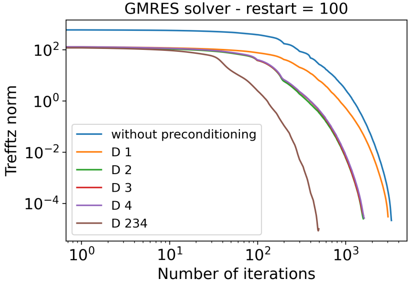


Eigenvalues of $\mathbf{D}_{234}$.

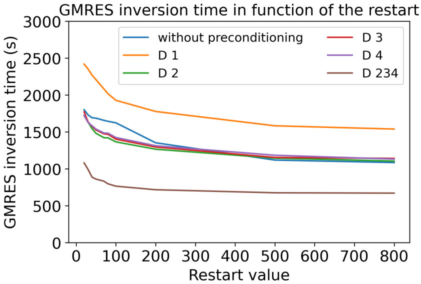
- Eigenvalues become centered around zero $\Longrightarrow$ **better conditioning**.
- Isolated eigenvalues close to unity circle **do not impact GMRES convergence**.

GMRES solver - comparison of strategies

- Number of elements : $20^3 = 8000$
- Reflexion coefficient : 0.9
- Left-preconditioning for decompositions 1, 2, 3, 4 and 234



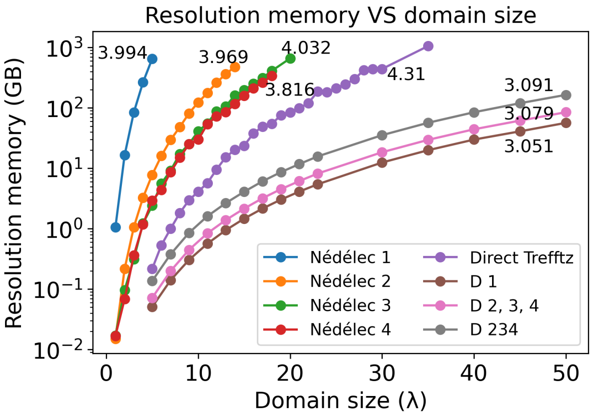
Comparison of decompositions in function of the number of iterations.



Comparison of GMRES inversion time for different sizes of Krylov space.

- 84% **less iterations** with D_{234} than with D_1
- 41% **less seconds** with D_{234} than with D_1

Memory cost for resolution



Memory cost for resolution according to the different methods at 1% precision error.

$\rightarrow$ **Trefftz GMRES solver can simulate electromagnetic waves in large domains.**

Outline

Conclusion

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- **3D Trefftz method** has been developed
- **Domain size up to 50λ** offer good results for homogeneous cases

Perspectives

- Consider different physical cases :
  - **Heterogeneous** cases with **interior domain boundaries**
  - **Trapped modes**
- Deal with **general numerical fluxes** for Trefftz thanks to flexible impedances
- Develop **HPC architecture** to reduce computation time $\rightarrow \mathbf{1000\lambda}$

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.

Contact : margot.sirdey@inria.fr

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Thank you for your attention

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