

A Quasi-Trefftz Method for the Iterative Solution of Time-Harmonic Wave Problems based on the Flux Reconstruction Method

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Context of the work

- Increasing need of 3D simulations of time-harmonic electromagnetic waves:
high-frequency, heterogeneous environments, wide domains (in terms of wavelengths)...

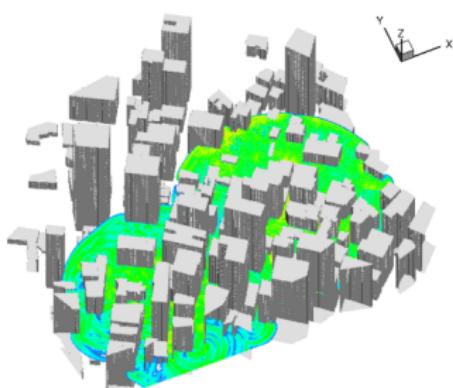


Figure: FDTD simulation on a
Manhattan mesh of $700 \times 600 \times 300$ m,
Thibault Volpert (DEMR ONERA)

Example of computation challenge:
field radiated by two antennas in Manhattan

- Large simulation domain.**
 - Wide range of frequencies (1-18 GHz).**
- ⇒ Need of **efficient methods** to solve such ambitious cases!

Plan of the talk

1. 3D Maxwell: limitations and (quasi-)Trefftz method
2. Quasi-Trefftz numerical analysis
3. Information transfer optimisation

The 3D Maxwell problem in wide domains: current limitations and (quasi-)Trefftz method interests

Current issues: memory and iterative resolution

Time-harmonic Maxwell equations for the electromagnetic field

$\mathbf{Y} := (\mathbf{E}, \mathbf{H}) \in [\mathbf{H}(\mathbf{curl}, \Omega)]^6$:

$$i\kappa \mathbf{M}\mathbf{Y} + \sum_{j=1}^3 \frac{\partial \mathbf{F}^j \mathbf{Y}}{\partial x_j} = \mathbf{0} \text{ in } \Omega, \quad (1)$$

with **impedance Boundary Conditions (BCs)**

$$(\mathbf{n}_{\partial\Omega} \times \mathbf{E}) \times \mathbf{n}_{\partial\Omega} + Z_{\partial\Omega} \mathbf{n}_{\partial\Omega} \times \mathbf{H} = \mathbf{g} \text{ on } \partial\Omega. \quad (2)$$

Current issues: memory and iterative resolution

Many classic methods as Finite Differences [Yee 1966], Finite Elements [Nédélec 1980], Discontinuous Galerkin [Fezoui et al. 2005], but limitations for current applications:

- Wide domains lead to **very large linear systems**.
- Traditional direct solvers induce a **prohibitive memory consumption**.
- Usual numerical methods are **not well adapted to iterative resolution**.

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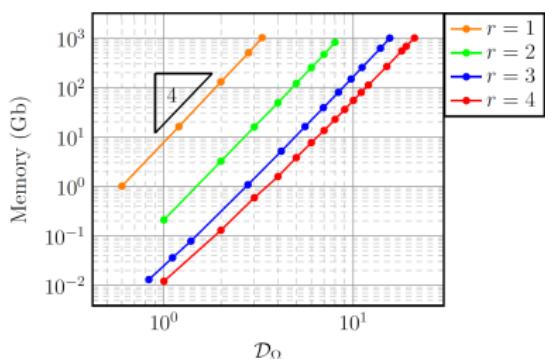


Figure: Memory consumption of a FEM w.r.t. the domain size (in wavelengths) [Sirdey 2022].

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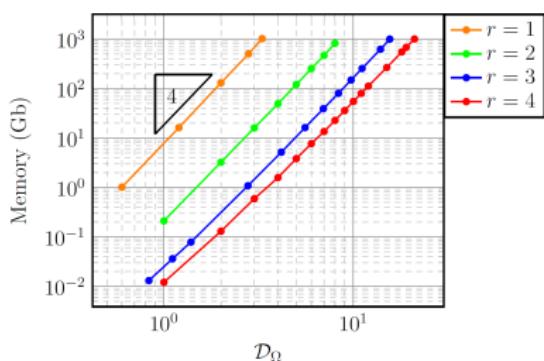


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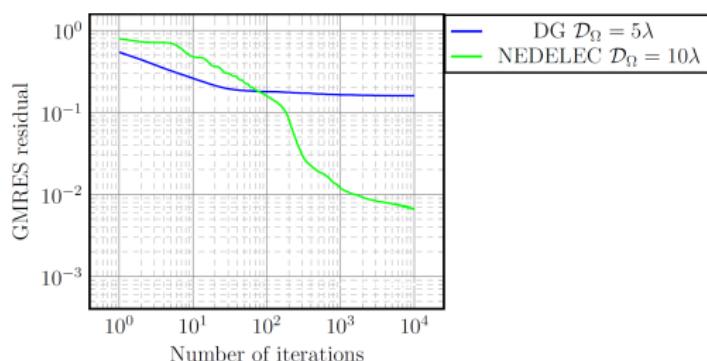


Figure: GMRES convergence of DG and FEM methods [Sirdey 2022].

Considered numerical method: the Trefftz approach

1. Belongs to the Discontinuous Galerkin methods, with the Galerkin space $\mathbb{X} := \prod_{T \in \mathcal{T}_h} \mathbb{X}_T$ made up of **local solutions** (i.e. in each mesh cell $T \in \mathcal{T}_h$) of the Maxwell equations.
2. Use of the **reciprocity formula** verified in each cell

$$\forall T \in \mathcal{T}_h, \int_{\partial T} \gamma_x^T \mathbf{H}^T \cdot \overline{\gamma_t \mathbf{E}'^T} + \gamma_t \mathbf{E}^T \cdot \overline{\gamma_x^T \mathbf{H}'^T} = 0, \quad (3)$$

in addition to the introduction of **numerical traces** [Sirdey 2022]:

Find $\mathbf{Y} = (\mathbf{E}, \mathbf{H}) \in \mathbb{X}$ such that $\forall \mathbf{Y}' = (\mathbf{E}', \mathbf{H}') \in \mathbb{X}$,

$$\sum_{T \in \mathcal{T}_h} \int_{\partial T} \widehat{\gamma_x^T \mathbf{H}^T} \cdot \overline{\gamma_t \mathbf{E}'^T} + \widehat{\gamma_t \mathbf{E}^T} \cdot \overline{\gamma_x^T \mathbf{H}'^T} = \ell(\mathbf{E}'),$$

where $\widehat{\cdot}$ stands for *upwind* (or Riemann) **numerical traces** and with

$$\gamma_t \mathbf{u}^T = \mathbf{u}^T - (\mathbf{u}^T \cdot \mathbf{n}_T) \mathbf{n}_T \text{ and } \gamma_x^T \mathbf{u}^T = \mathbf{n}_T \times \mathbf{u}^T.$$

The Trefftz approach: properties and classic limits

1. The formulation is posed on the **mesh skeleton** and adaptable to an **iterative resolution (contraction property)** [Cessenat, Després 1998].
2. A relevant choice of the numerical traces naturally implies formulation **coercivity**.
3. Basis functions have a **physical meaning**: leads to a **reduced numerical pollution** [Ihlenburg, Babuška 1995].

Limits of the classic **Plane Waves** (PWs) choice:

- Numerical dependence phenomena:
ill-conditioned basis [Congreve et al. 2019].
- **No adaptability of the basis** to the local properties: expected singularities, complex interference phenomena...

⇒ Possible algebraic adaptations [Barucq et al. 2021].

⇒ Introduction of **well-conditioned basis** by parameterising the space of local solutions by **polynomial boundary conditions**.

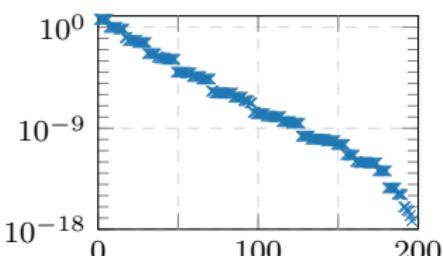


Figure: Eigenvalues of the mass matrix for 196 PWs.

A Quasi-Trefftz approach

Definition of the local problem

A local solution \mathbf{Y}^T in T is parameterised by a tangential field $\mathbf{g}^T \in \mathbb{V}^T$ such that

$$\gamma_t \mathbf{E}^T + Z_{\partial T} \gamma_x^T \mathbf{H}^T = \mathbf{g}^T \text{ on } \partial T. \quad (4)$$

⇒ Consider a finite-dimensional subspace $\mathbb{V}_h^T \subset \mathbb{V}^T$ and the associated Maxwell solutions as local basis [Fure et al. 2020].

Construction of \mathbb{V}_h :

- * Consider a cell $T \in \mathcal{T}_h^T$.
- * Define a mesh of $T(\partial T)$.
- * Consider a piecewise polynomial \mathbf{g}^T of degree k_{QT} on $T(\partial T)$.



Figure: 2D example of the mesh of ∂T for $k_{QT} = 1$.

⇒ Associated Maxwell solutions are unknown: need of an auxiliary solver to compute approximations!

⇒ Other Quasi-Trefftz approaches: generalised PWs [Imbert-Gérard, Després 2013], polynomial Quasi-Trefftz functions [Imbert-Gérard, Sylvand 2023], Embedded Trefftz DG [Lehrenfeld, Stocker 2023], BEM local solver [Barucq et al. 2017]...

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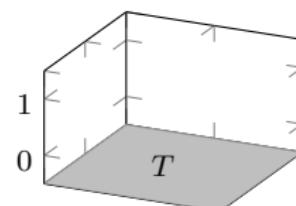


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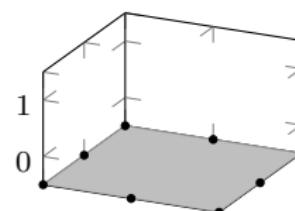


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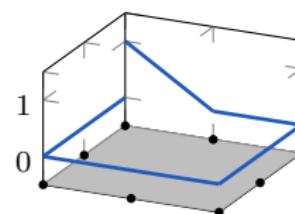


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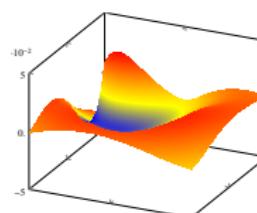


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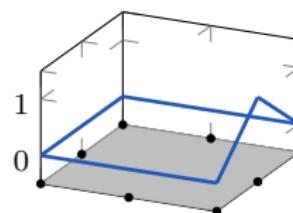


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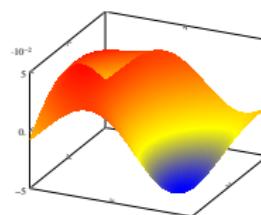


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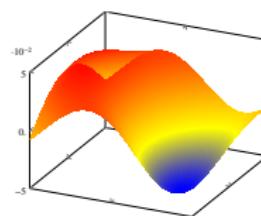


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Description of the FR local solver

Choice of the local solver: **the Flux Reconstruction method** [Huynh 2007]

- Based on the **first-order strong formulation** (solves both \mathbf{E} and \mathbf{H}): no dependence on a quadrature rule.
- Idea: copy the **strong equation in each cell** of the mesh, which is solved on **piecewise polynomials**: the flux is corrected at interfaces thanks to **numerical traces** and **correction polynomial functions**.

$$i\kappa \mathbf{y} + \frac{d\phi}{dx} = \mathbf{0} \text{ with } \phi = \mathcal{F}(\mathbf{y}) \implies \forall n \in \llbracket 1, N \rrbracket, i\kappa \mathbf{y}_h + \frac{d\tilde{\phi}_h}{dx} = \mathbf{0} \text{ in } [X_{n-1}, X_n].$$

- Natural **high-order** method and **adaptable to unstructured meshes**.
 - Choice of correction polynomials allows to **retrieve usual methods**: nodal DG (for Radau polynomials), Spectral Differences (for Lagrange polynomials)...
 - Choice of the correction polynomials to the user: possibility to **optimise them for wave propagation problems**, especially in pre-asymptotic regime [Rivet, Pernet, Tordeux 2024].
 - For identical cells, the **inversion has to be realised only once!**
- ⇒ **Any numerical method, solving the first-order system, may be used!**

A quasi-Trefftz approach based on a Flux Reconstruction auxiliary solver: numerical analysis

Summary of this Quasi-Trefftz approach

Variational formulation posed on $\mathbb{X} := \prod_{T \in \mathcal{T}_h} \mathbb{X}_T$ made up of local solutions.



Functions $(\mathbf{E}^T, \mathbf{H}^T)$ of \mathbb{X}_T parameterised by $\mathbf{g}^T \in \mathbb{V}^T$ such that:

$$\gamma_t \mathbf{E}^T + Z_{\partial T} \gamma_{\mathbb{X}}^T \mathbf{H}^T = \mathbf{g}^T \text{ on } \partial T. \quad (5)$$



Polynomial approximation of the trace space: $\mathbb{V}_h^T = \text{span}(\mathbf{g}_i^T)$.
For all i , the associated solutions $(\mathbf{E}_i^T, \mathbf{H}_i^T)$ are taken as basis functions of \mathbb{X}_T .



FR auxiliary solver to compute an approximation of $(\mathbf{E}_i^T, \mathbf{H}_i^T)$.

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Numerical experiments: basis quality

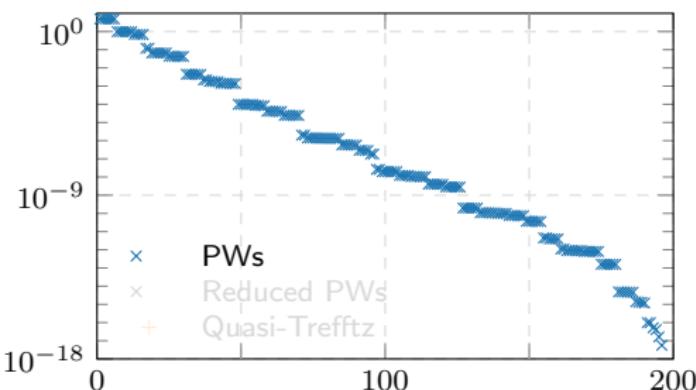


Figure: Eigenvalues of the mass matrix for 196 PWs (and reduction for $\epsilon = 10^{-6}$) and 192 Quasi-Trefftz basis functions.

Basis quality

- ⇒ Possible reduction techniques to restore the condition number.
- ⇒ Avoids spurious numerical modes and ill-conditioning of the mass matrix!

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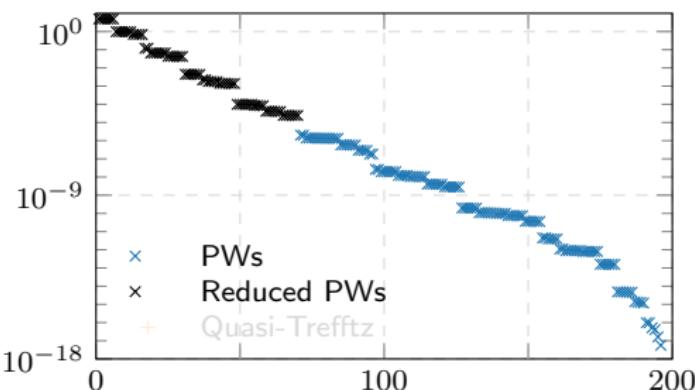


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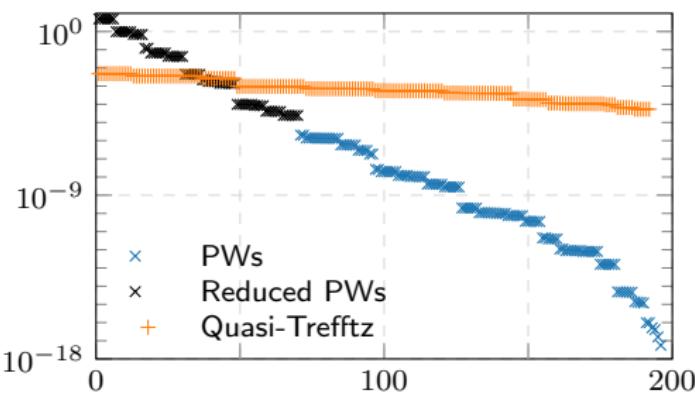


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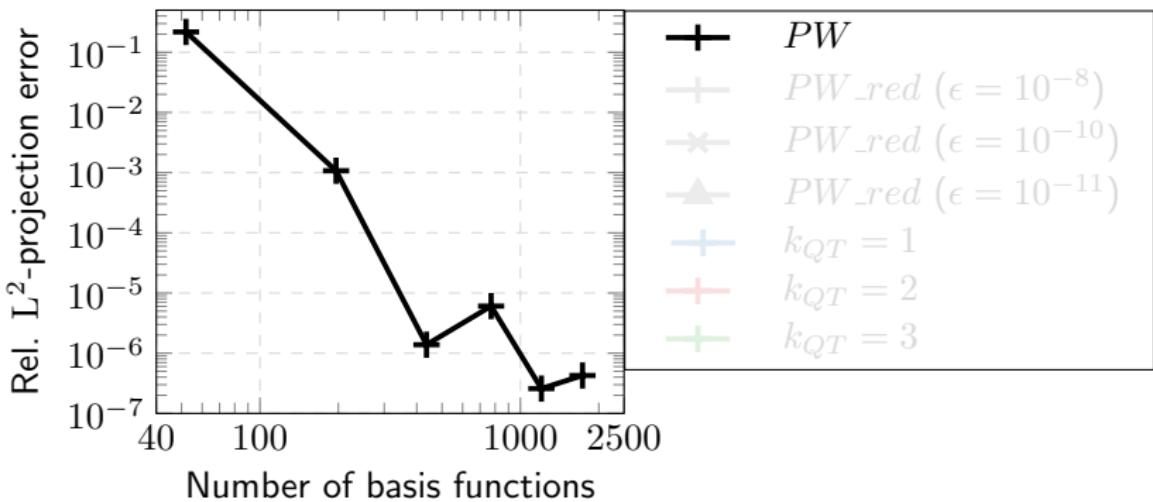


Figure: Projection error on the different basis for a sum of random PWs.

⇒ **Saturation phenomenon due to condition number.**

⇒ Reduction techniques avoid conditioning issues, but locked convergence because of rounding pollution error for an asked threshold.

⇒ Robust approximation by FR basis.

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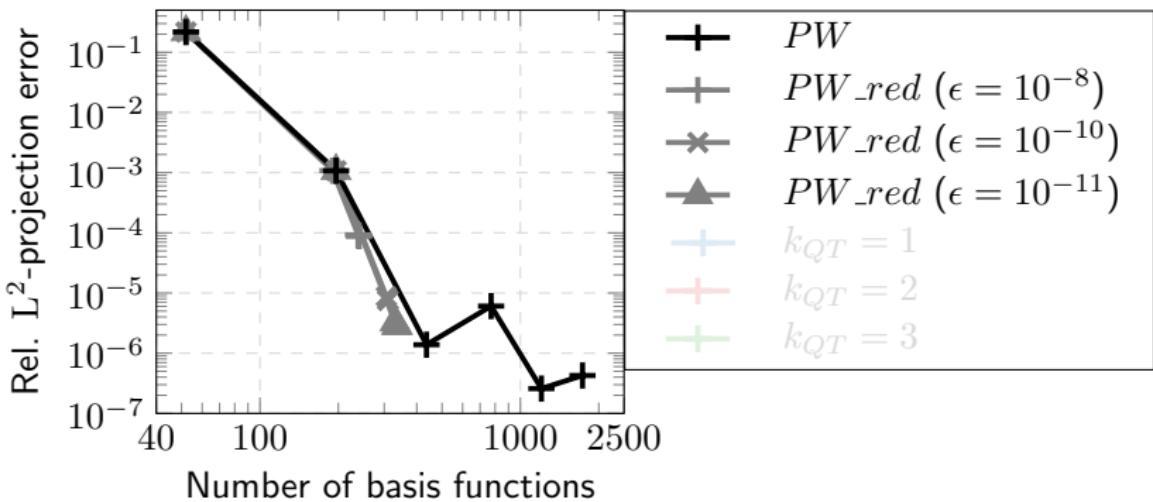


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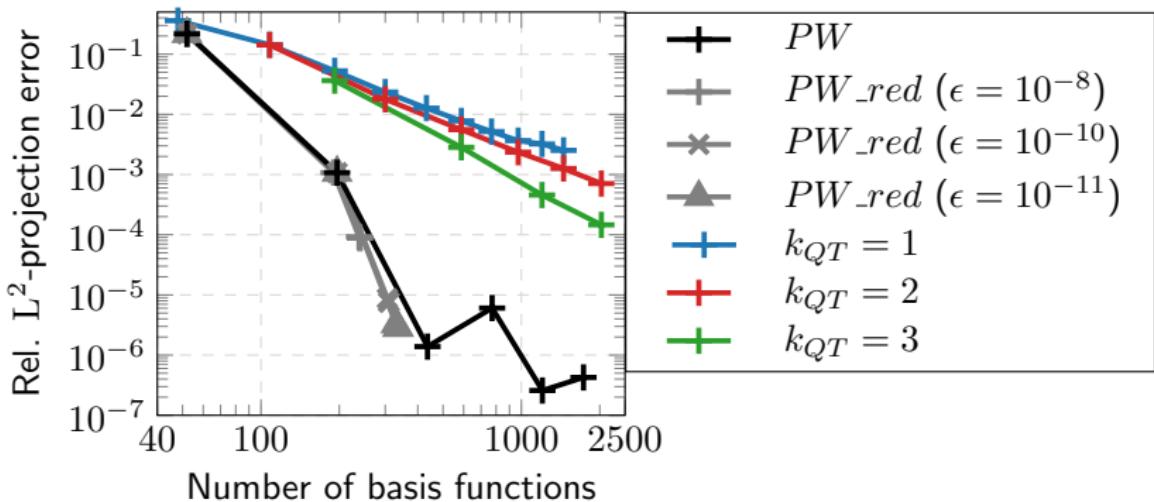


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Approximation properties of the basis for a 'non-smooth' solution: sum of random dipoles

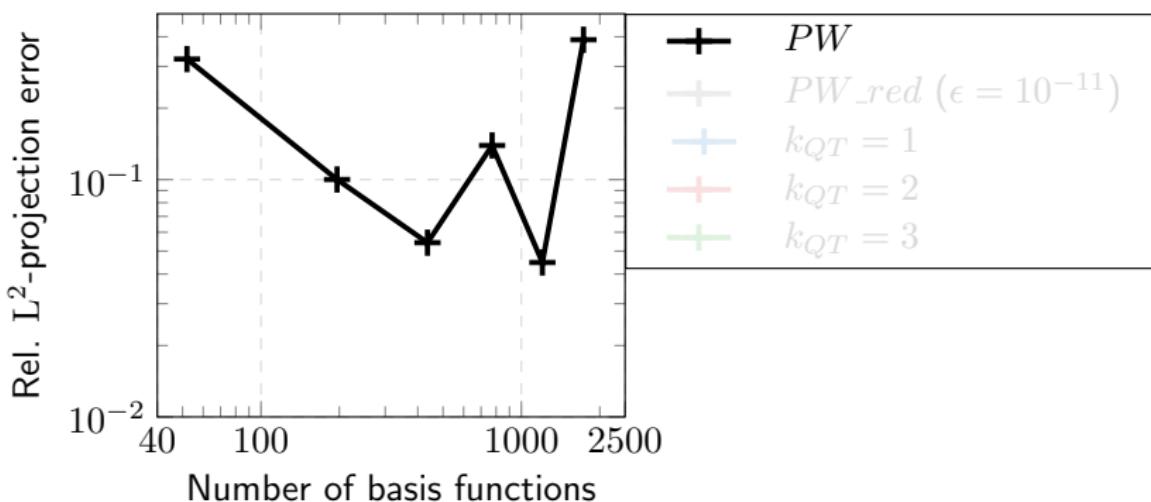


Figure: Projection error on the different basis for a sum of random dipoles.

⇒ **Saturation phenomenon** due to condition number: **difficult representation of complex local solutions with PWs.**

⇒ Reduction techniques avoid conditioning issues, but **locked convergence** because of rounding pollution error for an **asked threshold**.

⇒ Robust approximation by FR basis.

Approximation properties of the basis for a 'non-smooth' solution: sum of random dipoles

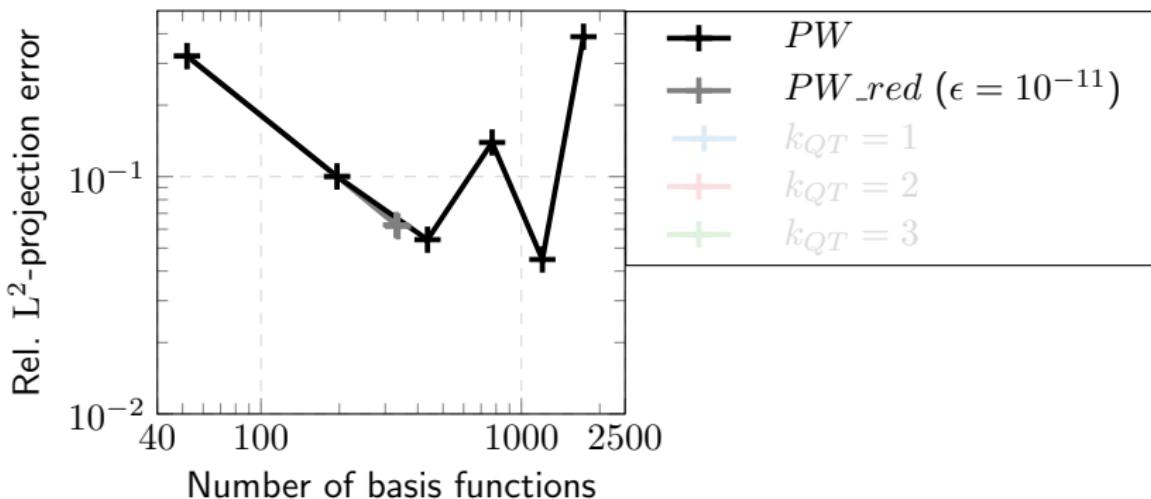


Figure: Projection error on the different basis for a sum of random dipoles.

⇒ **Saturation phenomenon** due to condition number: **difficult representation of complex local solutions with PWs.**

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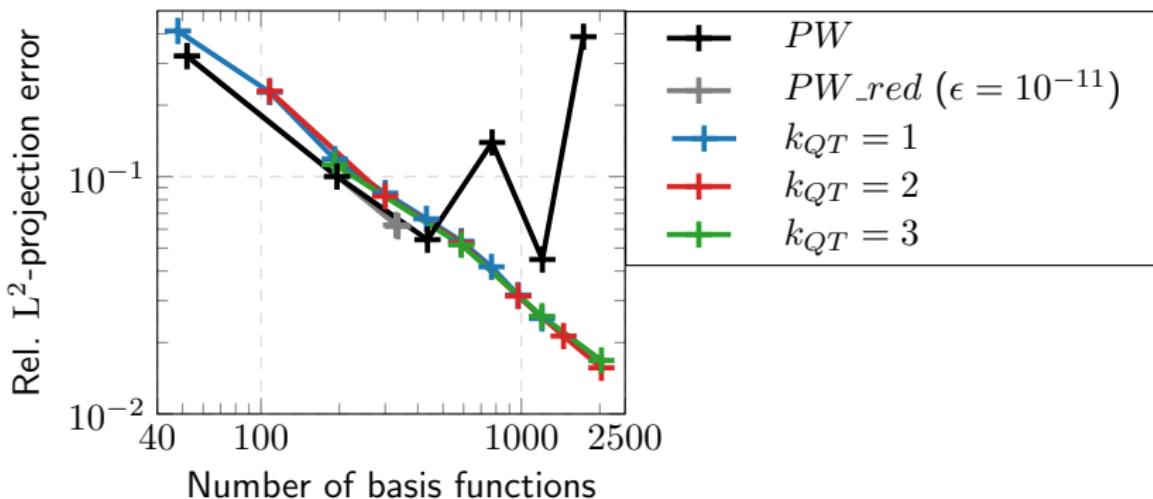


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Recovery of the Trefftz properties under local solver convergence

Trefftz approach rests on the use of **exact solutions** of the Maxwell equations:

Is using quasi-solutions enough?

Quasi-Trefftz properties at convergence

Hypothesis : the local solver verifies the **convergence property** for
 $\gamma_T \mathbf{E}^T + Z_{\partial T} \gamma_X^T \mathbf{H}^T = g^T$ on ∂T :

$$\|\gamma_T(\mathbf{E}^T - \mathbf{E}_h^T)\|_{L^2(\partial T)} + \|\gamma_X^T(\mathbf{H}^T - \mathbf{H}_h^T)\|_{L^2(\partial T)} \leq \varepsilon_{ls}^T \|\mathbf{g}^T\|_{L^2(\partial T)} \text{ with } \varepsilon_{ls}^T \rightarrow 0,$$

when the local solver mesh is refined.

If the local solver mesh is sufficiently refined, the quasi-Trefftz formulation verifies the

- weak-coercivity,
- contraction properties,

of the original Trefftz formulation.

Calibration of the FR auxiliary solver

Trefftz approach rests on the use of **exact solutions** of the Maxwell equations:

Is using quasi-solutions enough?
How to adapt the FR order to the Trefftz one?

- Uniform Cartesian mesh $\mathcal{T}_H(\Omega)$ of the domain Ω : N macro-cells per direction.
- Uniform Cartesian mesh $\mathcal{T}_h(\partial T)$ of ∂T : M micro-faces per direction.
- Piecewise polynomial BCs of degree $k_{QT} = 1$.



Figure: Mesh $\mathcal{T}_H(\Omega)$ for $N = 3$.



Figure: Mesh $\mathcal{T}_h(\partial T)$ for $M = 2$ and $k_{QT} = 1$.

⇒ No theoretical *a priori* error estimates in $L^2(\Omega)$ -norm: **numerical convergence in mesh and number of basis functions** [Fure et al. 2020].

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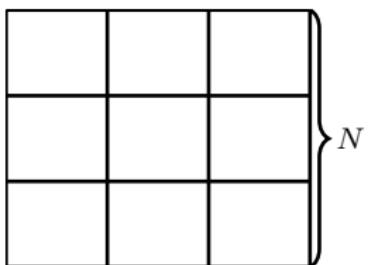


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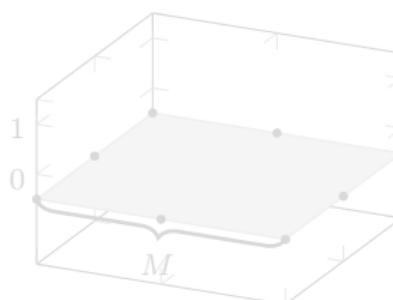


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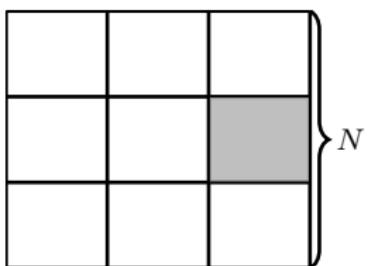


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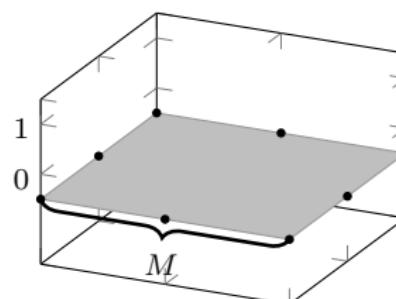


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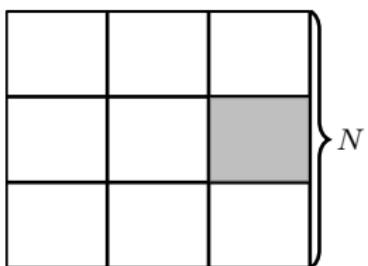


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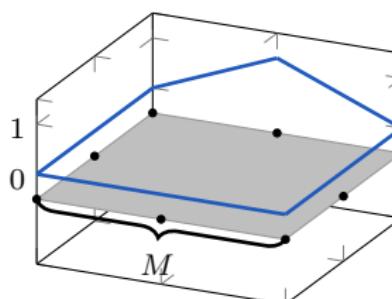


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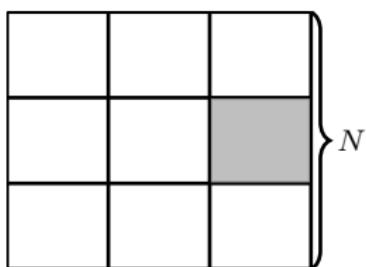


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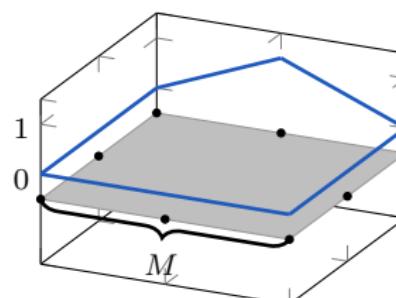


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Calibration of the FR auxiliary solver (2D Helmholtz)

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⇒ Mesh-convergence: refinement of the macro-mesh $\mathcal{T}_H(\Omega)$ for $M = 2$.

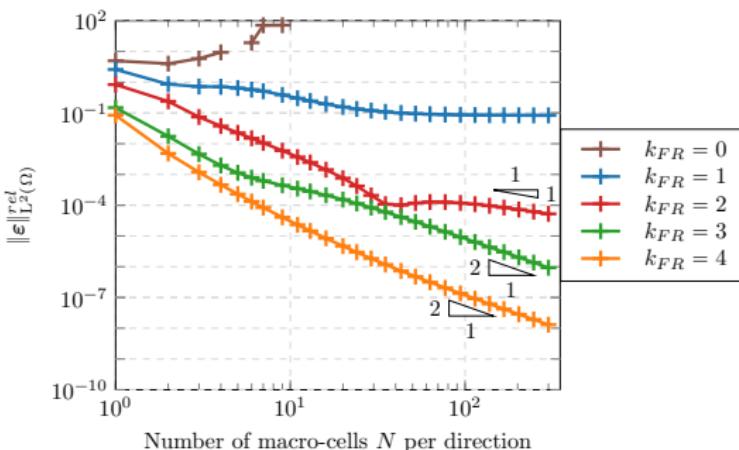


Figure: Evolution of the error for 1 nano-cell per micro-face.

Influence of the local solver precision (through the number of nano-cells):

- Regime 1 ('imperfect' local solver): quasi-optimal for $k_{FR} \geq k_{QT} + 2$ and the higher the order and the more refined the nano-mesh is, the later the transition.
- Regime 2 ('perfect' local solver): common super-convergence for $k_{FR} \geq k_{QT} + 1$.

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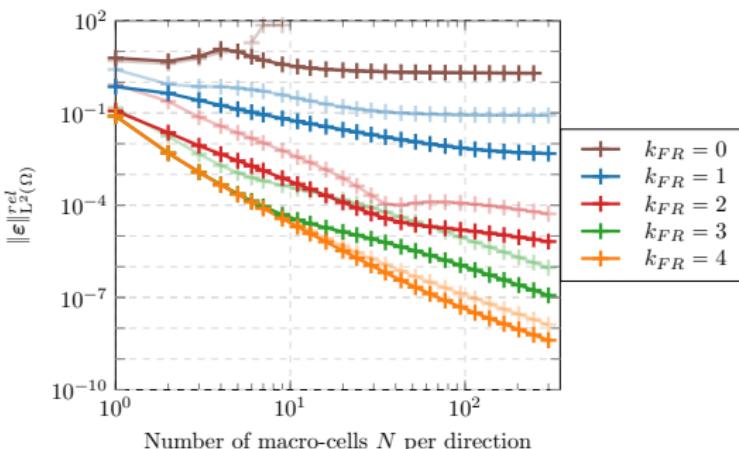


Figure: Evolution of the error for 2 nano-cells per micro-face.

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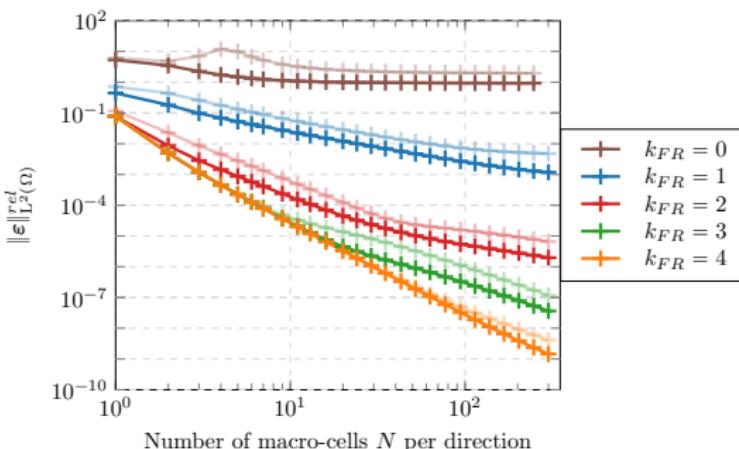


Figure: Evolution of the error for 3 nano-cells per micro-face.

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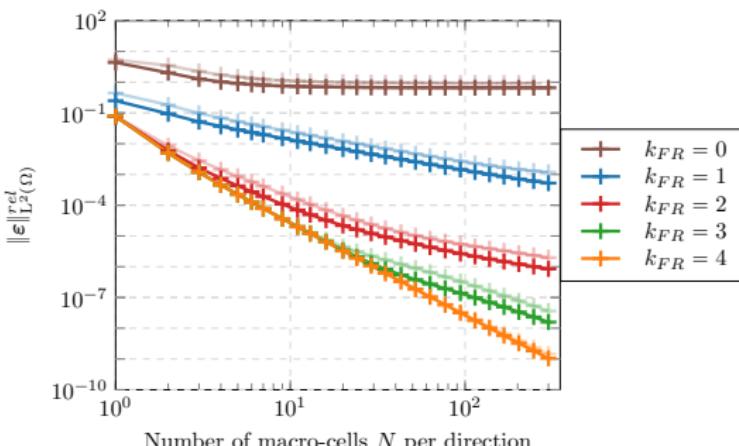


Figure: Evolution of the error for 4 nano-cells per micro-face.

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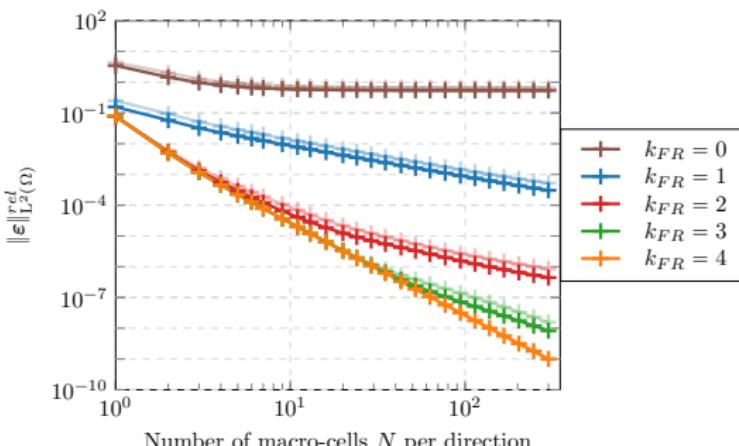


Figure: Evolution of the error for 5 nano-cells per micro-face.

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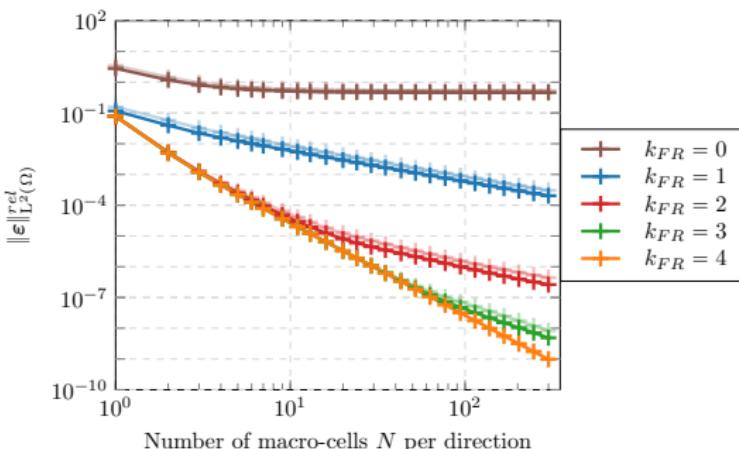


Figure: Evolution of the error for 6 nano-cells per micro-face.

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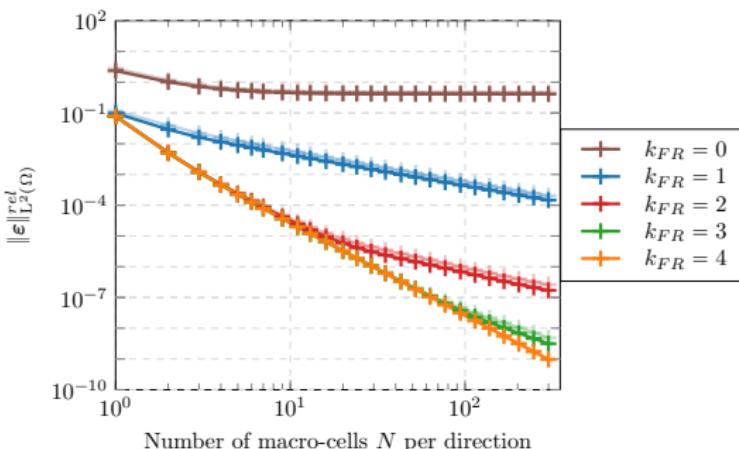


Figure: Evolution of the error for 7 nano-cells per micro-face.

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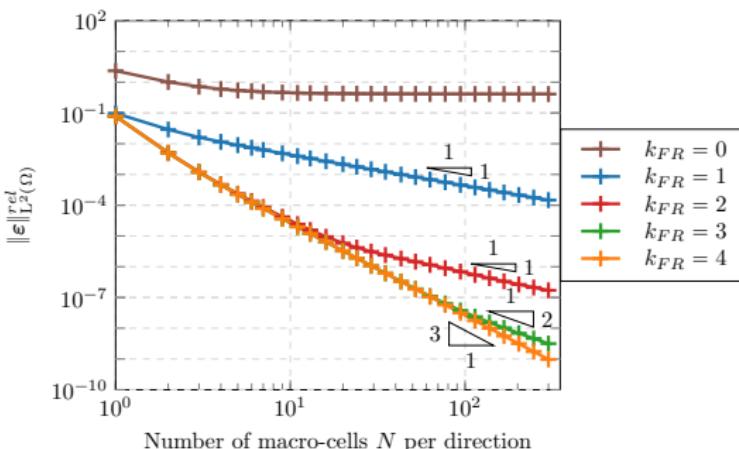


Figure: Evolution of the error for 7 nano-cells per micro-face.

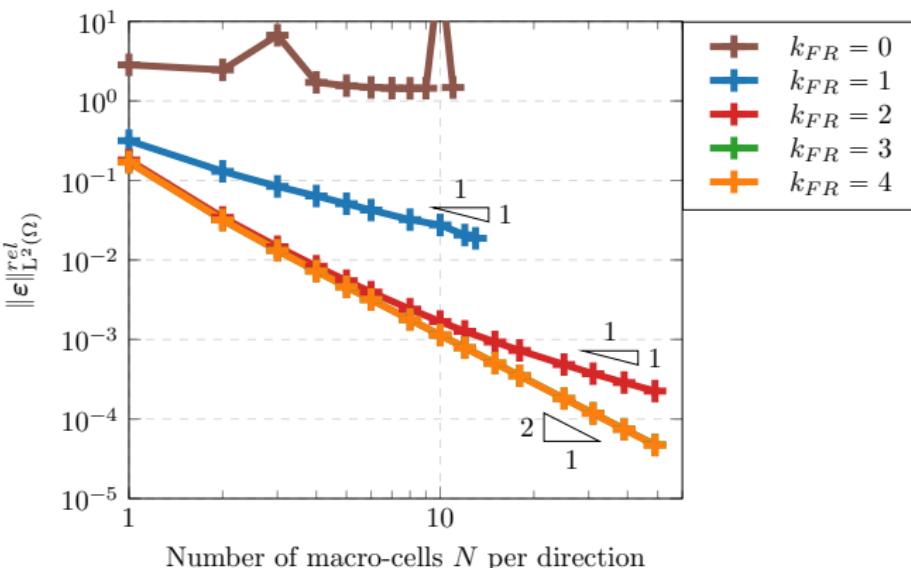
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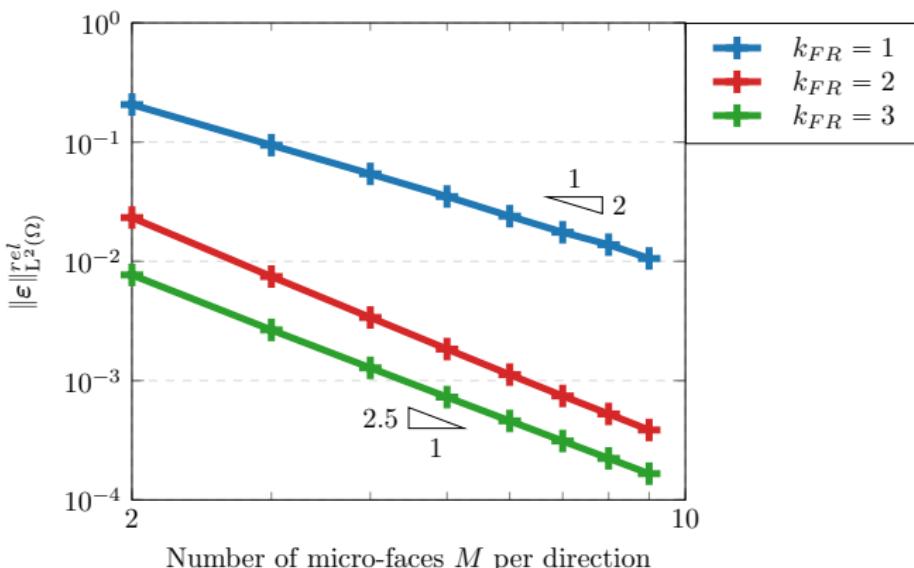
- Need of $k_{FR} \geq k_{QT} + 2$ for quasi-optimal orders, but no interest in over-resolving!

Numerical experiments: convergence in the number of basis functions

Is using quasi-solutions enough?

How to adapt the FR order to the Trefftz one?

⇒ Local basis enrichment through refinement of the micro-mesh $\mathcal{T}_h(\partial T)$ for $N = 2$.



- Need of $k_{FR} \geq k_{QT}$ to be sufficiently 'quasi-solution'.
- Improvement for $k_{FR} \geq k_{QT} + 1$, but limited interest in over-resolving!

Conclusions on the quasi-Trefftz approach

- Classic numerical schemes are **not well adapted to wide domain simulations**, contrary to the **Trefftz method**.
- The classic choice of **Plane Waves** leads to limitations: we introduce a **Quasi-Trefftz approach**, in which a FR solver computes approximate Maxwell solutions associated to polynomial BCs in each cell.
- Good numerical **independence properties** of the basis functions.
- **Robust approximation** properties of the basis, even for complex local solutions.
- Numerical calibration of the local solver: $k_{FR} \geq k_{QT} + 2$ for **asymptotic quasi-optimality**, but **no need to over-resolve!**
- **2 convergence regimes** according to the local solver resolution: **as refined as possible!**

Improvement of the transfer of information: DtN approximation and local optimisation

Problematic: reduce the number of iterations to convergence

Iterative solution of the linear system thanks to a Krylov method, as GMRES:
improving the information transfer would allow to **reduce the number of iterations to convergence**.

(i) Solution evolution

(ii) Solution modification

Figure: Iterative convergence: information propagation through iterations.

Trefftz formulation generalisation

Principle of the proposed generalisation for the 2D Helmholtz equation:

- Introduction of the **outgoing trace** from a cell T ($\mathcal{O}^T = i\kappa Id$ classically) :

$$\gamma_{out}^T \mathbf{y}^T = -v^T + \mathcal{O}^T(u^T) \quad \text{avec} \quad v^T = \frac{\kappa}{\kappa_T} \partial_{\mathbf{n}_T} u^T.$$

- **Consistent numerical traces** \widehat{u} and $\widehat{v^T}$ defined from $\gamma_{out}^T \mathbf{y}^T$ and $\gamma_{out}^K \mathbf{y}^K$.

⇒ Need to have \mathcal{O}^T in a **set of operators \mathcal{C} which ensures the formulation conserves classic properties** (coercivity and contraction):

$$\mathcal{C} \subset \{\mathcal{O}, \text{ there exists a definite linear operator } \Lambda, \mathcal{O} = i\Lambda\Lambda^* \text{ for each face}\}.$$

Approximation of the Dirichlet-to-Neumann operator

Trefftz method can be seen as the variational formulation of

$$v^T + \mathcal{O}^K(u^T) = -v^K + \mathcal{O}^K(u^K) \quad \text{on} \quad \partial T \cap \partial K.$$

The theory of Domain Decomposition Methods (DDM) ensures the **optimal** operator \mathcal{O}^T is the **exterior Dirichlet-to-Neumann** (DtN) one.

3 approximation types :

- Exact operator for classic outgoing waves with respect to the cell centre \mathbf{x}_0 :

$$\mathcal{O}^T = i\kappa \mathbf{d} \cdot \mathbf{n}_{\partial\Omega} \quad (\text{directive PWs}) \quad \text{and} \quad \mathcal{O}^T = -\kappa \frac{H_1^{(1)}(\kappa r)}{H_0^{(1)}(\kappa r)} \quad (\text{Green kernel}),$$

for $\mathbf{d} = (\mathbf{x} - \mathbf{x}_0)/r$ and $r = |\mathbf{x} - \mathbf{x}_0|$.

- Operator with same principal symbol as the classic approximation [El Bouajaji et al. 2014]

$$\mathcal{O}^T = i\kappa \sqrt{Id + \frac{\Delta_F}{\kappa^2}},$$

as Padé-type approximations [Després et al. 2021]

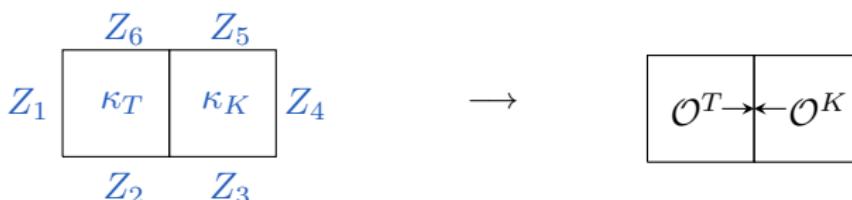
$$\mathcal{O}^T = i\kappa \left(Id - \frac{\Delta_F}{2\kappa^2} \right)^{-1}.$$

→ Face point of view: BCs for the Laplace-Beltrami operator?

- Approximation thanks to **neural networks** (NN): allows to enforce $\mathcal{O}^T \in \mathcal{C}$.

Local optimisation

Being given **local parameters P** , we want to **optimise** the operators \mathcal{O}^T and \mathcal{O}^K with respect to an **information transfer measure ρ_P** .



$$\mathcal{O}_P^{T,*}, \mathcal{O}_P^{K,*} = \underset{\mathcal{O}^T, \mathcal{O}^K \in \mathcal{C}}{\operatorname{argmin}} \rho_P(\mathcal{O}^T, \mathcal{O}^K).$$

Different problematics:

- Size of the local parameters P .
- Possibility to develop **interpolation approximations** of ρ_P for efficient optimisation.
- Which measure ρ_P ?
 - Reduce the distance of the eigenvalues to 1 (fixed point vision).
 - Increase the distance of the eigenvalues to 0 (GMRES point of view).
- Does local optimisation lead to a similar behaviour at the global level?

Preliminary results and conclusion

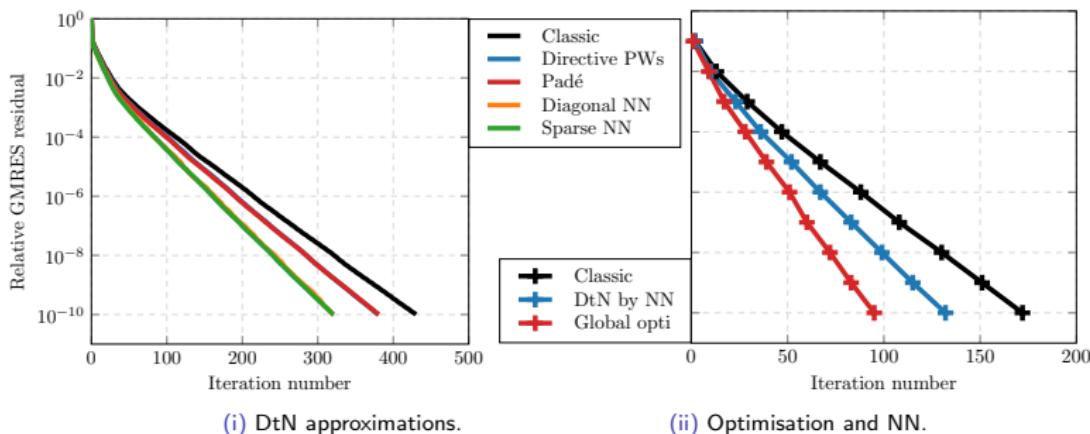


Figure: GMRES convergence for different generalisations: analytic, NN-based and optimisation-based.

- We proposed a generalisation of the Trefftz method, thanks to **general numerical fluxes** **keeping the original properties of the classic formulation**.
- Trefftz approach can be interpreted as a DDM one: we introduced **approximations of the Dirichlet-to-Neumann operator**, which is supposed to be optimal.
- Introduction of **local optimisation problems** for the operators, depending on the surrounding parameters.
- Promising preliminary results to reduce the number of iterations to convergence: **about 25% reduction by using NNs**.

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