A Quasi-Trefftz Method Based on a Flux Reconstruction Local Solver for the Time-Harmonic Maxwell System

Sébastien Pernet[1], Matthias Rivet[1,2], Sébastien Tordeux[2]

[1] DTIS, ONERA, Université de Toulouse, 31000, Toulouse, France
[2] EPI Makutu, INRIA, Université de Pau et des Pays de l'Adour, TotalEnergies, CNRS UMR 5142

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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)...

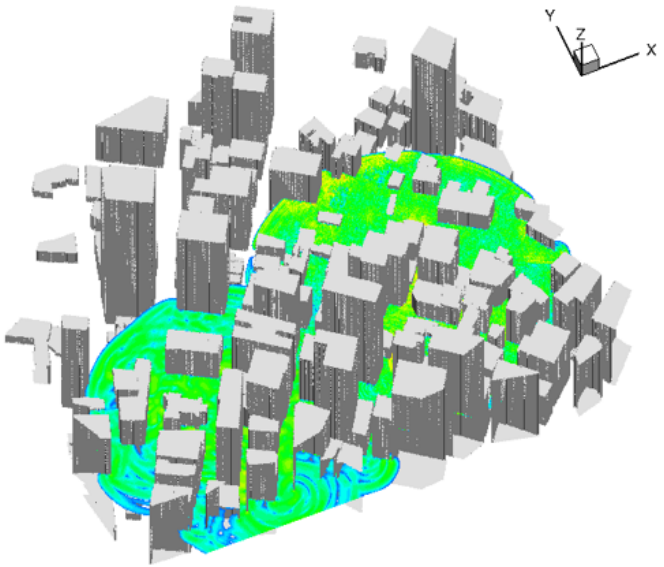

Figure: FDTD simulation on a Manhattan mesh of $700 \times 600 \times 300$m, Thibault Volpert (DEMR ONERA)

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

- **Large simulation domain**.
- **Wide range of frequencies** (1-18 GHz).

$\Longrightarrow$ Need of efficient methods to solve such ambitious cases!

Plan of the talk

1. 3D Maxwell: limitations and Trefftz method

2. FR for wave propagation problems

3. Quasi-Trefftz numerical analysis

The 3D Maxwell problem: current limitations and Trefftz method interests

Current issues: memory and iterative resolution

Time-harmonic Maxwell equations for the electromagnetic field $\mathbf{Y} := (\mathbf{E}, \mathbf{H}) \in [\mathrm{H}(\mathrm{curl}, \Omega)]^6$:

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

with impedance Boundary Conditions (BCs)

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

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**.

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

$$\forall\, T \in \mathcal{T}_h,\ \int_{\partial T} \gamma_\times^T \mathbf{H}^T \cdot \overline{\gamma_t \mathbf{E}'^T} + \gamma_t \mathbf{E}^T \cdot \overline{\gamma_\times^T \mathbf{H}'^T} = 0, \tag{3}$$

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

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

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

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

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

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...

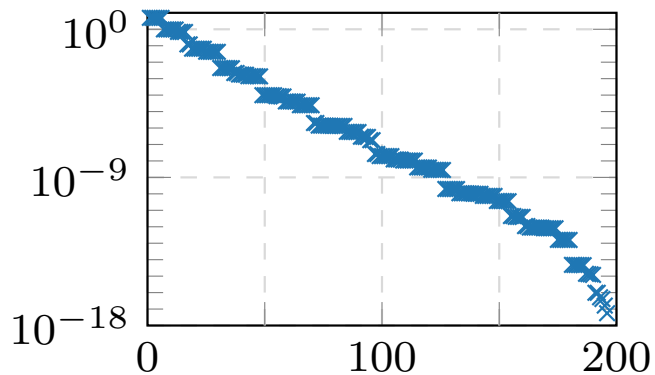

Figure: Eigenvalues of the mass matrix for 196 PWs.

$\Longrightarrow$ Possible algebraic adaptations [Barucq et al. 2021].

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

A Quasi-Trefftz approach

Definition of the local problem

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

$$\gamma_t \mathbf{E}^T + Z_{\partial T}\, \gamma_\times^T \mathbf{H}^T = \mathbf{g}^T \text{ on } \partial T. \tag{4}$$

$\Longrightarrow$ Consider a finite-dimensional subspace $\mathbb{V}_h \subset \mathbb{V}$ and the associated Maxwell solutions [Fure et al. 2020].

Construction of $\mathbb{V}_h$:

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

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

$\Longrightarrow$ **Associated Maxwell solutions are unknown**: need of an auxiliary solver to compute approximations!

$\Longrightarrow$ **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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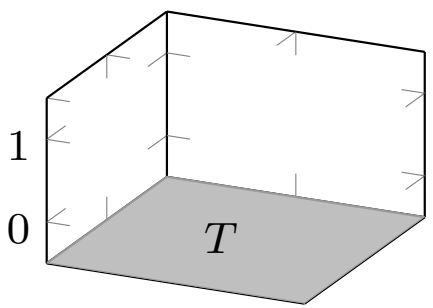

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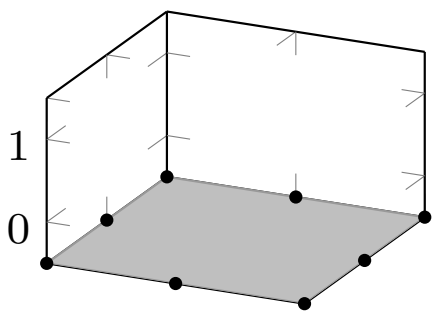

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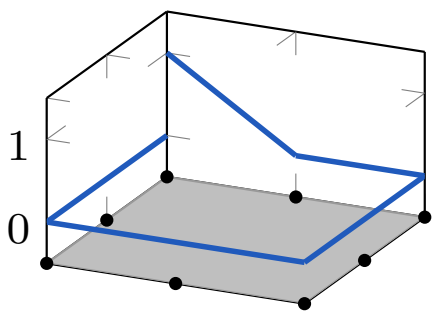

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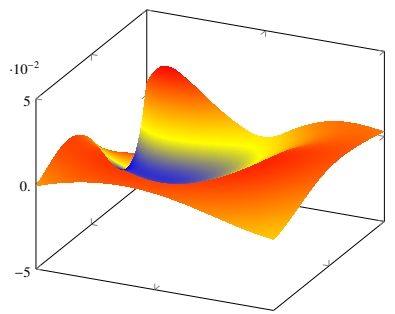

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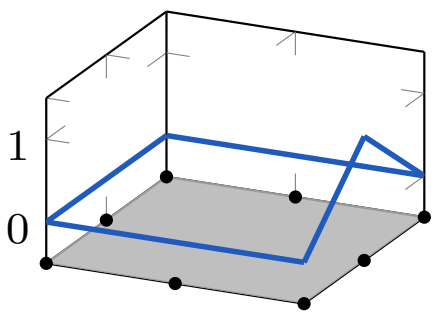

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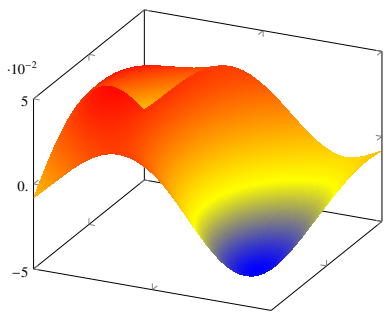

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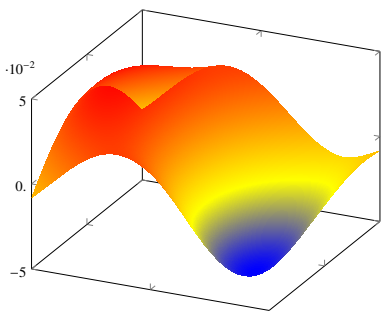

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The Flux Reconstruction method for wave propagation problems

FR principle

Consider the homogeneous 1D model system on $\Omega = [0, L]$:
Find $\mathbf{y} = (u, v) : \Omega \to \mathbb{C}^2$ such that

$$\begin{cases} i\kappa\mathbf{y} + \dfrac{\mathrm{d}\boldsymbol{\phi}}{\mathrm{d}x} = \mathbf{0}, \\ \boldsymbol{\phi} = \mathbf{F}\mathbf{y}, \end{cases} \quad \text{in } \Omega \text{ with } \mathbf{F} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \tag{5}$$

and the BCs

$$\begin{cases} u(0) - Z_1 v(0) = g_1, \\ u(L) + Z_2 v(L) = g_2. \end{cases} \tag{6}$$

Presentation for a **linear** equation!

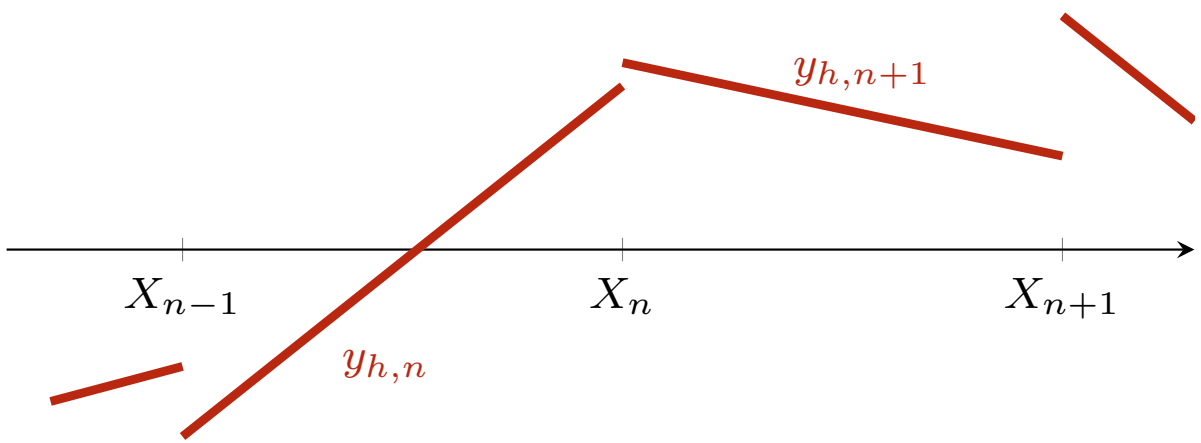
$\Longrightarrow$ Copy this equation at the discrete level on each cell of the mesh [Huynh 2007]:

$$\forall\, n \in [\![1, N]\!],\ i\kappa\mathbf{y}_h + \frac{\mathrm{d}\widetilde{\boldsymbol{\phi}}_h}{\mathrm{d}x} = \mathbf{0} \text{ in } [X_{n-1}, X_n]\,. \tag{7}$$

FR construction steps and properties

$$\forall\, n \in [\![1, N]\!],\ i\kappa \mathbf{y}_h + \frac{\mathrm{d}\widetilde{\boldsymbol{\phi}}_h}{\mathrm{d}x} = \mathbf{0} \text{ in } [X_{n-1}, X_n]\,. \tag{8}$$

1. Approximation $\mathbf{y}_h$ as piecewise polynomial of degree k_{FR}.
2. Natural flux approximation $\boldsymbol{\phi}_h = \mathbf{F}\mathbf{y}_h$.
3. Numerical fluxes $\widehat{\boldsymbol{\phi}}_n$ as a mean of $\boldsymbol{\phi}_n^-$ and $\boldsymbol{\phi}_n^+$.
4. Correction polynomials $P_n^{\rightarrow}$ and $P_n^{\leftarrow}$ of degree $k_{FR}+1$.
5. Correction $\widetilde{\boldsymbol{\phi}}_{h,n} = \boldsymbol{\phi}_{h,n} + \delta_{n-1}^{\rightarrow} P_n^{\rightarrow} + \delta_n^{\leftarrow} P_n^{\leftarrow}$.



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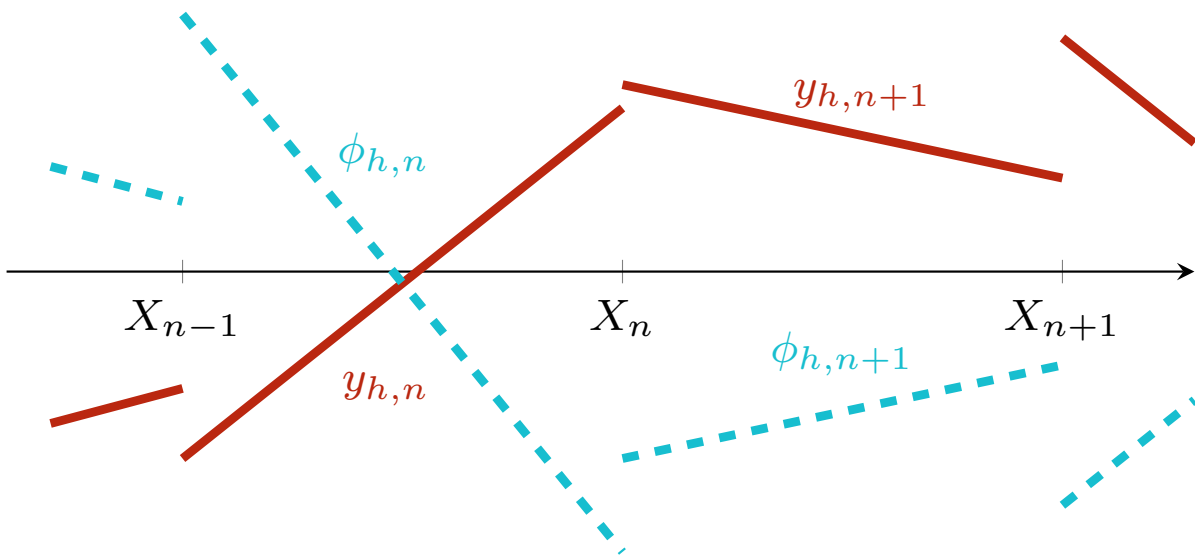

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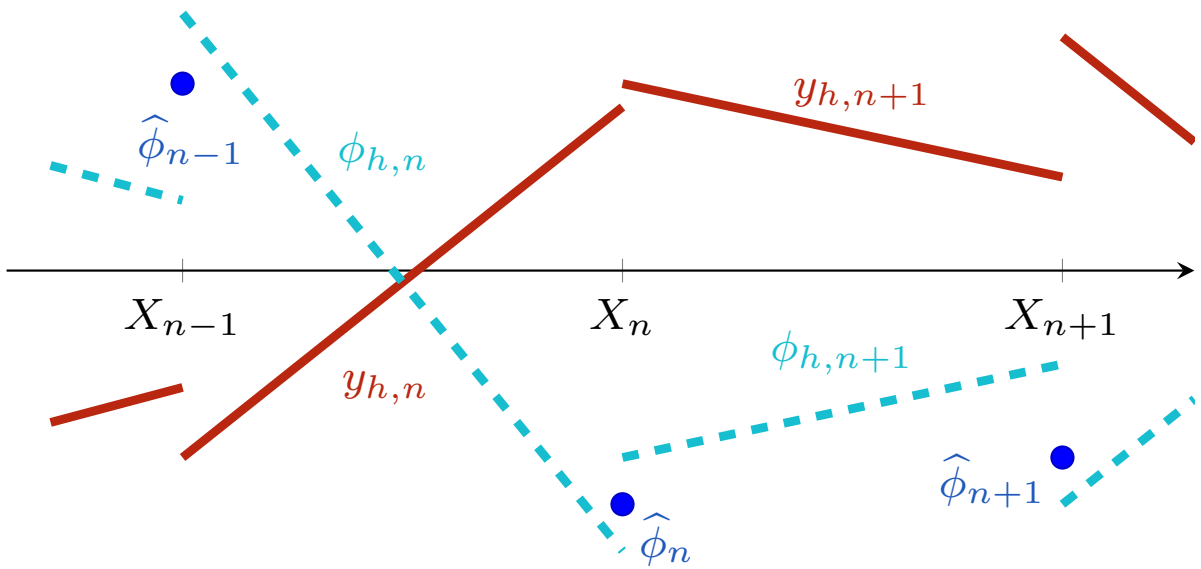

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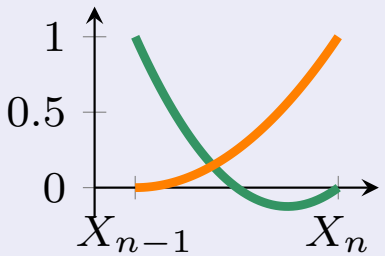

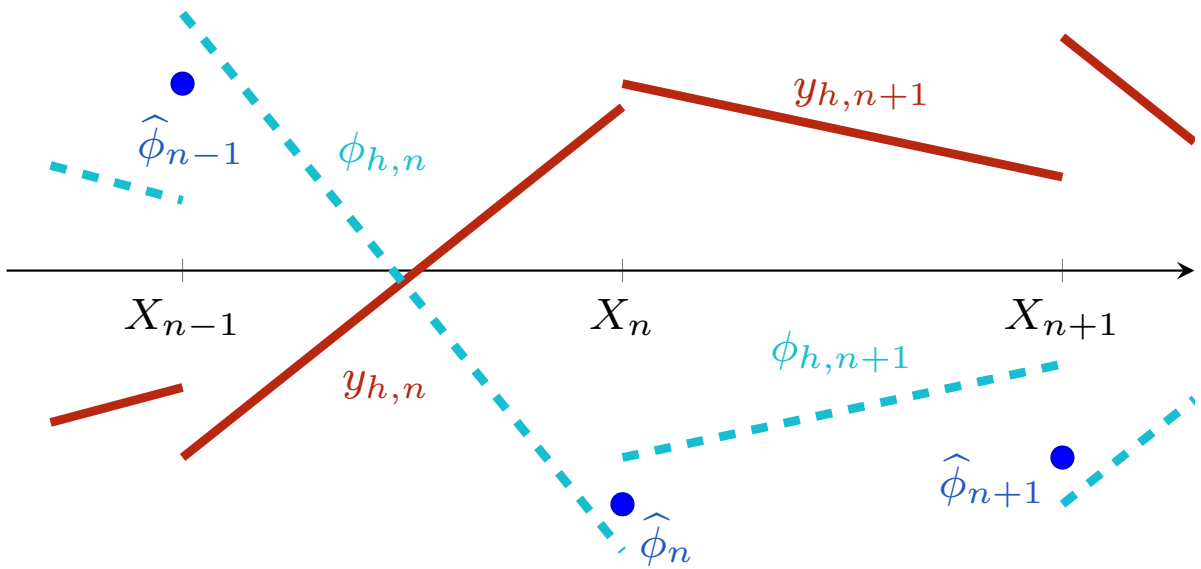

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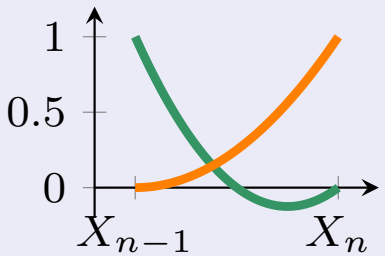

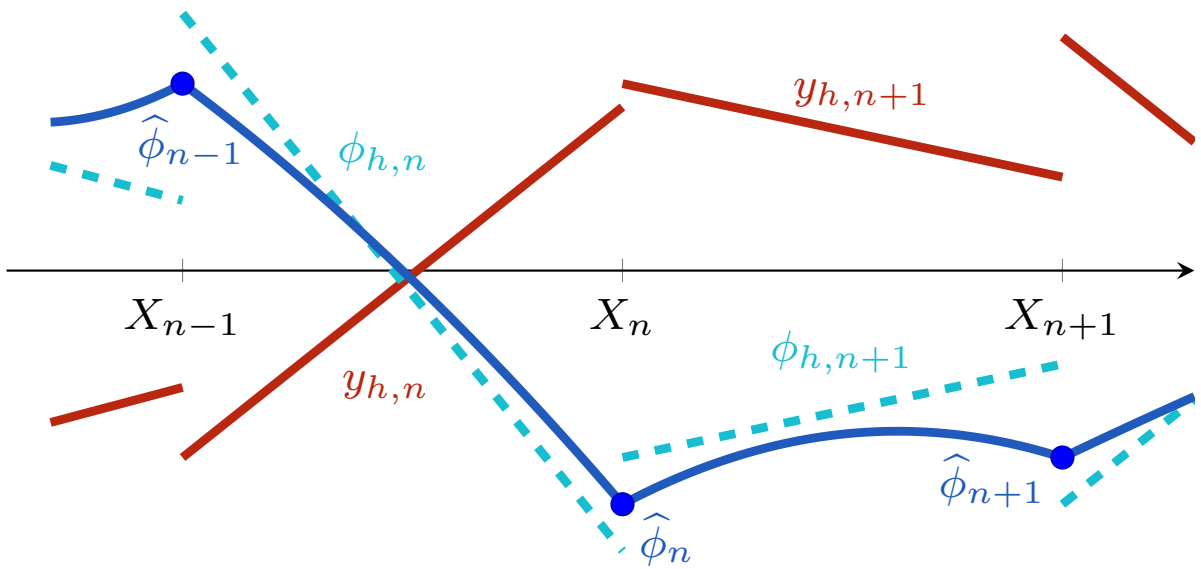

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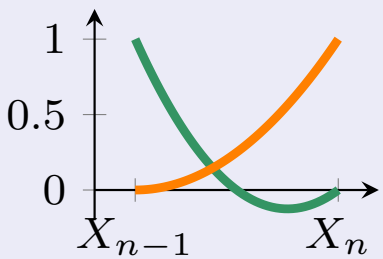

- **Strong formulation**: no dependence on a quadrature rule.
- Choice of correction polynomials allows to **retrieve usual methods**: classic choice of Radau polynomials (nodal DG).
- Natural **generalisation to 3D** and adaptable to **unstructured meshes**.

Numerical results

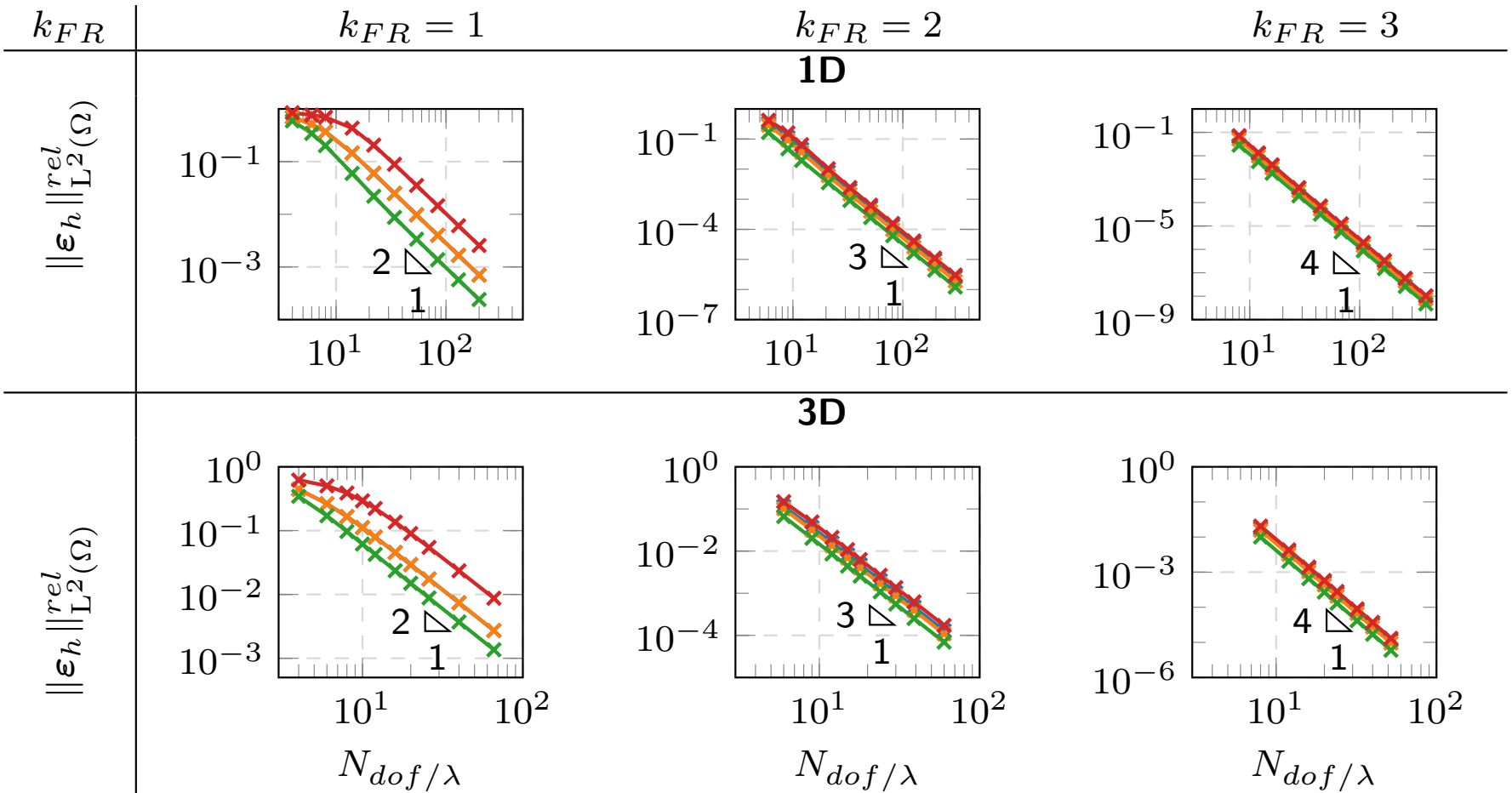

Table: h-convergence of the FR method in 1D and 3D for different correction polynomials (SD_CLo (—×—), SD_IG (—×—), FR_Rad (—×—) and FR_G2 (—×—)).

$\Longrightarrow$ Dependence on the choice of the correction polynomials: what is the **best choice**?

Error estimate and optimised correction polynomials

Developed an **explicit a priori error estimate** with incoming BCs, *i.e.* $Z_1 = Z_2 = 1$ [Rivet et al. 2023]:

$$\|\mathbf{y} - \mathbf{y}_h\|^2_{\mathrm{L}^2(\Omega)} \leq \mathsf{C}\left(\kappa, h, L, P^{\rightarrow}\right)\left(|\mathbf{g}_1|^2 + |\mathbf{g}_2|^2\right) \tag{9}$$

$\Longrightarrow$ Choose the correction polynomial $P^{\rightarrow}$ as [Rivet et al. 2024]

$$P^{\rightarrow} = \underset{\widetilde{P} \in \mathbb{P}^{adm}}{\operatorname{argmin}}\, \mathsf{C}\left(\kappa, h, L, \widetilde{P}\right). \tag{10}$$

Error estimate and optimised correction polynomials

$\Longrightarrow$ Direction-wise optimisation in the 3D case: **applicable even for general BCs**!

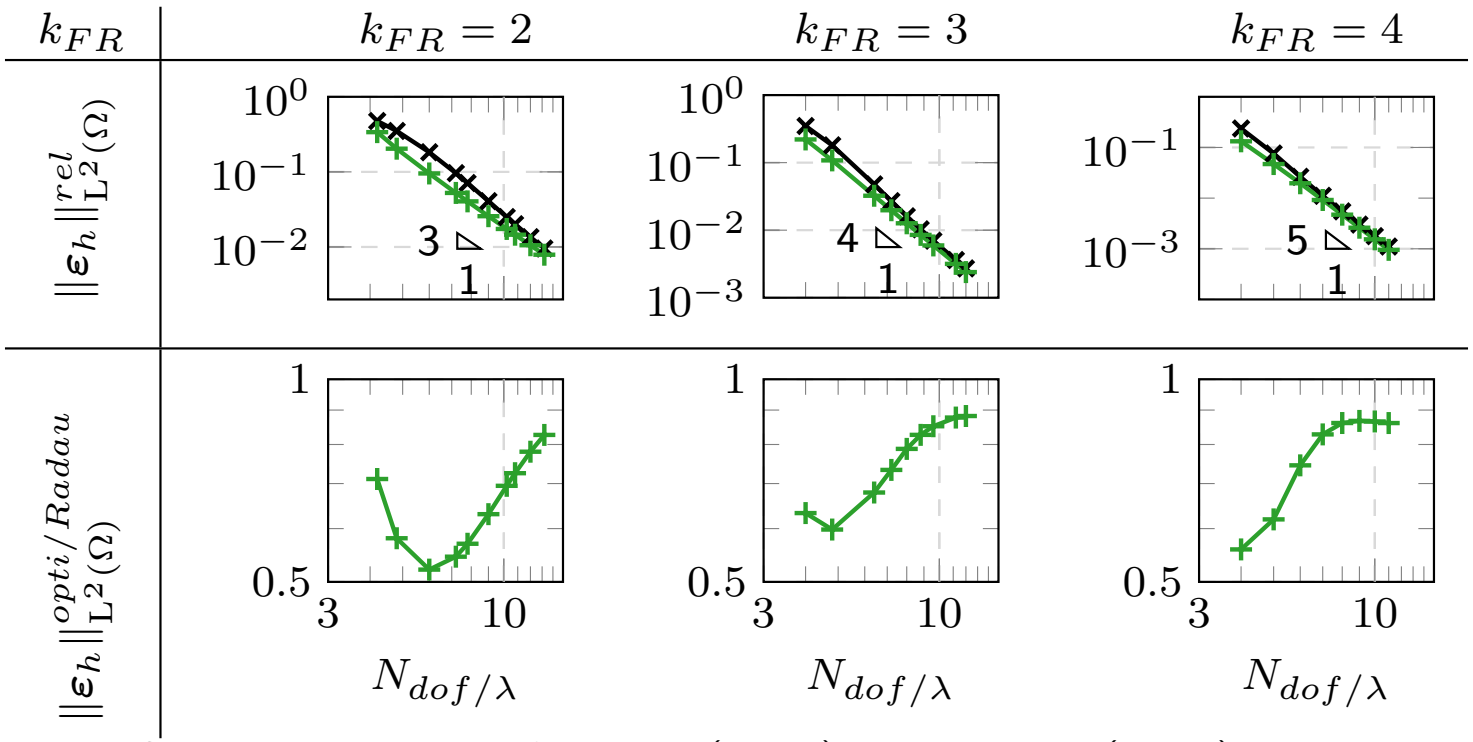

Table: General 3D simulation for Radau (—×—) and optimised (—+—) polynomials.

$\Longrightarrow$ Possible to find better polynomials than the classic ones!

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 $\mathbf{g}^T \in \mathbb{V}$ such that:

$$\gamma_t \mathbf{E}^T + Z_{\partial T}\, \gamma_\times^T \mathbf{H}^T = \mathbf{g}^T \text{ on } \partial T. \tag{11}$$

↓

Polynomial approximation of the trace space: $\mathbb{V}_h = \mathrm{span}(\mathbf{g}_i^T)$.
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 $(\mathbf{E}_h^T, \mathbf{H}_h^T)$.

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Numerical experiments: basis quality

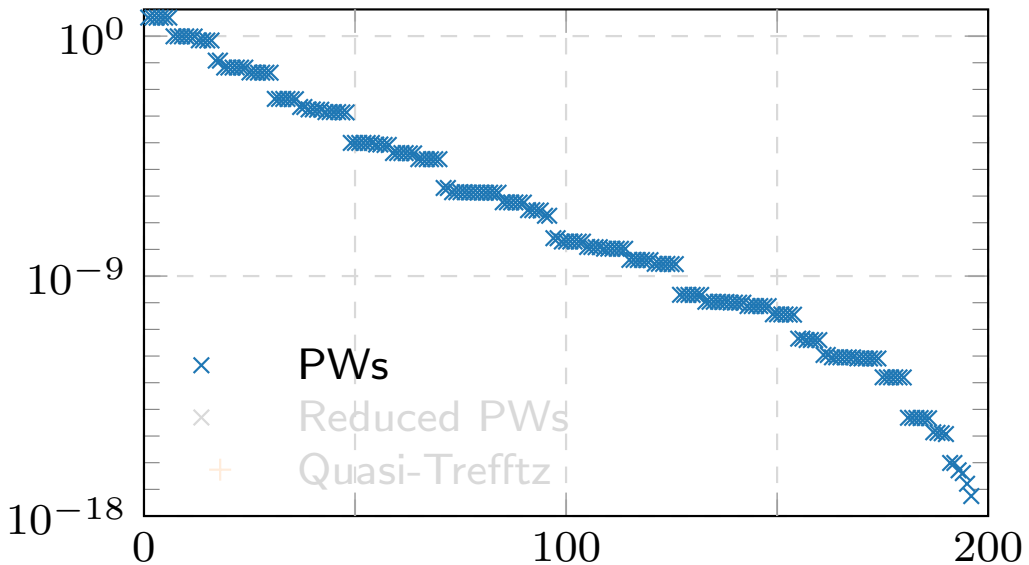

Figure: Eigenvalues of the mass matrix for 196 PWs (and reduction for $\epsilon = 10^{-6}$) and 192 Quasi-Trefftz basis functions.

Basis quality

$\Longrightarrow$ Possible **reduction techniques** to restore the condition number.

$\Longrightarrow$ Avoids spurious numerical modes and ill-conditioning of the mass matrix!

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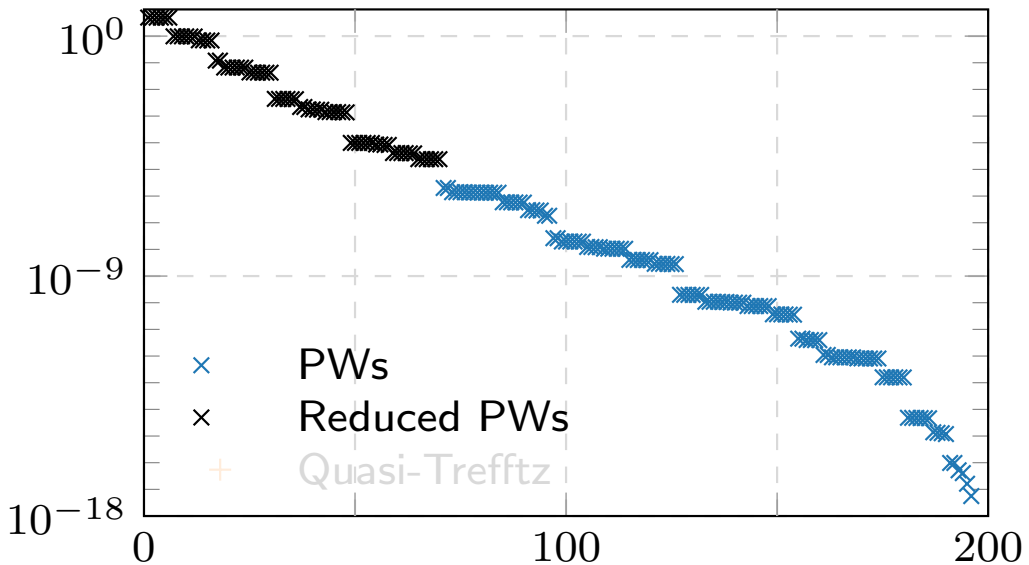

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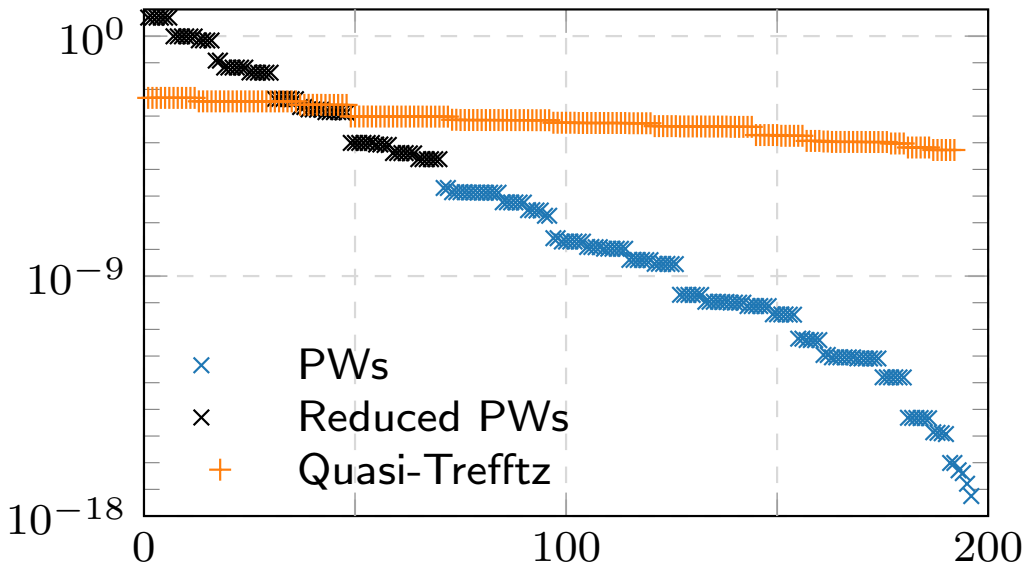

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Approximation properties of the basis for a smooth solution: sum of random PWs

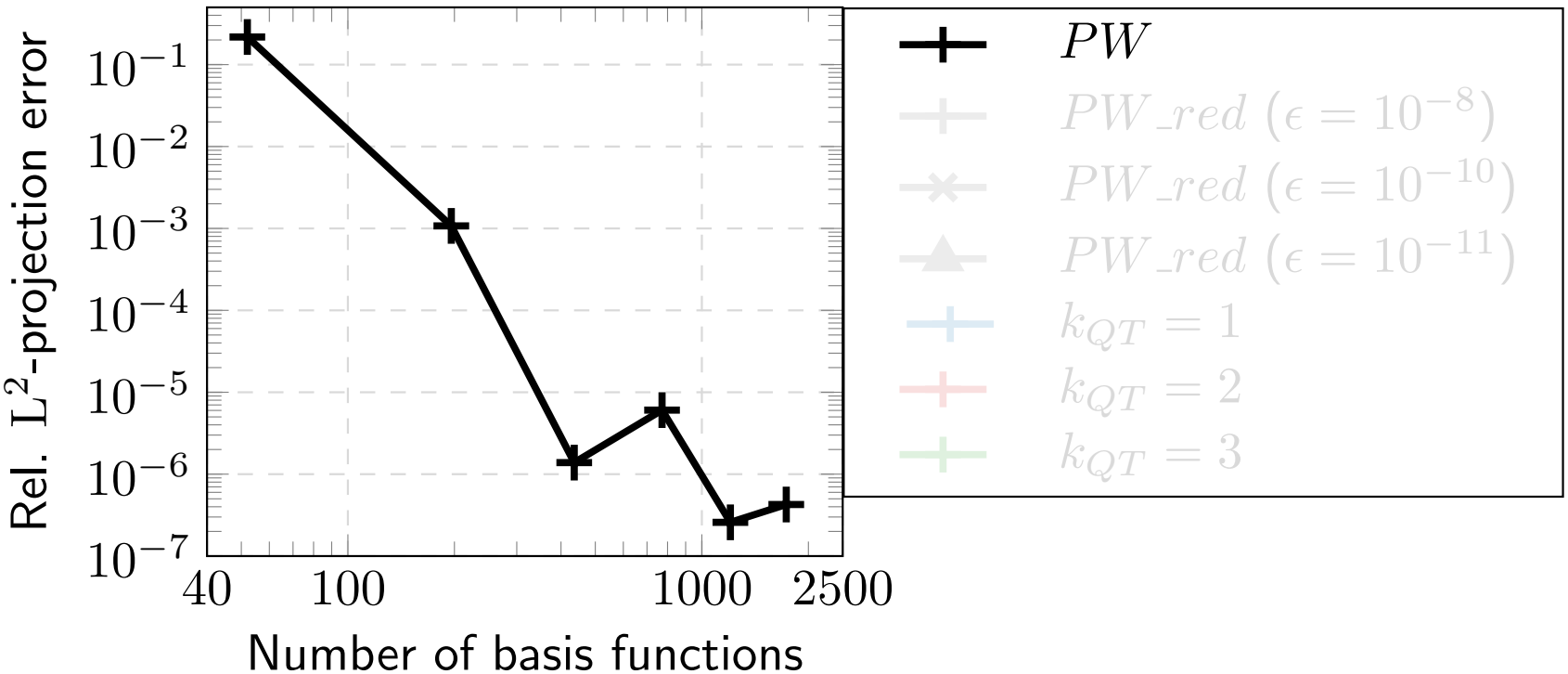

Figure: Projection error on the different basis for a sum of random PWs.

$\Longrightarrow$ Saturation phenomenon due to condition number.

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

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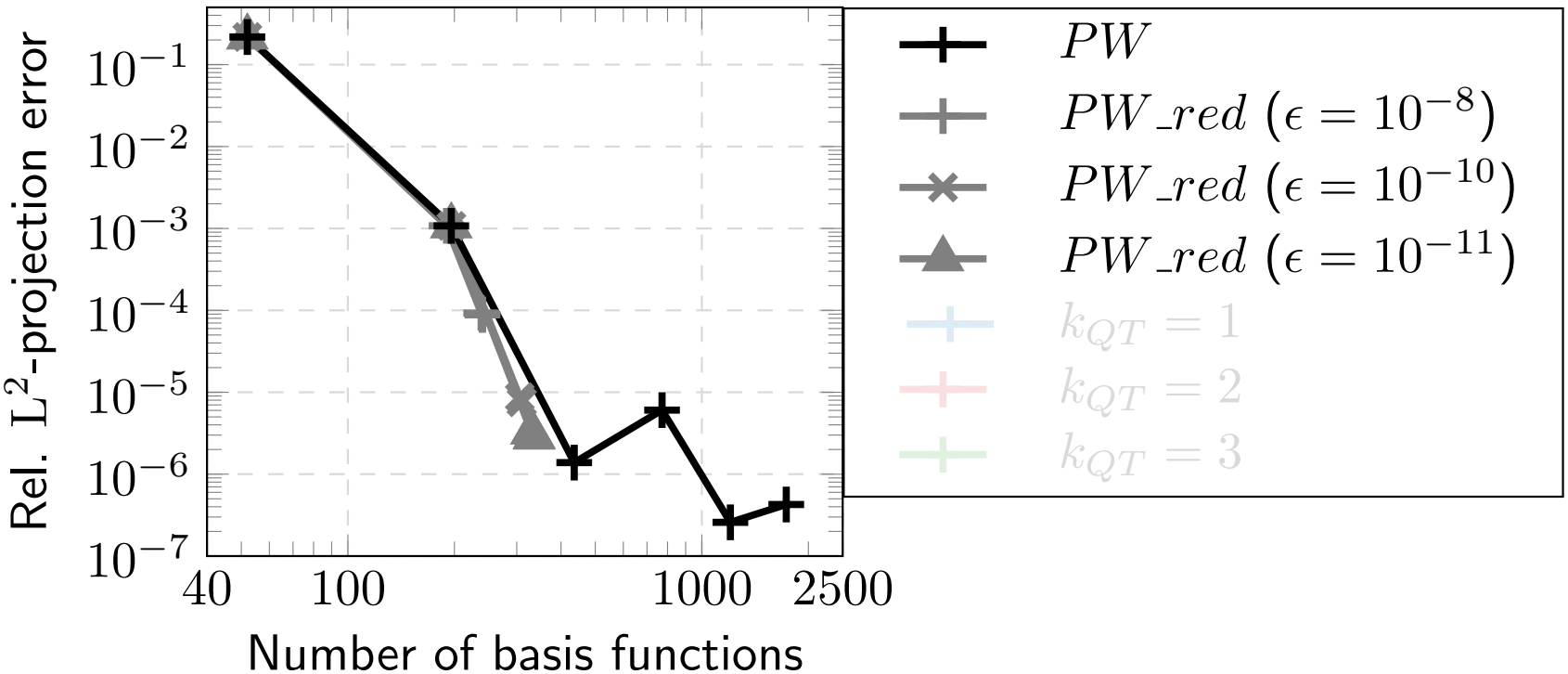

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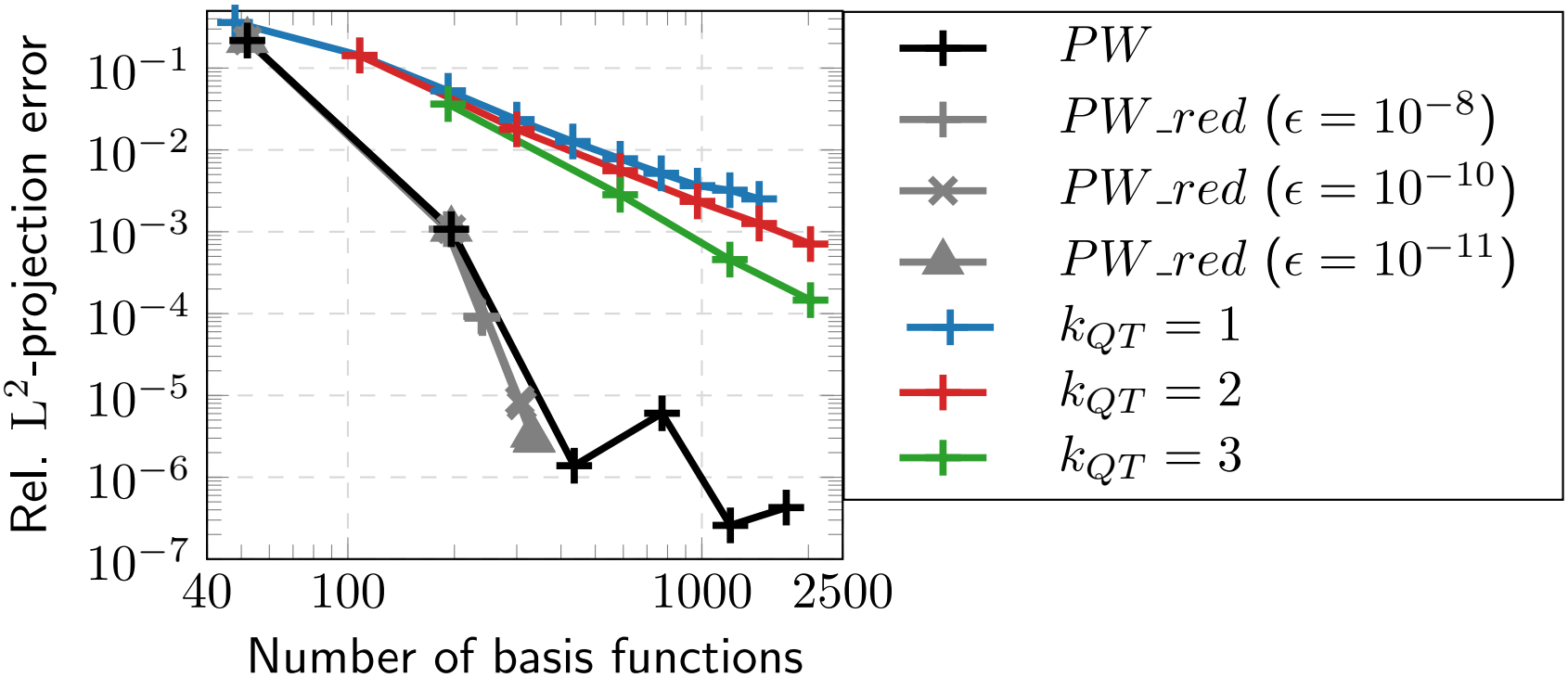

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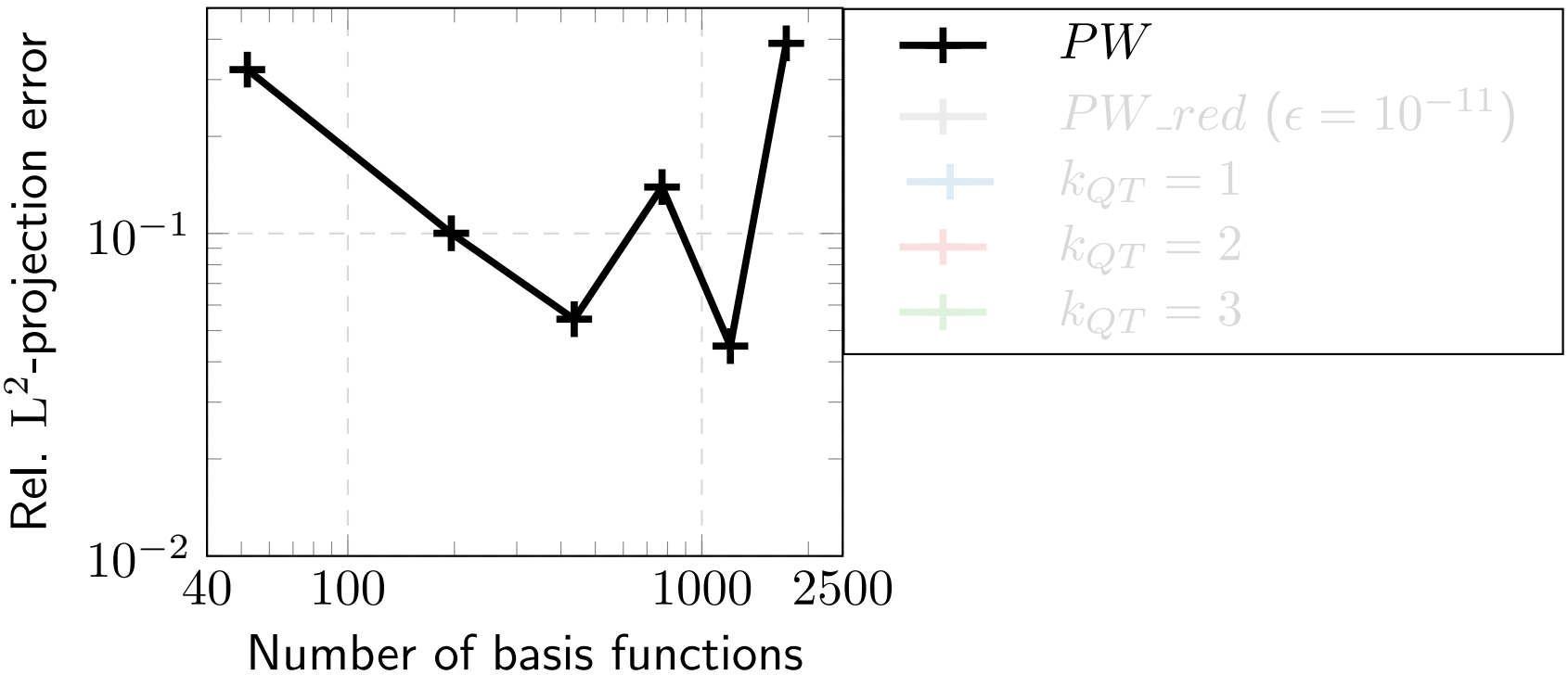

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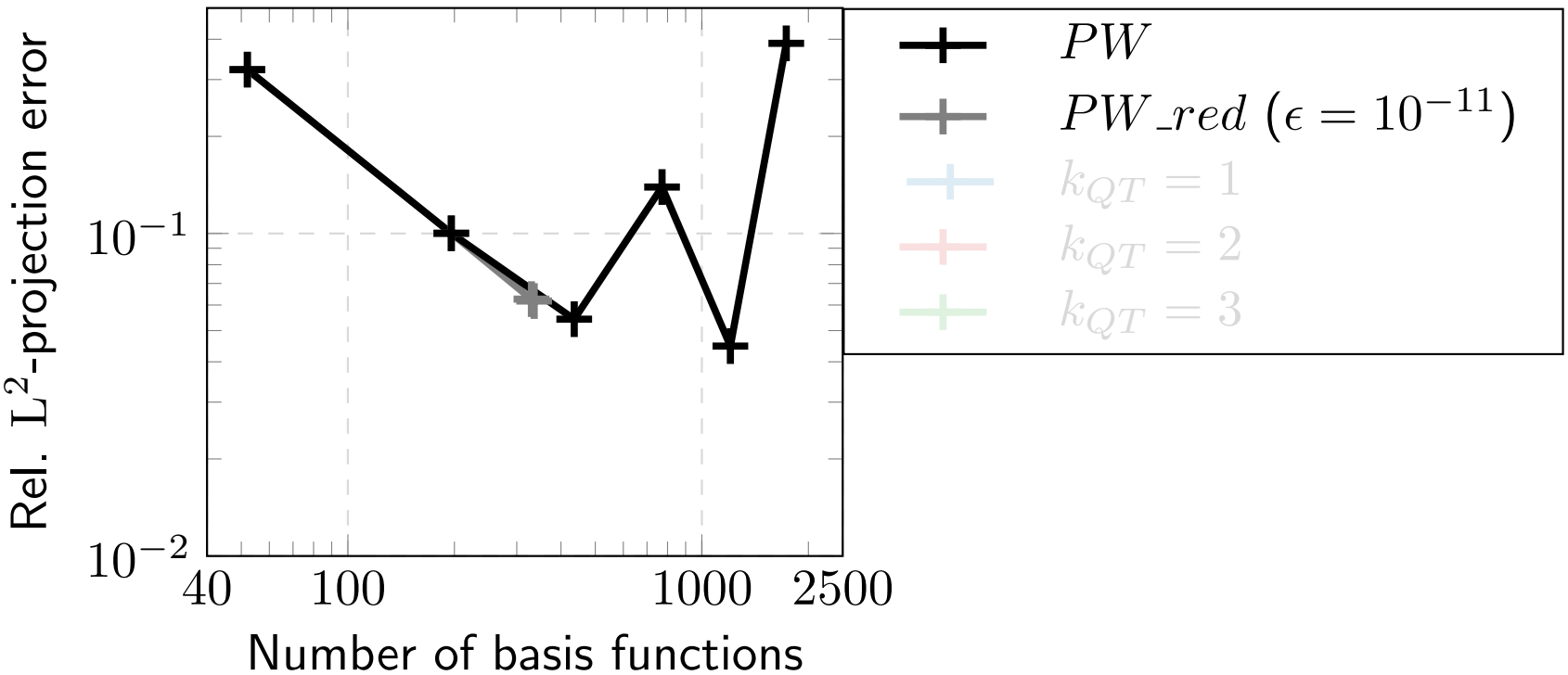

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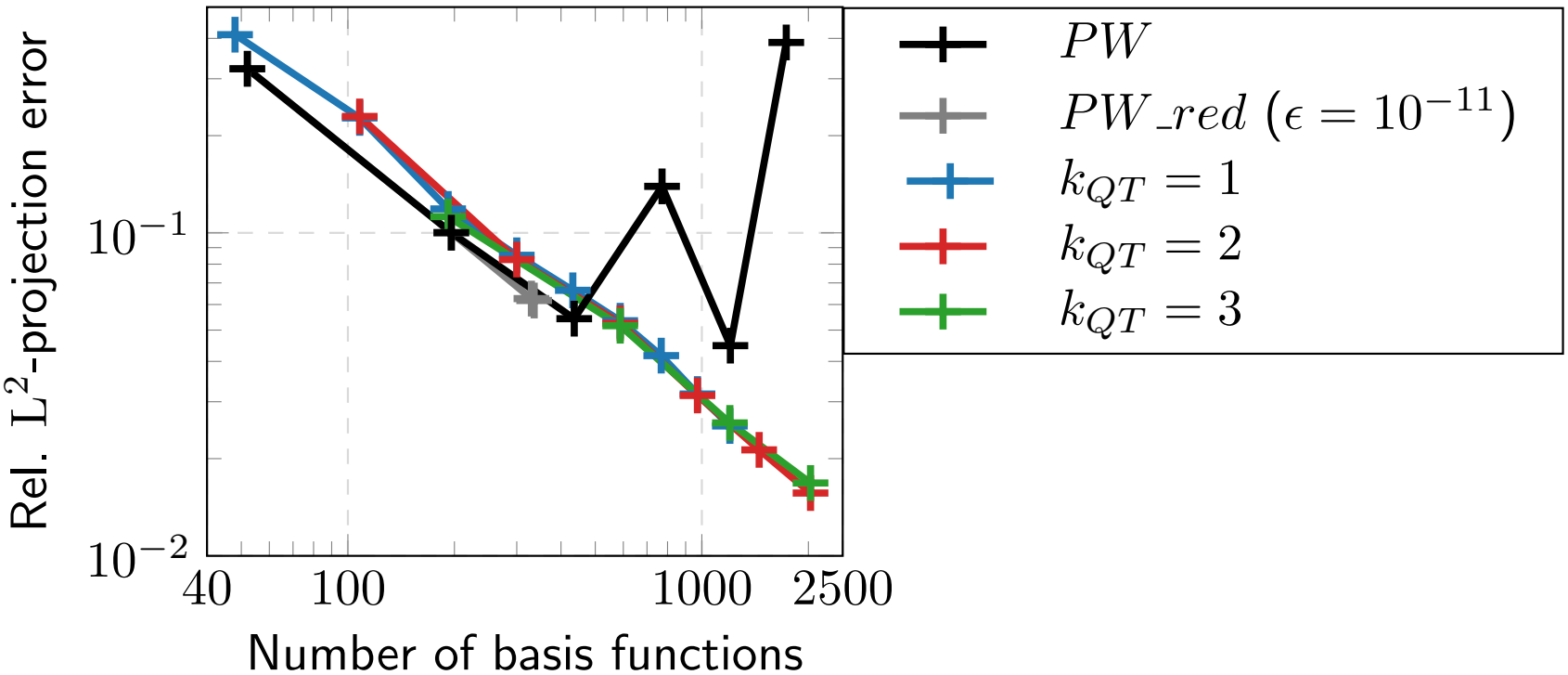

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Calibration of the FR auxiliary solver

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 $N = 3$.

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

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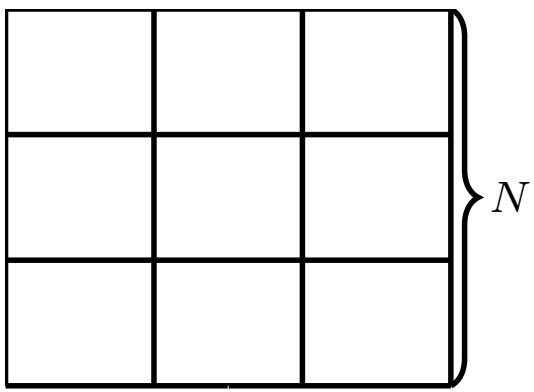

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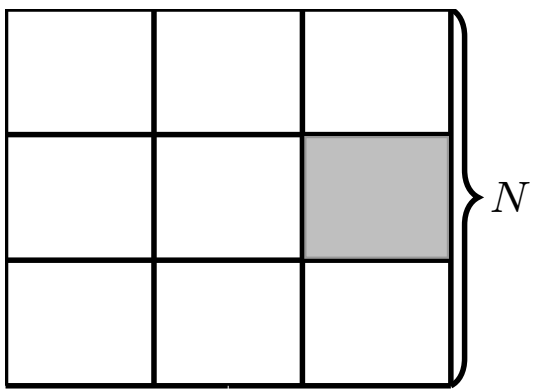

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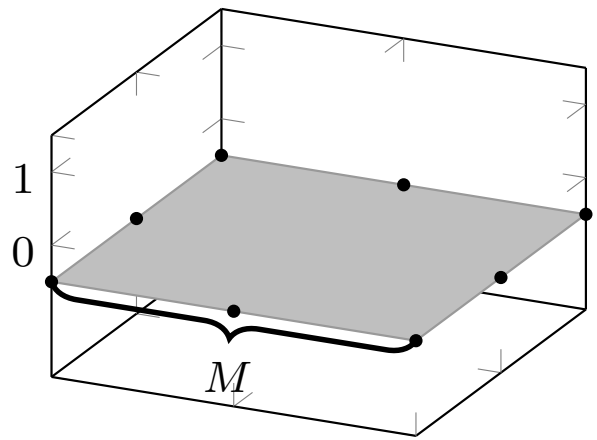

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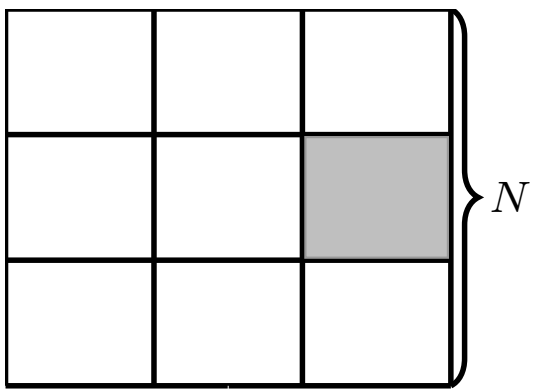

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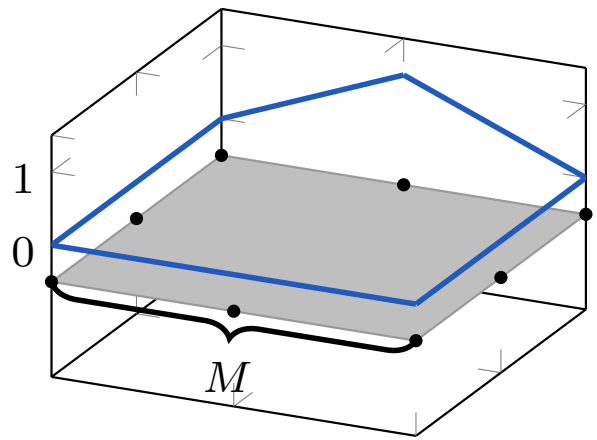

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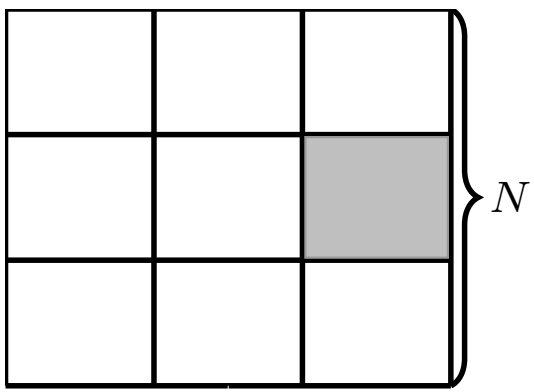

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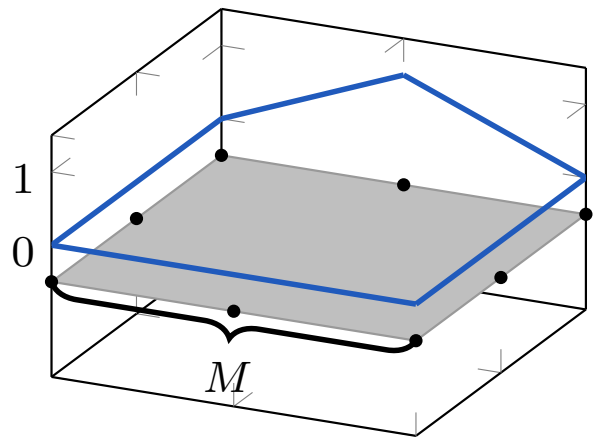

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Is using quasi-solutions enough?
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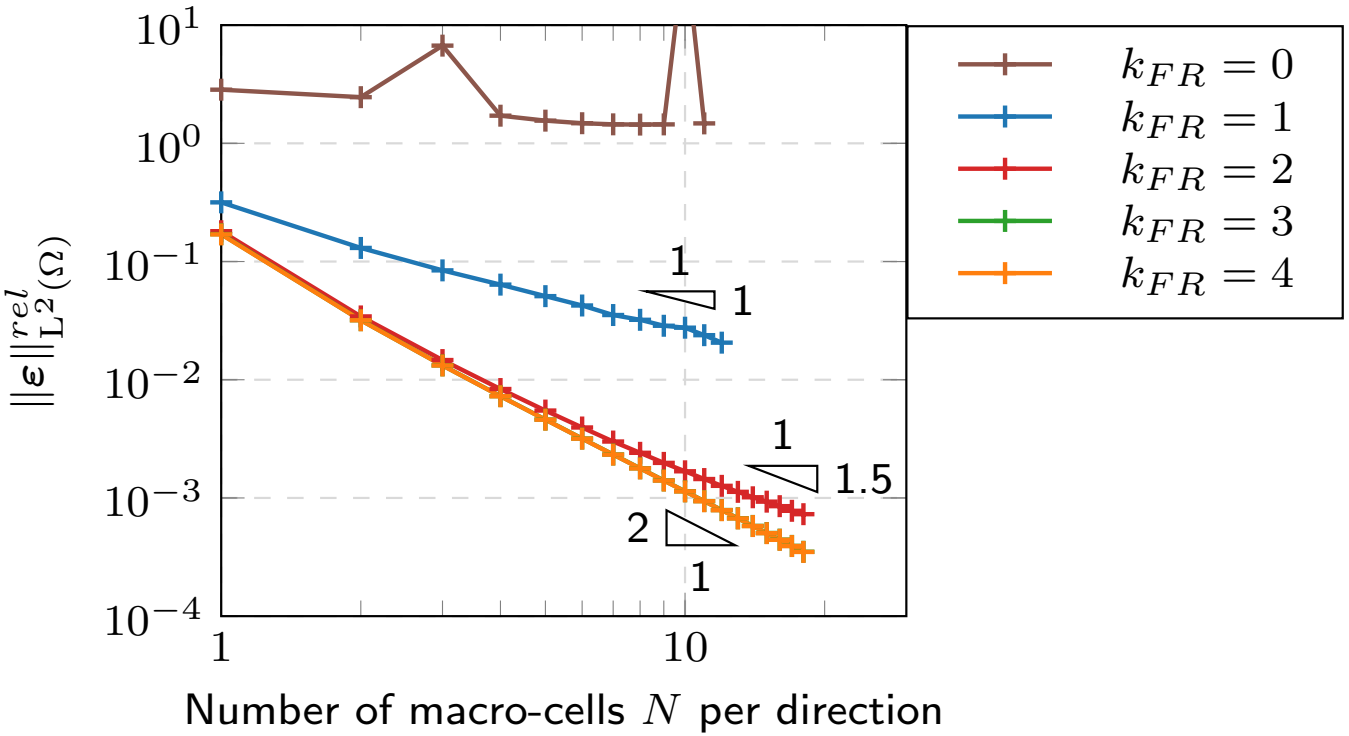
$\Longrightarrow$ Mesh-convergence: refinement of the macro-mesh $\mathcal{T}_H(\Omega)$.

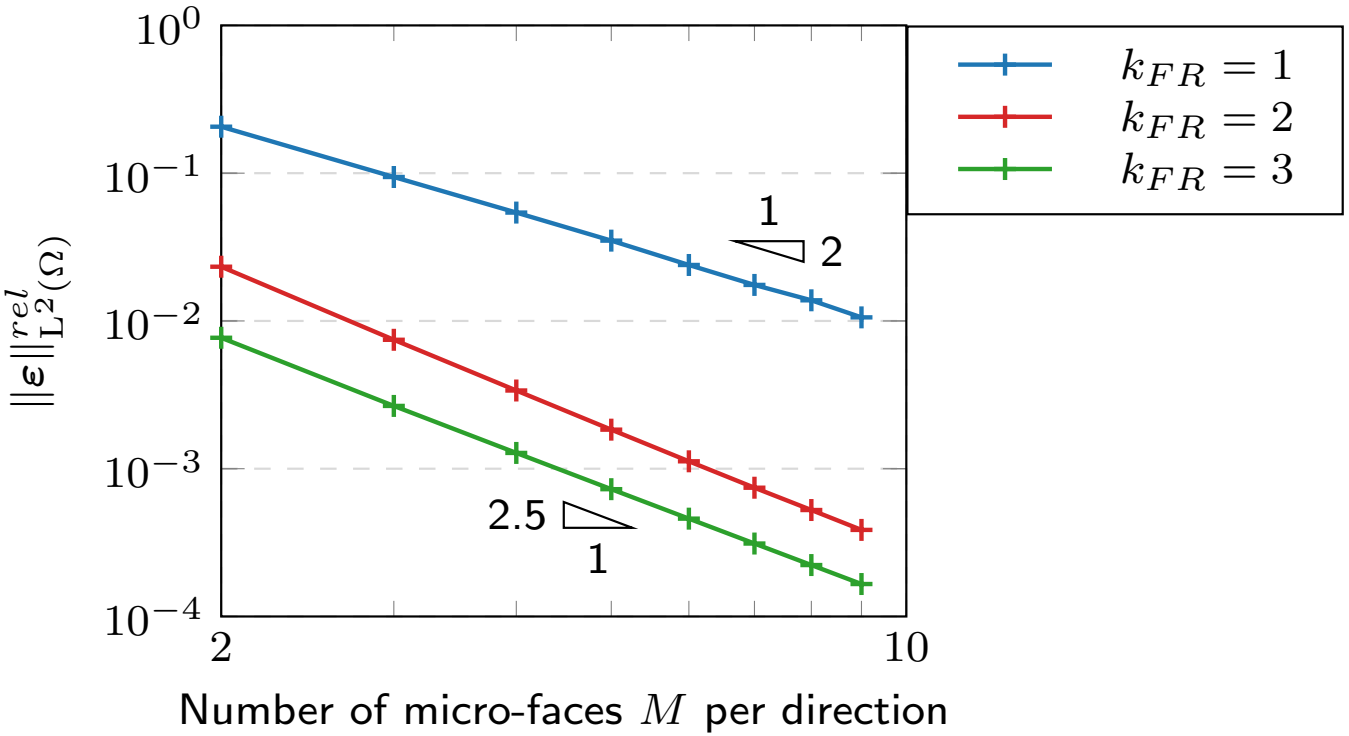


- Need of $k_{FR} \geq k_{QT} + 2$ for quasi-optimal orders, but **no interest in over-resolving**!

Numerical experiments: convergence in the number of basis functions

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

$\Longrightarrow$ **Local basis enrichment** through refinement of the micro-mesh $\mathcal{T}_h(\partial T)$.



- 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**!

Conclusion and perspectives

- 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.
- Numerically, $k_{FR} \geq k_{QT} + 2$ for quasi-optimality, but no need to over-resolve!

Perspectives:

- **Theoretical well-posedness conditions and a priori error estimates** in progress.
- Adaptable for (piecewise constant) **heterogeneous** configurations.
- Possible **hybrid approach** by mixing with PW basis.
- Development of **optimised transmission conditions** to reduce the number of iterations for convergence.

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