Implementation aspects of polytoptal methods and handling of polytopal meshes in HArDCore

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NEMESIS
New generation methods
for numerical simulations

Towards polytopal meshes in GMSH
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Outline

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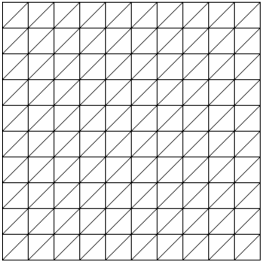
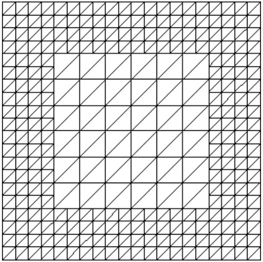
Established by the European Commission

Reissner–Mindlin plate problem

[Di Pietro and Droniou, 2022]

Stabilised $\mathcal{P}^2$-($\mathcal{P}^1 + \mathcal{B}^3$) scheme		DDR scheme	
			
nb. DOFs	Error	nb. DOFs	Error
2403	0.138	550	0.161
9603	6.82e-2	2121	6.77e-2
38402	3.40e-2	8329	3.1e-2

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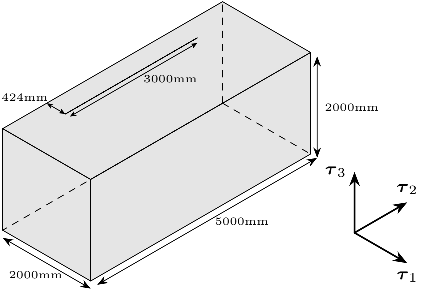
Electromagnetic wave I

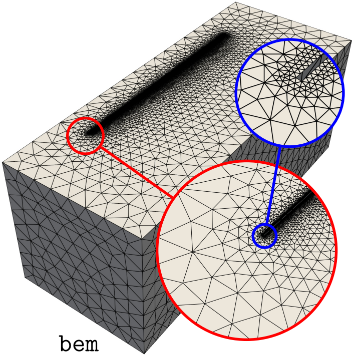
[Touzalin, 2025]

Problem: use a boundary element method to analyse the shielding effectiveness of a perfectly conductive box with a very small slit.

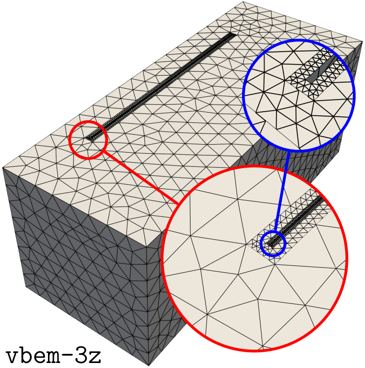


Electromagnetic wave II

Meshes: conforming triangular for finite-element boundary method (bem), non-conforming triangular (polygonal) for virtual element boundary method (vbem-3z).



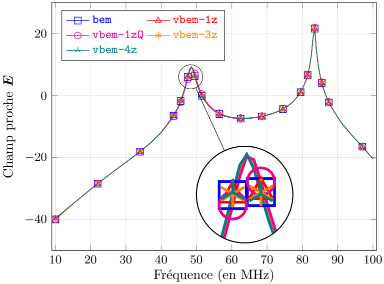
bem

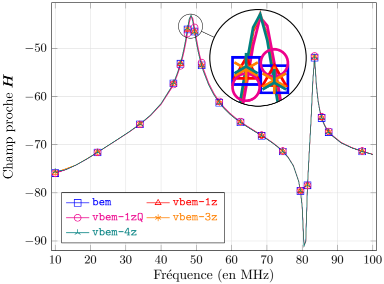


vbem-3z

Electromagnetic wave III

Accuracy: comparison of modulus of reflected near fields at the top.





Computational cost

Method	*Assembly*	*Resolution*
bem	813s	125s
vbem-3z	321s	19s

Outline

Algebraic realisation of potential

- Space: $\underline{V}_T^k = \{\underline{v}_T = (v_T, (v_F)_{F\in\mathcal{F}_T}) \,:\, v_T \in \mathcal{P}^{k-1}(T)\,,\ v_F \in \mathcal{P}^k(F)\}$.
- Potential reconstruction ($k \geq 1$):

$$\int_T \nabla p_T^{k+1}\underline{v}_T \cdot \nabla w = -\int_T v_T \Delta w + \sum_{F\in\mathcal{F}_T} \int_F v_F\,(\nabla w \cdot \boldsymbol{n}_{TF}) \quad \forall w \in \mathcal{P}^{k+1}(T),$$

$$\int_T p_T^{k+1}\underline{v}_T = \int_T v_T.$$

- Recast as: for all $w \in \mathcal{P}^{k+1}(T)$,

$$(\nabla p_T^{k+1}\underline{v}_T, \nabla w)_T + (p_T^{k+1}\underline{v}_T, 1)_T (w,1)_T = -(v_T, \Delta w)_T + \sum_{F\in\mathcal{F}_T} (v_F, \nabla w \cdot \boldsymbol{n}_{TF})_F + (v_T, 1)_T (w,1)_T.$$

(Solution of a Riesz representation problem)

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Matrix of $p_T^{k+1} : \underline{V}_T^k \to \mathcal{P}^{k+1}(T)$ on selected bases

- Pick bases Φ_F^k of $\mathcal{P}^k(F)$ for $F \in \mathcal{F}_T$ and Φ_T^{k-1} of $\mathcal{P}^{k-1}(T)$.

$$\text{Basis of } \underline{V}_T^k : \Phi_{F_1}^k \times \cdots \times \Phi_{F_{N_{\partial T}}}^k \times \Phi_T^{k-1}.$$

(Increasing dimension of mesh entities)

- Pick basis $\widehat{\Phi}_T^{k+1}$ of $\mathcal{P}^{k+1}(T)$.

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(Increasing dimension of mesh entities)

- Pick basis $\widehat{\Phi}_T^{k+1}$ of $\mathcal{P}^{k+1}(T)$.

- Notations:

$$\begin{aligned}
\Phi_F^k &= \{\varphi_1^F, \ldots, \varphi_{N_{k,F}}^F\},\\
\Phi_T^{k-1} &= \{\varphi_1^T, \ldots, \varphi_{N_{k,T}}^T\},\\
\widehat{\Phi}_T^{k+1} &= \{\widehat{\varphi}_1^T, \ldots, \widehat{\varphi}_{N_{k+1,T}}^T\}.
\end{aligned}$$

Matrix of $p_T^{k+1} : \underline{V}_T^k \to \mathcal{P}^{k+1}(T)$ on selected bases

- Pick bases Φ_F^k of $\mathcal{P}^k(F)$ for $F \in \mathcal{F}_T$ and Φ_T^{k-1} of $\mathcal{P}^{k-1}(T)$.

$$\text{Basis of } \underline{V}_T^k : \Phi_{F_1}^k \times \cdots \times \Phi_{F_{N_{\partial T}}}^k \times \Phi_T^{k-1}.$$

(Increasing dimension of mesh entities)

- Pick basis $\widehat{\Phi}_T^{k+1}$ of $\mathcal{P}^{k+1}(T)$.

- Notations: vector $\underline{\mathsf{V}}_T$ of $\underline{v}_T \in \underline{V}_T^k$ written as:

$$\underline{\mathsf{V}}_T = \begin{bmatrix} \mathsf{V}_{F_1} \\ \vdots \\ \mathsf{V}_{F_{N_{\partial T}}} \\ \mathsf{V}_T \end{bmatrix} \quad \text{with} \quad \begin{array}{l} \mathsf{V}_F = [V_i^F]_{i=1,\ldots,N_{k,F}} \text{ coefficients on } \Phi_F^k, \\ \mathsf{V}_T = [V_i^T]_{i=1,\ldots,N_{k-1,T}} \text{ coefficients on } \Phi_T^{k-1}. \end{array}$$

Matrix of $p_T^{k+1} : \underline{V}_T^k \to \mathcal{P}^{k+1}(T)$ on selected bases

- Definition:

$$(\nabla p_T^{k+1}\underline{v}_T, \nabla w)_T + (p_T^{k+1}\underline{v}_T, 1)_T(w,1)_T$$
$$= -(v_T, \Delta w)_T + (v_T, 1)_T(w,1)_T + \sum_{F\in\mathcal{F}_T}(v_F, \nabla w\cdot \boldsymbol{n}_{TF})_F.$$

- Algebraic translation: the coefficients P_T of $p_T^{k+1}\underline{v}_T$ on $\widehat{\Phi}_T^{k+1}$ satisfy

$$\left(\mathbf{S}_T + \widehat{\mathsf{L}}_T^{k+1}(\widehat{\mathsf{L}}_T^{k+1})^\intercal\right)\mathsf{P}_T = \left(\mathbf{B}_{P,T} + \widehat{\mathsf{L}}_T^{k+1}(\mathsf{L}_T^{k-1})^\intercal\right)\mathsf{V}_T + \sum_{F\in\mathcal{F}_T}\mathbf{B}_{P,F}\mathsf{V}_F,$$

with

$$\mathbf{S}_T := \left[(\nabla\widehat{\varphi}_i^T, \nabla\widehat{\varphi}_j^T)_T\right]_{1\le i,j\le N_{k+1,T}}, \quad \widehat{\mathsf{L}}_T^{k+1} := [(\widehat{\varphi}_i^T, 1)_T]_{1\le i\le N_{k+1,T}},$$
$$\mathbf{B}_{P,T} := \left[-(\Delta\widehat{\varphi}_i^T, \varphi_j^T)_T\right]_{1\le i\le N_{k+1,T}, 1\le j\le N_{k-1,T}}, \quad \mathsf{L}_T^{k-1} := [(\varphi_i^T, 1)_T]_{1\le i\le N_{k-1,T}}$$
$$\mathbf{B}_{P,F} := \left[(\nabla\widehat{\varphi}_i^T\cdot\boldsymbol{n}_{TF}, \varphi_j^F)_F\right]_{1\le i\le N_{k+1,T}, 1\le j\le N_{k,F}}.$$

Matrix of $p_T^{k+1} : \underline{V}_T^k \to \mathcal{P}^{k+1}(T)$ on selected bases

- The coefficients P_T of $p_T^{k+1}\underline{v}_T$ on $\widehat{\Phi}_T^{k+1}$ satisfy

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$$\mathbf{B}_{P,F} := \left[(\nabla\widehat{\varphi}_i^T\cdot\boldsymbol{n}_{TF},\varphi_j^F)_F\right]_{1\le i\le N_{k+1,T},1\le j\le N_{k,F}}.$$

- The matrix $\mathbf{P}_T$ of p_T^{k+1} is thus obtained by solving

$$\left(\mathbf{S}_T + \widehat{\mathsf{L}}_T^{k+1}(\widehat{\mathsf{L}}_T^{k+1})^\intercal\right)\mathbf{P}_T = \left[\mathbf{B}_{P,F_1} \quad \cdots \quad \mathbf{B}_{P,F_{N_{\partial T}}} \quad \mathbf{B}_{P,T} + \widehat{\mathsf{L}}_T^{k+1}(\mathsf{L}_T^{k-1})^\intercal\right].$$

Matrix of $p_T^{k+1} : \underline{V}_T^k \to \mathcal{P}^{k+1}(T)$ on selected bases

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$$\mathbf{S}_T := \left[(\nabla\widehat{\varphi}_i^T, \nabla\widehat{\varphi}_j^T)_T\right]_{1\le i,j\le N_{k+1,T}}, \quad \widehat{\mathsf{L}}_T^{k+1} := [(\widehat{\varphi}_i^T, 1)_T]_{1\le i\le N_{k+1,T}},$$

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- A few requirements for the library:
  - Gram matrices of families of polynomials (integrate products).
  - Differential operators between families of polynomials.
  - Direct access to faces of an elements, and integrate on them.

HArDCore library (`https://github.com/jdroniou/HArDCore`)

- Linear algebra: via Eigen (`https://gitlab.com/libeigen/eigen`).
- In-house Mesh classes and Polynomial family classes.
- Fast integration rules [Chin et al., 2015]: essential for polytopal methods, requires full connectivity from element to vertices, as well as geometric information (outer normal, etc.).

  (In some instances, quadrature-based integration is still required.)
- Various interfaces:
  - ⋆ PaSTiX (`https://solverstack.gitlabpages.inria.fr/pastix/`),
  - ⋆ PETSc (`https://petsc.org/release/`),
  - ⋆ etc.
- Many polytopal methods and schemes : HHO, DDR, VEM, elasticity with Tresca contact, plates, Yang–Mills, etc.

Outline

Construction of polynomial bases

- Store vectors of powers up to degree ℓ

$$\{\boldsymbol{\alpha} = (\omega_1, \ldots, \omega_d) \in \mathbb{N}^d \;:\; \sum_i \omega_i = \ell\} = \{\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \ldots, \boldsymbol{\alpha}_{N_\ell}\},$$

which define the monomials ($\boldsymbol{x}_T$ = center of mass of T, h_T = diameter)

$$m_j(\boldsymbol{x}) = \left(\frac{x_1 - x_{T,1}}{h_T}\right)^{\alpha_{j,1}} \cdots \left(\frac{x_1 - x_{T,d}}{h_T}\right)^{\alpha_{j,d}}.$$

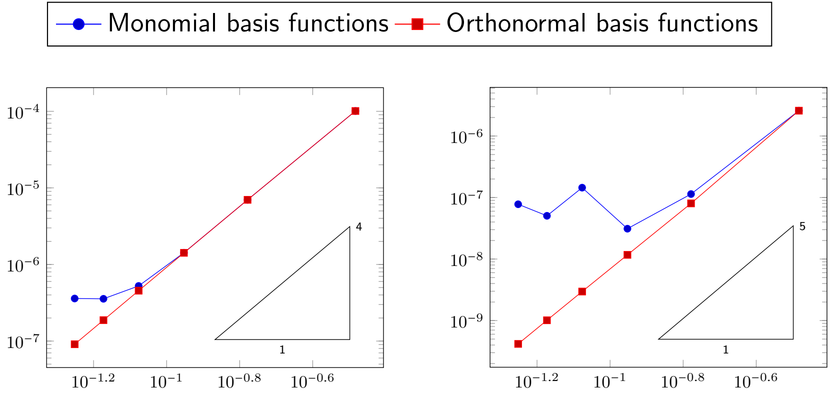
- Basis $\Phi_T^\ell = \{\phi_1, \ldots, \phi_{N_\ell}\}$ of $\mathcal{P}^\ell(T)$: linear combination of monomials

$$\phi_r = \sum_{j=1}^{N_\ell} M_{rj} m_j.$$

- Extensions: vector- or matrix-valued polynomials by tensorisation.
- **`PolynomialFamily`**: defined by degree ℓ, mesh entity (T, F, etc.), generators (list of scalars, vectors, matrices) and matrix M.

Construction of polynomial bases

Local polynomial bases on $\mathcal{P}^k(T)$, $\mathcal{P}^k(F)$ are orthonormalised!



(a) Energy norm vs. h, Kershaw meshes, $k = 3$.

(b) L^2-norm vs. h, Kershaw meshes, $k = 3$.

Unified class for all kinds of polynomial spaces

- **`PolynomialFamily`**: defined by degree ℓ, mesh entity (T, F, etc.), generators (list of scalars, vectors, matrices) and matrix M.
- Suitable choices of generators and matrix describe **`PolynomialFamilies`** that are not $\mathcal{P}^{\ell}(X)$.
  For example, for PF *polynomial family:*
  - ⋆ **`gradient`**(PF), **`divergence`**(PF), **`curl`**(PF), *etc.*
  - ⋆ L(PF) *if L linear map acting on generators.*
  - ⋆ $\mathrm{PF}_1 + \mathrm{PF}_2$ *(sum of spanned vector spaces).*

Unified class for all kinds of polynomial spaces

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  - ⋆ L(PF) *if* L *linear map acting on generators.*
  - ⋆ $\text{PF}_1 + \text{PF}_2$ *(sum of spanned vector spaces).*
- Koszul complements are also described as **`PolynomialFamilies`**, e.g.:

$$\mathcal{R}^{c,\ell}(T) = (\boldsymbol{x} - \boldsymbol{x}_T)\mathcal{P}^{\ell-1}(T)\,, \quad \mathcal{G}^{c,\ell}(T) = (\boldsymbol{x} - \boldsymbol{x}_T) \times \mathcal{P}^{\ell-1}(T)^3.$$

  (leads to straightforward description of arbitrary-order Nédélec and Raviart–Thomas elements)
- Unified class of polynomials means unified (fast) integration rules.

Outline

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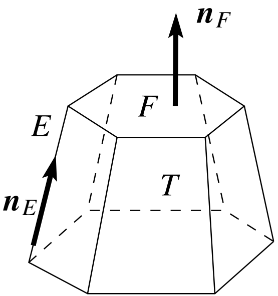
Classes for mesh entities

- Classes for **`Cell`**, **`Face`**, **`Edge`**, **`Vertex`**.
  All templated versions of the same **`MeshObject`** *class.*
- Full connectivity, for example each **`Face`** embeds (pointers to) its neighbouring **`Cells`**, and the **`Edges`**, **`Vertex`** it contains.
  Useful for local constructions of operators, and fast integration rule.
- Lots of additional embedded information (where relevant): global index; diameter, volume/area/length; center of mass; outer normal, tangent vector; relative orientations of sub-mesh entities; etc.



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- Lots of additional embedded information (where relevant): global index; diameter, volume/area/length; center of mass; outer normal, tangent vector; relative orientations of sub-mesh entities; etc.

- Other features:
  - ★ Each cell/face has a simplicial subdivision.
  - ★ 2-level meshes can be handled (coarsened mesh from fine mesh).
  - ★ Mesh transformation/handlers: move vertices; split non-planar faces; etc.

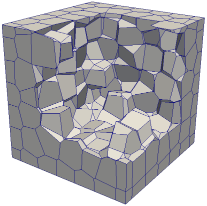
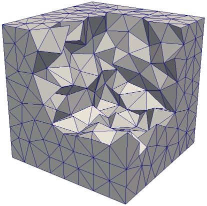
Mesh construction

- Full mesh described in (large) "RF" mesh files with minimal (non-redundant) information.
- **`MeshBuilder`** takes care of creating all the connectivity.

Since last October, the development version of `HArDCore` also has an interface with `GMesh` (`https://gmsh.info/`).

RF mesh file data structure

- Two files for each 3D mesh: `M.node` for vertices, `M.ele` for cells.
- In `M.node`, one line per vertex:
  <vertex id> <x coordinate> <y coordinate> <z coordinate>
- In `M.ele`, each cell is given by:
  - ⋆ Header line: <cell id> <number of faces>
  - ⋆ For each face in the cell:
    <local face id> <number of vertices> <id of first vertex> <id of second vertex> ...
    (vertices listed in order around the face boundary)

Mesh builder

- From RF file or GMesh mesh, creates **`std::vector`** to list vertices and cells (as in RF file format).
- To create a mesh entity in **`Mesh`**, it is split into simplices:
  - ⋆ ensures that orientation will be correct,
  - ⋆ allows for calculation of center of mass, measure, etc.

  (Assumes that faces and cells are star-shaped w.r.t. average of their vertices).
- Entities (partially) created and added by increasing dimension:
  - ⋆ Vertices (no connectivity at this stage).
  - ⋆ Edges (connected to vertices and gives connexion between vertices).
  - ⋆ etc.

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Conclusion and transition

- Building polytopal schemes requires:
  - ⋆ Selecting degrees of freedom *(polynomials on vertices, edges, faces, elements)*.
  - ⋆ Implementing reconstruction operators as the solutions to local problems *(Riez representation problems)*.

  No need for explicit shape functions.

- Same approach can be applied to (complex) finite elements, without having to know their shape functions *(typically challenging in some FE for elasticity)*.

- Coding polytopal methods is facilitated by a rich mesh structure, well-suite polynomial bases and efficient libraries for polynomial integration.

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Thank you for your attention!

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