Adding a new finite element to FreeFem++:
the example of edge elements

Marcella Bonazzoli[1→2], Victorita Dolean[1,3], Frédéric Hecht[2], Francesca Rapetti[1], Pierre-Henri Tournier[2]

[1]LJAD, University of Nice Sophia Antipolis, Nice, France
[2]LJLL, Pierre and Marie Curie University, Paris, France - Inria Alpines
[3]University of Strathclyde, Glasgow, UK

December 15, 2017

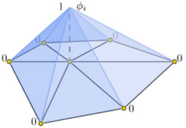
Definition of a finite element

A finite element (FE) is a triple (K, P, Σ):

- K - geometrical element of the mesh $\mathcal{T}_h$ over Ω
  ex: triangle in $2d$, tetrahedron in $3d$,
- P - finite-dimensional space of functions on K,
- Σ - set of linear *functionals* ξ_i acting on P (degrees of freedom).

Example of $\mathbb{P}_1$ Lagrange finite element (in 2d):

- K - triangle,
- P - space of polynomials of degree 1 on a triangle
  basis functions: barycentric coordinates
  $\lambda_{n_1}, \lambda_{n_2}, \lambda_{n_3}$ (hat functions)
- Σ - functionals giving the *values at mesh nodes*:
  $\xi_{n_i} : w \mapsto w(\mathbf{x}_{n_i})$



Definition of a finite element

$\mathbb{P}_1$ Lagrange finite element:

- basis functions: barycentric coordinates $\lambda_{n_1}, \lambda_{n_2}, \lambda_{n_3}$ (hat functions)
- degrees of freedom: values at mesh nodes $\quad \xi_{n_i} : w \mapsto w(\mathbf{x}_{n_i})$

Property (duality)

$$\xi_{n_i}(\lambda_{n_j}) = \lambda_{n_j}(\mathbf{x}_{n_i}) = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

Consequence: the coefficients of the interpolation operator Π_h are the values at mesh nodes

$$\Pi_h \colon H^1(T) \to V_h(T), \quad u \mapsto u_h = \sum_{j=1}^{m} c_j \, \lambda_{n_j}, \text{ with } c_j = \xi_{n_j}(u) = u(\mathbf{x}_{n_j})$$

Indeed if $\xi_{n_i}(\lambda_{n_j}) = \delta_{ij}$, then $\xi_{n_i}(u_h) = \sum_{j=1}^{m} c_j \, \xi_{n_i}(\lambda_{n_j}) = c_i$

Adding a new finite element to FreeFem++

To add a new finite element to FreeFem++, write a C++ plugin that defines a *C++ class*. Main ingredients

- the basis functions and their derivatives (class function `FB`): defined *locally* in a triangle/tetrahedron K,
- the interpolation operator (class constructor): define the computation of the degrees of freedom
  (quadrature formulas for more complicated FE)

  It requires degrees of freedom ξ_i in *duality* with the basis functions!

Edge finite elements

Edge finite elements are well suited for the approximation of the electric field in *Maxwell's equations*: conformal discretization of

$$H(\mathrm{curl}, \Omega) = \{\mathbf{v} \in L^2(\Omega)^3, \nabla \times \mathbf{v} \in L^2(\Omega)^3\}$$

In FreeFem++

- edge finite elements of degree 1 in 3d: keyword `Edge03d`,
- we added the edge elements of degree $2, 3$ in 3d $\Rightarrow$ to use them:
  - `load "Element_Mixte3d";`
  - keywords `Edge13d`, `Edge23d`.

[Bonazzoli, Dolean, Hecht, Rapetti, An example of explicit implementation strategy and preconditioning for the high order edge finite elements applied to the time-harmonic Maxwell's equations. *Accepted for publication in CAMWA. Preprint HAL <hal-01298938>*]

Edge finite elements

Tetrahedral mesh $\mathcal{T}_h$ of Ω, $V_h \subset H(\mathrm{curl}, \Omega)$

Low order edge finite elements (degree $r = 1$, Nédélec)

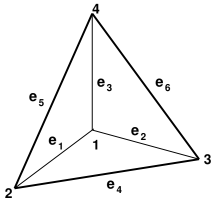
Given a tetrahedron $T \in \mathcal{T}_h$, the local *basis functions* are associated with the oriented *edges* $e = \{n_i, n_j\}$ of T:

$$\mathbf{w}^e = \lambda_{n_i} \nabla \lambda_{n_j} - \lambda_{n_j} \nabla \lambda_{n_i},$$

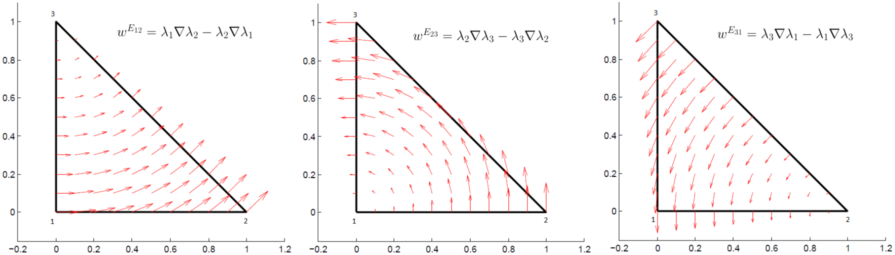
(the λ_{n_ℓ} are the barycentric coordinates).

- *oriented* edges,
- they are *vector* functions,
- they ensure the *continuity* of the *tangential* component across inter-element interfaces,
- degrees of freedom: $\xi_e : \mathbf{w} \mapsto \frac{1}{|e|} \int_e \mathbf{w} \cdot \mathbf{t}_e$,

duality: $\xi_e(\mathbf{w}^{e'}) = \delta_{ee'}$



Visualization of basis functions in 2d:



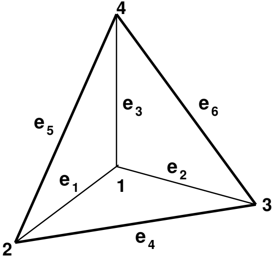
$$\xi_e : \mathbf{w} \mapsto \frac{1}{|e|} \int_e \mathbf{w} \cdot \mathbf{t}_e, \quad \xi_e(\mathbf{w}^{e'}) = \delta_{ee'} = \begin{cases} 1 & \text{if } e' = e \\ 0 & \text{if } e' \neq e \end{cases}$$

Generators of degree $r = k + 1$

Given $T \in \mathcal{T}_h$, for all oriented edges e of T and for all multi-indices $\mathbf{k} = (k_1, k_2, k_3, k_4)$ of weight $k = k_1 + k_2 + k_3 + k_4$, define:

$$\mathbf{w}^{\{\mathbf{k},e\}} = \lambda^{\mathbf{k}} \mathbf{w}^e, \qquad \text{where } \lambda^{\mathbf{k}} = (\lambda_{n_1})^{k_1} (\lambda_{n_2})^{k_2} (\lambda_{n_3})^{k_3} (\lambda_{n_4})^{k_4}.$$

Only barycentric coordinates! Still $V_h \subset H(\text{curl}, \Omega)$



E.g. degree $r = 2 \rightarrow k = 1$

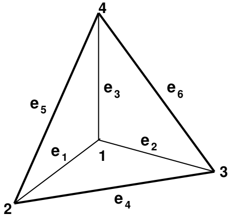
$\lambda_1 \mathbf{w}^{e_1}, \lambda_2 \mathbf{w}^{e_1}, \lambda_3 \mathbf{w}^{e_1}, \lambda_4 \mathbf{w}^{e_1},$
$\lambda_1 \mathbf{w}^{e_2}, \lambda_2 \mathbf{w}^{e_2}, \lambda_3 \mathbf{w}^{e_2}, \lambda_4 \mathbf{w}^{e_2},$
$\lambda_1 \mathbf{w}^{e_3}, \lambda_2 \mathbf{w}^{e_3}, \lambda_3 \mathbf{w}^{e_3}, \lambda_4 \mathbf{w}^{e_3},$
$\lambda_1 \mathbf{w}^{e_4}, \lambda_2 \mathbf{w}^{e_4}, \lambda_3 \mathbf{w}^{e_4}, \lambda_4 \mathbf{w}^{e_4},$
$\lambda_1 \mathbf{w}^{e_5}, \lambda_2 \mathbf{w}^{e_5}, \lambda_3 \mathbf{w}^{e_5}, \lambda_4 \mathbf{w}^{e_5},$
$\lambda_1 \mathbf{w}^{e_6}, \lambda_2 \mathbf{w}^{e_6}, \lambda_3 \mathbf{w}^{e_6}, \lambda_4 \mathbf{w}^{e_6}.$

Select linearly independent basis functions! (dim = 20)

[Rapetti, Bossavit, Whitney forms of higher degree, *SIAM J. Num. Anal.*, 47(3), 2009]

High order edge finite elements

The basis functions



$e_1 = \{1,2\}$, $e_2 = \{1,3\}$, $e_3 = \{1,4\}$, $e_4 = \{2,3\}$,
$e_5 = \{2,4\}$, $e_6 = \{3,4\}$,
$f_1 = \{2,3,4\}$, $f_2 = \{1,3,4\}$, $f_3 = \{1,2,4\}$, $f_4 = \{1,2,3\}$.

degree $r = 2$:

- *Edge-type* basis functions:

  $\mathbf{w}_1 = \lambda_1 \mathbf{w}^{e_1}$, $\mathbf{w}_2 = \lambda_2 \mathbf{w}^{e_1}$, $\quad \mathbf{w}_3 = \lambda_1 \mathbf{w}^{e_2}$, $\mathbf{w}_4 = \lambda_3 \mathbf{w}^{e_2}$,

  $\mathbf{w}_5 = \lambda_1 \mathbf{w}^{e_3}$, $\mathbf{w}_6 = \lambda_4 \mathbf{w}^{e_3}$, $\quad \mathbf{w}_7 = \lambda_2 \mathbf{w}^{e_4}$, $\mathbf{w}_8 = \lambda_3 \mathbf{w}^{e_4}$,

  $\mathbf{w}_9 = \lambda_2 \mathbf{w}^{e_5}$, $\mathbf{w}_{10} = \lambda_4 \mathbf{w}^{e_5}$, $\quad \mathbf{w}_{11} = \lambda_3 \mathbf{w}^{e_6}$, $\mathbf{w}_{12} = \lambda_4 \mathbf{w}^{e_6}$,

- *Face-type* basis functions:

  $\mathbf{w}_{13} = \lambda_4 \mathbf{w}^{e_4}$, $\mathbf{w}_{14} = \lambda_3 \mathbf{w}^{e_5}$, $\quad \mathbf{w}_{15} = \lambda_4 \mathbf{w}^{e_2}$, $\mathbf{w}_{16} = \lambda_3 \mathbf{w}^{e_3}$,

  $\mathbf{w}_{17} = \lambda_4 \mathbf{w}^{e_1}$, $\mathbf{w}_{18} = \lambda_2 \mathbf{w}^{e_3}$, $\quad \mathbf{w}_{19} = \lambda_3 \mathbf{w}^{e_1}$, $\mathbf{w}_{20} = \lambda_2 \mathbf{w}^{e_2}$.

  Choice using the *global numbers* of the vertices!

Revisitation of classical dofs

Define the dofs on $T \in \mathcal{T}_h$ for degree $r \geq 1$ as the functionals:

$$\xi_e : \mathbf{w} \mapsto \frac{1}{|e|} \int_e (\mathbf{w} \cdot \mathbf{t}_e)\, q, \qquad \forall\, q \in \mathbb{P}_{r-1}(e),\ \forall\, e \in \mathcal{E}(T),$$

$$\xi_f : \mathbf{w} \mapsto \frac{1}{|f|} \int_f (\mathbf{w} \cdot \mathbf{t}_{f,i})\, q, \qquad \forall\, q \in \mathbb{P}_{r-2}(f),\ \forall\, f \in \mathcal{F}(T),$$

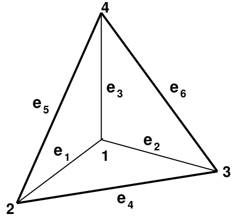
$\mathbf{t}_{f,i}$ two sides of f, $i = 1, 2$,

$$\xi_T : \mathbf{w} \mapsto \frac{1}{|T|} \int_T (\mathbf{w} \cdot \mathbf{t}_{T,i})\, q, \qquad \forall\, q \in \mathbb{P}_{r-3}(T),$$

$\mathbf{t}_{T,i}$ three sides of T, $i = 1, 2, 3$.

As polynomials q, use *products of barycentric coordinates*

[Bonazzoli, Rapetti, High order finite elements in numerical electromagnetism: dofs and generators in duality, *NUMA* 2017]



$e_1 = \{1,2\}$, $e_2 = \{1,3\}$, $e_3 = \{1,4\}$, $e_4 = \{2,3\}$,
$e_5 = \{2,4\}$, $e_6 = \{3,4\}$,
$f_1 = \{2,3,4\}$, $f_2 = \{1,3,4\}$, $f_3 = \{1,2,4\}$, $f_4 = \{1,2,3\}$.

degree $r = 2$:
for $e = \{n_i, n_j\}$, $\mathbb{P}_1(e) = \text{span}(\lambda_{n_i}, \lambda_{n_j})$;
$\mathbb{P}_0(f) = \text{span}(1)$; no volume dofs

- *Edge-type* dofs:

$$\xi_1 : \mathbf{w} \mapsto \frac{1}{|e_1|} \int_{e_1} (\mathbf{w} \cdot \mathbf{t}_{e_1})\, \lambda_1, \quad \xi_2 : \mathbf{w} \mapsto \frac{1}{|e_1|} \int_{e_1} (\mathbf{w} \cdot \mathbf{t}_{e_1})\, \lambda_2, \quad \ldots$$

$$\xi_{11} : \mathbf{w} \mapsto \frac{1}{|e_6|} \int_{e_6} (\mathbf{w} \cdot \mathbf{t}_{e_6})\, \lambda_3, \quad \xi_{12} : \mathbf{w} \mapsto \frac{1}{|e_6|} \int_{e_6} (\mathbf{w} \cdot \mathbf{t}_{e_6})\, \lambda_4,$$

- *Face-type* dofs:

$$\xi_{13} : \mathbf{w} \mapsto \frac{1}{|f_1|} \int_{f_1} (\mathbf{w} \cdot \mathbf{t}_{e_4}), \quad \xi_{14} : \mathbf{w} \mapsto \frac{1}{|f_1|} \int_{f_1} (\mathbf{w} \cdot \mathbf{t}_{e_5}), \quad \ldots$$

$$\xi_{19} : \mathbf{w} \mapsto \frac{1}{|f_4|} \int_{f_4} (\mathbf{w} \cdot \mathbf{t}_{e_1}), \quad \xi_{20} : \mathbf{w} \mapsto \frac{1}{|f_4|} \int_{f_4} (\mathbf{w} \cdot \mathbf{t}_{e_2}).$$

Same choice as for generators

To restore duality between basis functions $\tilde{\mathbf{w}}_j$ and dofs ξ_i:

$$\tilde{V}_{ij} = \xi_i(\tilde{\mathbf{w}}_j) = \delta_{ij}$$

take *linear combinations* of the old basis functions $\mathbf{w}_j$ with coefficients given by the entries of V^{-1}.

Properties of the matrix $V_{ij} = \xi_i(\mathbf{w}_j)$:

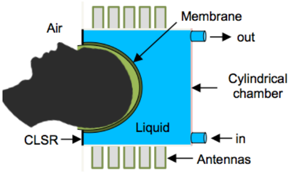
- V does not depend on the metrics of the tetrahedron T (but pay attention to orientation!),
- V is blockwise lower triangular,
- V^{-1} entries are integer numbers.

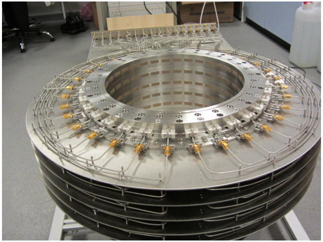
[Bonazzoli, Dolean, Hecht, Rapetti, An example of explicit implementation strategy and preconditioning for the high order edge finite elements applied to the time-harmonic Maxwell's equations. *Accepted for publication in CAMWA. Preprint HAL <hal-01298938>*]

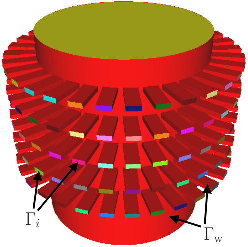
degree $r = 2$,
basis functions and dofs listed as before (ordering and choice!):

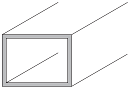
$$V^{-1} = \begin{bmatrix}
4 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-2 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 4 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -2 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 4 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -2 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 4 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -2 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -4 & -2 & 2 & -2 & 2 & 4 & 8 & -4 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2 & -2 & -4 & -2 & -4 & -2 & -4 & 8 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -4 & -2 & 2 & -2 & 0 & 0 & 0 & 0 & 2 & 4 & 0 & 0 & 8 & -4 & 0 & 0 & 0 & 0 \\
0 & 0 & 2 & -2 & -4 & -2 & 0 & 0 & 0 & 0 & -4 & -2 & 0 & 0 & -4 & 8 & 0 & 0 & 0 & 0 \\
-4 & -2 & 0 & 0 & 2 & -2 & 0 & 0 & 2 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & -4 & 0 & 0 \\
2 & -2 & 0 & 0 & -4 & -2 & 0 & 0 & -4 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & -4 & 8 & 0 & 0 \\
-4 & -2 & 2 & -2 & 0 & 0 & 2 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & -4 \\
2 & -2 & -4 & -2 & 0 & 0 & -4 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -4 & 8
\end{bmatrix}$$

Microwave brain imaging system prototype (EMTensor, Austria):
cylindrical chamber with 5 rings of 32 antennas (rectangular waveguides)









Numerical results

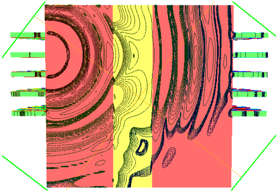
Variational formulation in FreeFem++

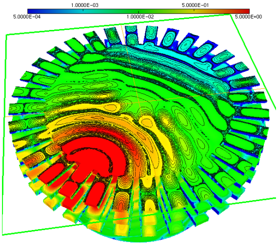
$$\int_\Omega \left[(\nabla \times \mathbf{E}) \cdot (\nabla \times \mathbf{v}) - \gamma^2 \mathbf{E} \cdot \mathbf{v}\right] + \int_{\bigcup_{i=1}^{160} \Gamma_i} \mathrm{i}\beta(\mathbf{E} \times \mathbf{n}) \cdot (\mathbf{v} \times \mathbf{n})$$
$$= \int_{\Gamma_j} \mathbf{g}_j \cdot \mathbf{v}, \qquad \forall \mathbf{v} \in V_h \subset V, \quad V = \{\mathbf{v} \in H(\mathrm{curl}, \Omega), \mathbf{v} \times \mathbf{n} = 0 \text{ on } \Gamma_w\}.$$

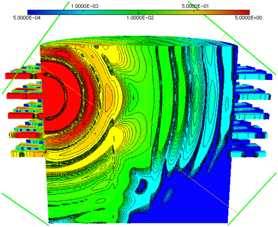
```
load "Element_Mixte3d"
fespace Vh(Th,Edge13d);  // Edge03d, Edge13d, Edge23d
Vh<complex> [Ex,Ey,Ez], [vx,vy,vz];

macro Curl(ux,uy,uz) [dy(uz)-dz(uy),dz(ux)-dx(uz),dx(uy)-dy(ux)] // EOM
macro Nvec(ux,uy,uz) [uy*N.z-uz*N.y,uz*N.x-ux*N.z,ux*N.y-uy*N.x] // EOM

varf medimax([Ex,Ey,Ez], [vx,vy,vz]) =
                 int3d(Th)(Curl(Ex,Ey,Ez)'*Curl(vx,vy,vz)
                                  - gamma^2*[Ex,Ey,Ez]'*[vx,vy,vz])
               + int2d(Th,ports)(1i*beta*Nvec(Ex,Ey,Ez)'*Nvec(vx,vy,vz))
               + on(guide,Ex=0,Ey=0,Ez=0);
varf medimaxRhs([Ex,Ey,Ez], [vx,vy,vz]) =
                 int2d(Th,portj)([vx,vy,vz]'*[Gjx,Gjy,Gjz])
               + on(guide,Ex=0,Ey=0,Ez=0);
```

Plastic-filled cylinder (non dissipative!) immersed in the matching solution inside the imaging chamber.
One transmitting antenna in the second ring from the top.

Norm of the real part of the solution field:





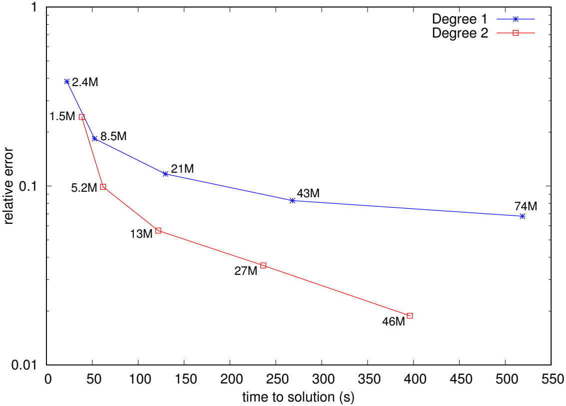


[Bonazzoli, Dolean, Rapetti, Tournier. Parallel preconditioners for high order discretizations arising from full system modeling for brain microwave imaging. 2017]

Numerical results (FreeFem++ with HPDDM)

Solve 32 linear systems (same matrix, different right-hand sides)
Pseudo-block GMRES with a Domain Decomposition preconditioner
1024 cores on Curie supercomputer

Reference solution with 114 million (complex-valued) unknowns.
Edge finite elements of degree $1, 2$ for different mesh sizes:



Relative error

$$\text{Err} = \frac{\sqrt{\sum_{j,i} |S_{ij} - S_{ij}^{\mathbf{ref}}|^2}}{\sqrt{\sum_{j,i} |S_{ij}^{\mathbf{ref}}|^2}}$$

(the S_{ij} are the measurable quantities, calculated from the solution $\mathbf{E}$)

For Err ~ 0.1
degree 1: 21 M unks, 130 s
degree 2: 5 M unks, 62 s

Conclusion

- The user can *add new finite elements* to FreeFem++: define basis functions and interpolation operator (need duality!).
- FreeFem++ is based on a *natural transcription* of the variational formulation of the considered boundary value problem.
- The *high order* finite elements make it possible to attain a given accuracy with much fewer unknowns and much less computing time than the degree 1 approximation.
- The *parallel* implementation in HPDDM of the *domain decomposition preconditioner* is essential to be able to solve the considered large scale linear systems.

Conclusion

Thank you for your attention!