Hybrid iterative/direct strategies for solving the three-dimensional time-harmonic Maxwell equations discretized by discontinuous Galerkin methods

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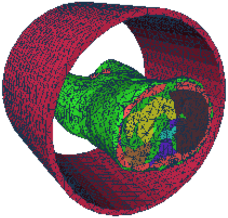
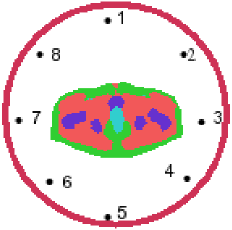
Hyperthermia example

Local hyperthermia using electromagnetic waves

Treatment of a cancerous tumour by a local increase of the temperature inside the tumour.
Means: use of a radio-frequency or microwave electromagnetic field.



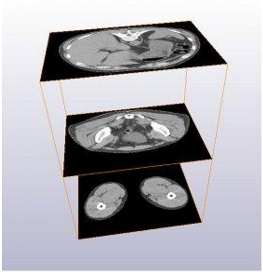


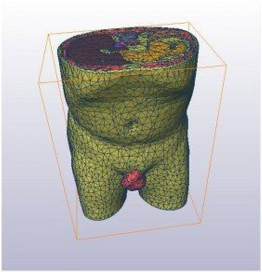
(ZIB, Lab. AMPERE, ...)

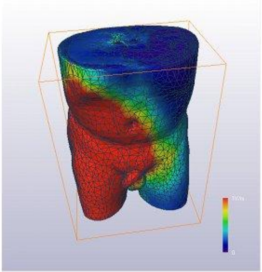
Hyperthermia example

Therapeutic planification

1. Segmenting the scanar cuts,
2. Meshing the body,
3. Electromagnetic and thermal computing + optimization of the parameters.







Problem under consideration

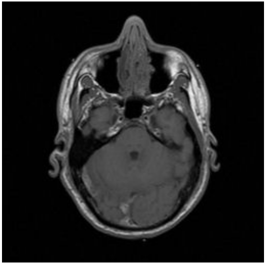
- First-order time-harmonic Maxwell's system (dimensionless):

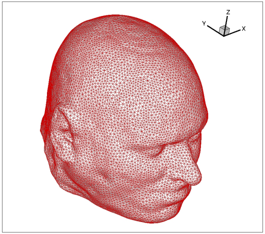
$$\begin{cases} \mathrm{i}\omega\varepsilon_r \mathbf{E} - \operatorname{rot} \mathbf{H} = -\mathbf{J}_{\mathrm{imp}}, \\ \mathrm{i}\omega\mu_r \mathbf{H} + \operatorname{rot} \mathbf{E} = 0. \end{cases}$$

  ω: angular wave frequency, μ_r: relative permeability, ε_r: relative permittivity, $\mathbf{J}_{\mathrm{imp}}$: imposed current, $(\mathbf{E}, \mathbf{H})$: electromagnetic field.

- Other features:
  - Free space,
  - Antenna: source term in current, internal to the domain. (Incident plane wave also considered in the following),
  - Linear isotropic material at a given frequency,
  - Complex-shaped geometry (unstructured mesh) and heterogeneous media.

Mobile phone example





(HEADEXP collaborative research team.)

Normalization purpose

1. Segmenting the scanar cuts,
2. Meshing the head,
3. Electromagnetic and thermal computing,
4. Generating statistics among a lot of configurations.

Outline of the talk

General approach

- A Lot of work about optimized Schwarz methods for scalar problems: Laplacian, convection-diffusion, Helmholtz, ...
- Some Separate works led concerning problem with underlying systems of PDEs.
  Ex.: for Maxwell, several works concerning the second-order vector wave equation.

A more systematic approach

1. Find a systematic way to reduce a system of PDEs to a scalar PDE,
2. Apply the optimized Schwarz to the scalar PDE deduced,
3. Go back to the system of PDEs with the optimized conditions.

(V. Dolean, F. Nataf and G. Rapin, New constructions of domain decomposition methods for systems of PDEs. CRAS, 340, (2005), no 9, 693–696.)

Application to the Maxwell's system in 2D

- Maxwell equations in the whole space:

$$\mathcal{A}(\mathbf{E}, H_z) = \begin{pmatrix} \mathrm{i}\varepsilon_r\omega & 0 & -\partial_y \\ 0 & \mathrm{i}\varepsilon_r\omega & \partial_x \\ -\partial_y & \partial_x & \mathrm{i}\mu_r\omega \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ H_z \end{pmatrix} = \mathbf{J}. \qquad (1)$$

- Fourier transform with respect to y, $\partial_y \to \mathrm{i}k$

$$\hat{\mathcal{A}}(\hat{\mathbf{E}}, \hat{H}_z) = \begin{pmatrix} \mathrm{i}\varepsilon_r\omega & 0 & -ik \\ 0 & \mathrm{i}\varepsilon_r\omega & \partial_x \\ -ik & \partial_x & \mathrm{i}\mu_r\omega \end{pmatrix} \begin{pmatrix} \hat{E}_x \\ \hat{E}_y \\ \hat{H}_z \end{pmatrix}. \qquad (2)$$

Application to the Maxwell's system in 2D

Using the Smith factorization, it can also be written under the form:

$$\hat{\mathcal{A}} = \hat{E}\hat{D}\hat{F}, \tag{3}$$

with:

$$\hat{D} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & (\varepsilon_r \mu_r \omega^2 - k^2 + \partial_{xx}) \end{pmatrix}$$

$$\hat{E} = \begin{pmatrix} \mathrm{i}\varepsilon_r\omega & \frac{\varepsilon_r\omega\partial_x}{k} & \frac{i}{k} \\ 0 & \mathrm{i}\varepsilon_r\omega & 0 \\ -ik & 0 & 0 \end{pmatrix} \text{ and } \hat{F} = \begin{pmatrix} 1 & \frac{\mathrm{i}\partial_x}{k} & -\frac{\mu_r\omega}{k} \\ 0 & 1 & -\frac{\mathrm{i}\partial_x}{\varepsilon_r\omega} \\ 0 & 0 & 1 \end{pmatrix}$$

Using this factorization, the Fourier transformed version of problem (1) can be formally written as:

$$\hat{D}\hat{\mathbf{U}} = \hat{E}^{-1}\hat{\mathbf{J}},\ \hat{\mathbf{U}} = \hat{F}\hat{\mathbf{W}}. \tag{4}$$

Brief overview of the strategy

- Using the previous equivalence, the following problem is considered:
  - the Helmholtz equation on the domain $\Omega = \mathbb{R}^2$

$$-\left(\tilde{\omega}^2 + \Delta\right) H_z = \tilde{f}, \qquad (5)$$

  - the Sommerfeld radiation conditions

$$\lim_{r\to\infty} r\left(\frac{\partial H_z}{\partial r} - \mathrm{i}\tilde{\omega} u\right) = 0, \qquad (6)$$

    where $r = |\mathbf{x}|$.
- Decomposition in two half-space $\Omega_1 = (-\infty, b) \times \mathbb{R}$ and $\Omega_2 = (a, \infty) \times \mathbb{R}$. $L = b - a$: overlap.

Brief overview of the strategy

- An initial magnetic field component $H_z^{l,0}$ on each subdomain Ω_l, $l = 1, 2$.
- The n-th iterates $H_z^{1,n}$ and $H_z^{2,n}$ are the solutions of:

$$\begin{cases} -(\tilde{\omega}^2 + \Delta)H_z^{1,n} = \tilde{f}, & \text{in } \Omega_1 \\ \mathcal{B}_1(H_z^{1,n})(b, y) = \mathcal{B}_1(H_z^{2,n-1})(b, y), & y \in \mathbb{R}, \end{cases}$$
$$\begin{cases} -(\tilde{\omega}^2 + \Delta)H_z^{2,n} = \tilde{f}, & \text{in } \Omega_2 \\ \mathcal{B}_2(H_z^{2,n})(a, y) = \mathcal{B}_2(H_z^{1,n-1})(a, y), & y \in \mathbb{R}, \end{cases} \quad (7)$$

with, moreover, Sommerfeld radiation conditions on the unbounded part of each subdomain.

Optimized Schwarz question

How to find the most efficient interface operators $\mathcal{B}_1$ and $\mathcal{B}_2$?

Brief overview of the strategy

The canonical approach to determine the nicest transmission operator:

1. Fourier transform following the variables tangential to the interfaces, *i.e.* here y.
2. Find the analytic solution of the equations on each subdomain and express the convergence rate ρ.
   $\rightarrow$ the best operator is non local :-(.
3. Find the best approximant into a class of simple interface operators: order 0 or order 2.
   Ex.: order 0 operators. $\mathcal{B}_1 = \partial_x + \alpha_1$ and $\mathcal{B}_2 = \partial_x + \alpha_2$.
   - Express ρ with this particular local operator,
   - Minimize ρ on the a range of frequency valid on the discretization grid: $(k_{\min}, k_-) \cup (k_+, k_{\max})$.
     $k_{\min} = C_1/L$ (L: diameter of the subdomain), $k_{\max} = C_2/h$, k_- and k_- used to exclude ω from the range.

Brief overview of the strategy

Different choices:

- $\alpha_1 = \alpha_2 = \mathrm{i}\tilde{\omega}$. Després interface conditions (1991).
- $\alpha_1 = \alpha_2$ Symmetric optimized Robin interface conditions.
- $\alpha_1 \neq \alpha_2$ Two-sided optimized Robin interface conditions (Gander, Nataf and Magoulès, 2002).

	With overlap, $L = h$		Without overlap, $L = 0$	
Case	ρ	parameters	ρ	parameters
Després	$1 - \sqrt{k_+ - \tilde{\omega}^2}h$	None	1	None
Symmetric	$1 - 2C_{\tilde{\omega}}^{\frac{1}{6}} h^{\frac{1}{3}}$	$p = \frac{C_{\tilde{\omega}}^{\frac{1}{3}}}{2h^{\frac{1}{3}}}$	$1 - \frac{\sqrt{2}C_{\tilde{\omega}}^{\frac{1}{4}}}{\sqrt{C}}\sqrt{h}$	$p = \frac{\sqrt{C}C_{\tilde{\omega}}^{\frac{1}{4}}}{\sqrt{2}\sqrt{h}}$
Two-sided	$1 - 2^{\frac{2}{5}} C_{\tilde{\omega}}^{\frac{1}{10}} h^{\frac{1}{5}}$	$\begin{cases} p_1 = \frac{C_{\tilde{\omega}}^{\frac{2}{5}}}{2^{\frac{7}{5}} h^{\frac{1}{5}}} \\ p_2 = \frac{C_{\tilde{\omega}}^{\frac{1}{5}}}{2^{\frac{6}{5}} h^{\frac{3}{5}}} \end{cases}$	$1 - \frac{C_{\tilde{\omega}}^{\frac{1}{8}}}{C^{\frac{1}{4}}} h^{\frac{1}{4}}$	$\begin{cases} p_1 = \frac{C_{\tilde{\omega}}^{\frac{3}{8}} C^{\frac{1}{4}}}{2h^{\frac{1}{4}}} \\ p_2 = \frac{C_{\tilde{\omega}}^{\frac{1}{8}} C^{\frac{3}{4}}}{h^{\frac{3}{4}}} \end{cases}$

Asymptotic convergence factor and optimal choice of the parameters for the transmission conditions. $\alpha_l = p_l(1 - \mathrm{i})$, $l = 1, 2$.

Optimized transmission conditions for Maxwell's system

The following algorithm applied to Maxwell's equations with Silver-Müller radiation conditions on the unbounded part of the domain:

$$\lim_{r\to\infty} r\left(\mathbf{H}\times\mathbf{n}-\mathbf{E}\right)=0 \tag{8}$$

where $r=|\mathbf{x}|$, $\mathbf{n}=\mathbf{x}/|\mathbf{x}|$ and $\mathbf{H}=(0,0,H_z)^t$, $\mathbf{E}=(E_x,E_y,0)^t$

$$\left\{\begin{array}{rcll} \mathcal{A}(\mathbf{E},H_z)^{1,n} & = & \tilde{\mathbf{J}}_1, & \text{in } \Omega_1 \\ (-E_y+\frac{\alpha_1}{\mathrm{i}\varepsilon_r\omega}H_z)^{1,n}(b,y) & = & (-E_y+\frac{\alpha_1}{\mathrm{i}\varepsilon_r\omega}H_z)^{2,n-1}(b,y), & y\in\mathbb{R}, \end{array}\right.$$

$$\left\{\begin{array}{rcll} \mathcal{A}(\mathbf{E},H_z)^{2,n} & = & \tilde{\mathbf{J}}_2, & \text{in } \Omega_2 \\ (E_y+\frac{\alpha_2}{\mathrm{i}\varepsilon_r\omega}H_z)^{2,n}(a,y) & = & (E_y+\frac{\alpha_2}{\mathrm{i}\varepsilon_r\omega}H_z)^{1,n-1}(a,y), & y\in\mathbb{R}, \end{array}\right. \tag{9}$$

is equivalent to the iterative procedure (7).

Schwarz algorithm: algorithmic aspects

- Global system (two-sudomain case)

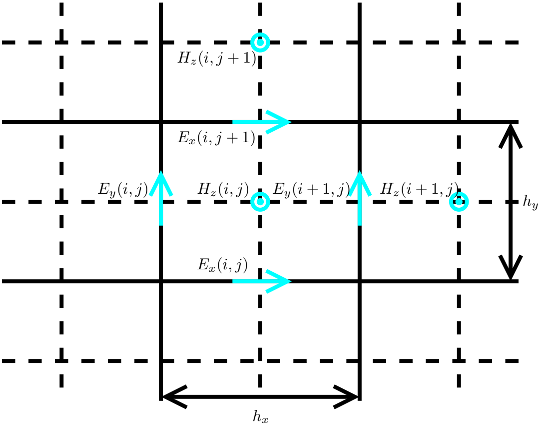
$$\begin{pmatrix} A_1 & 0 & R_1 & 0 \\ 0 & A_2 & 0 & R_2 \\ 0 & -B_2 & \mathrm{Id} & 0 \\ -B_1 & 0 & 0 & \mathrm{Id} \end{pmatrix} \begin{pmatrix} \mathbf{W}_h^1 \\ \mathbf{W}_h^2 \\ \lambda_h^1 \\ \lambda_h^2 \end{pmatrix} = \begin{pmatrix} \mathbf{f}_h^1 \\ \mathbf{f}_h^2 \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}$$

- Interface system: $\mathcal{T}_h \lambda_h = \mathbf{g}_h$

$$\mathcal{T}_h = \begin{pmatrix} \mathrm{Id} & B_2 A_2^{-1} R_2 \\ B_1 A_1^{-1} R_1 & \mathrm{Id} \end{pmatrix} \quad \text{and} \quad \mathbf{g}_h = \begin{pmatrix} B_2 A_2^{-1} F^2 \\ B_1 A_1^{-1} F^1 \end{pmatrix}$$

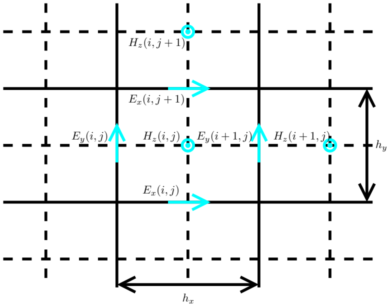
  - Schwarz iteration $\Leftrightarrow \lambda_h^{p+1} = (\mathrm{Id} - \mathcal{T}_h)\lambda_h^p + \mathbf{d}_h$
  - Accelerated iteration: Krylov method

A widely used discretization for Maxwell's system



Primal (solid lines) and dual (dashed lines) grids for discretizing the Maxwell equations. The component H_z is approximated on the dual grid contrary to $\mathbf{E}$ which is approximated on the primal grid.

A widely used discretization for Maxwell's system



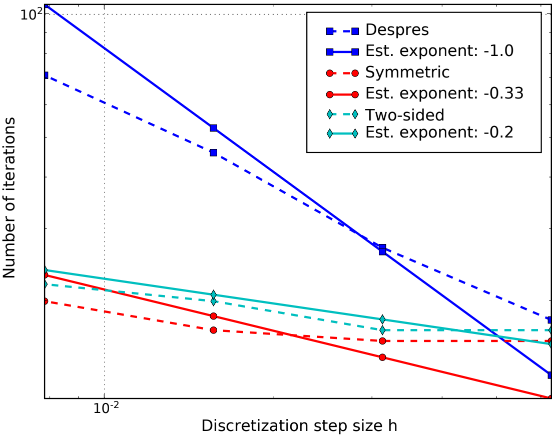
$$\left\{\begin{array}{lcl} \mathrm{i}\varepsilon_r\omega E_x(i,j) - (D_y^- H_z)(i,j) & = & 0, \\ \mathrm{i}\varepsilon_r\omega E_y(i,j) + (D_x^- H_z)(i,j) & = & 0, \\ \mathrm{i}\mu_r\omega H_z(i,j) - (D_y^+ E_x)(i,j) - (D_x^+ E_y)(i,j) & = & 0, \ \forall i,j \in \mathbb{Z}. \end{array}\right. \quad (10)$$

where $D_x^\pm$ and $D_y^\pm$ are the classical finite difference operators.

Toy problem for testing the theory

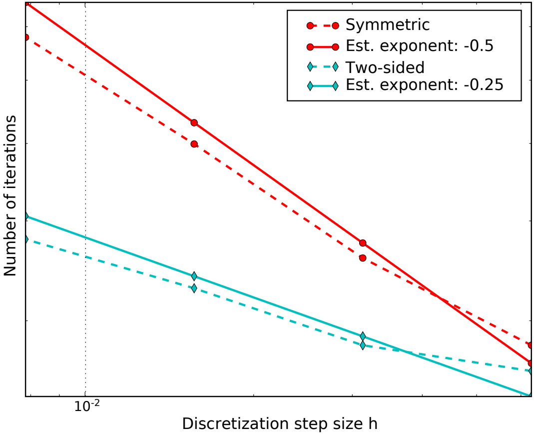
- $\Omega = (0;1)^2$, $\Omega_1 = (0;\alpha) \times (0;1)$, $\Omega_2 = (\beta;1) \times (0;1)$.
- Incident plane wave $(\mathbf{E}^{\rm inc}, H^{\rm inc}) = \exp(-\mathrm{i}\omega x)(0,1,1)$ with $\omega = 2\pi$.
- Overlapping when used is equal to h.

Results obtained



Overlapping subdomains.

Results obtained



Non-overlapping subdomains.

A non-conforming approximation space

The approximate solution $(\mathbf{E}_h, H_{z,h})$ of the Maxwell system is an element of V_h^3 where V_h:

$$V_h = \left\{ V \in L^2(\Omega) \ / \ \forall K \in T_h, \quad V_{|K} \in P_k(K) \right\}. \qquad (11)$$

No particular continuity constraint is enforced at the interface of each element.

- A total flexibility for the approximation inside each element:
  - makes easier *hp*-adaptivity,
  - treatment of non-admissible mesh is included.
- Main drawback: a huge number of unknowns compared to conforming finite element methods.

Weak formulation

$$\begin{cases} a(H_{z,h},\mathrm{G}) + \overline{b(\mathrm{G},\mathbf{E}_h)} = \displaystyle\int_{\partial\Omega} \frac{1}{2}\left(\mathbf{H}^{\mathrm{inc}} - N_{\mathbf{n}}^t\mathbf{E}^{\mathrm{inc}}\right)\overline{\mathrm{G}}ds, \\ b(H_{z,h},\mathbf{F}) - c(\mathbf{E}_h,\mathbf{F}) = \displaystyle\int_{\partial\Omega} \frac{1}{2}(N_{\mathbf{n}}\mathbf{H}^{\mathrm{inc}} - N_{\mathbf{n}}N_{\mathbf{n}}^t\mathbf{E}^{\mathrm{inc}})^t\overline{\mathbf{F}}ds, \\ \forall \mathbf{F} \in V_h^2, \mathbf{G} \in V_h. \end{cases}$$

where $N_{\mathbf{n}} = \begin{pmatrix} n_x & n_y \end{pmatrix}^t$, $[\![\cdot]\!]_T$: jump of the tangential component, $\{\cdot\}$: average.

$$a(H_{z,h},\mathrm{G}) = \int_{\Omega_h} \mathrm{i}\omega\mu H_{z,h}\overline{\mathrm{G}}dv + \sum_{F\in\Gamma^0}\int_F \alpha H_{z,h}\overline{\mathrm{G}}ds + \int_{\partial\Omega}\frac{1}{2}H_{z,h}\overline{\mathrm{G}}ds,$$

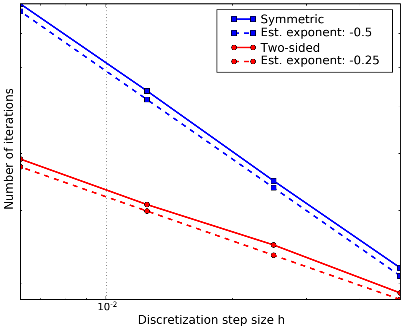
$$b(\mathrm{G},\mathbf{E}_h) = \sum_{K\in\mathcal{T}_h}\int_K \mathrm{G}\,\mathrm{rot}(\overline{\mathbf{E}_h})dv - \sum_{F\in\Gamma^0}\int_F \{\mathrm{G}\}^t[\![\overline{\mathbf{E}_h}]\!]_T ds - \int_{\partial\Omega}\frac{1}{2}\mathrm{G}(N_{\mathbf{n}}^t\overline{\mathbf{E}_h})ds,$$

and finally:

$$c(\mathbf{E}_h,\mathbf{F}) = \int_{\Omega_h} \mathrm{i}\omega\varepsilon\mathbf{E}_h^t\overline{\mathbf{F}}dv + \sum_{F\in\Gamma^0}\int_F \alpha[\![\mathbf{E}_h]\!]_T^t[\![\overline{\mathbf{F}}]\!]_T ds + \int_{\partial\Omega}\frac{1}{2}(N_{\mathbf{n}}^t\mathbf{E}_h)(N_{\mathbf{n}}^t\overline{\mathbf{F}})ds.$$

Validation of the optimized transmission conditions

Triangular uniform mesh. $P_1(K)$ as the local space in each element K.
Upwind flux is considered.



Number of iterations against the mesh size h. Logarithmic scale.

Validation of the optimized transmission conditions

Three polynomial orders for the element interpolation (here quadrilateral elements are considered) and two different fluxes.

Flux	Q_0	Q_1	Q_2
Centered symmetric	0.48	0.46	0.49
Centered two-sided	0.27	0.26	0.23
Upwind symmetric	0.45	0.47	0.47
Upwind two-sided	0.37	0.26	0.25

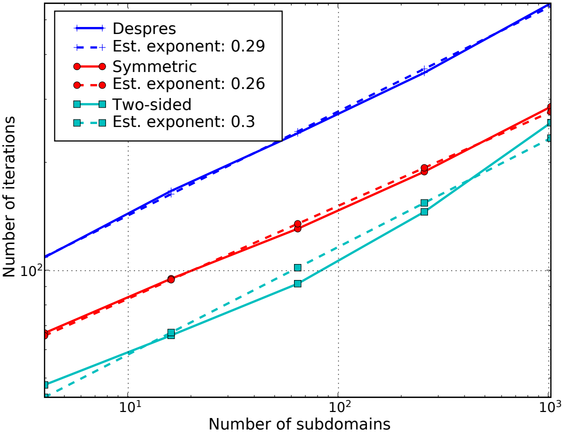
Estimated value of δ where $\rho = 1 - Ch^{\delta}$.

Summary

It seems that the behavior predicted by the theory is:

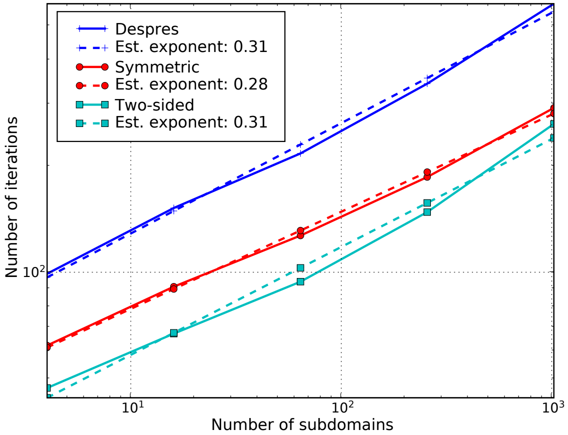
- roughly independent of the polynomial approximation,
- roughly independent of the numerical flux used.

Variation of the number of subdomains



Number of iterations against the number of subdomains. The number of dof is constant. Results for the centered flux.

Variation of the number of subdomains



Number of iterations against the number of subdomains. The number of dof is constant. Results for the upwind flux.

Schwarz algorithm: numerical and parallel performances

- Diffraction of a plane wave (F=1800 MHz)
- Model (artificial) problem

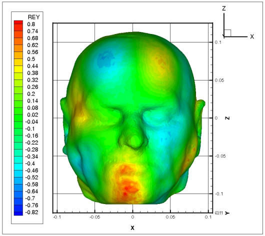
Tissue	ε_r	σ (S/m)	ρ (Kg/m^3)	λ (mm)
Skin	4.0	0.0	1100.0	26.73
Skull	1.5	0.0	1200.0	42.25
CSF	6.5	0.0	1000.0	20.33
Brain	4.0	0.0	1050.0	25.26

- Characteristics of the tetrahedral meshes (no telephone model)

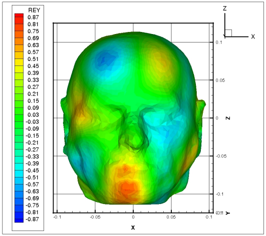
Mesh	# tetrahedra	L_{min} (mm)	Lmax (mm)	Lavg (mm)
M1	361,848	1.85	45.37	11.65
M2	1,853,832	1.15	24.76	6.93

Overview of the solutions

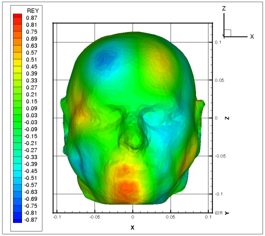
Real part of E_y



Mesh M2, $\mathbb{P}_0$-DGTH method



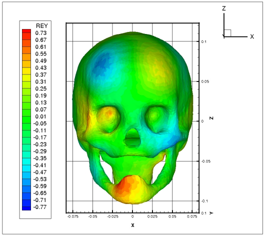
Mesh M1, $\mathbb{P}_1$-DGTH-c method



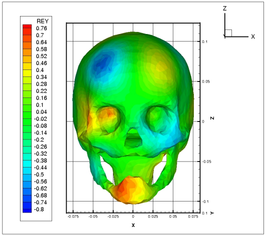
Mesh M1, $\mathbb{P}_1$-DGTH-u method

Overview of the solutions

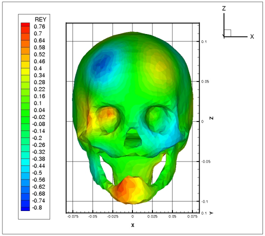
Real part of E_y



Mesh M2, $\mathbb{P}_0$-DGTH method



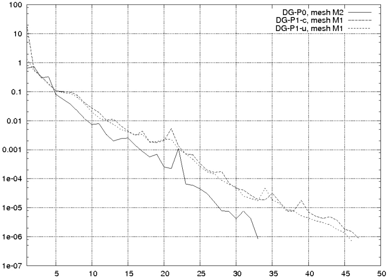
Mesh M1, $\mathbb{P}_1$-DGTH-c method



Mesh M1, $\mathbb{P}_1$-DGTH-u method

Details for the solution

- Interface system
  - BiCGstab(ℓ) (G.L.G. Sleijpen and D.R. Fokkema, ETNA, Vol.1, 1993)
  - $\ell = 6$
- Local systems
  - MUMPS multifrontal sparse solver (P.R. Amestoy, I.S. Duff and J.-Y. L'Excellent Comput. Meth. App. Mech. Engng., Vol 184, 2000)
  - L and U factors in 32 bit accuracy



Computational results

- Cluster of AMD Opteron/2.6 GHz nodes, Gigabit Ethernet/Myrinet
    - DG-$\mathbb{P}_1$-c: DGTH method with centered flux
    - DG-$\mathbb{P}_1$-u: DGTH method with upwind flux

Mesh	Method	Strategy	N_s	# it	CPU (min/max)	REAL
M1	DG-$\mathbb{P}_1$-c	DD-itref	96	47	346 sec/466 sec	714 sec
-	-	-	-	-	524 sec/715 sec	717 sec
-	DG-$\mathbb{P}_1$-u	DD-itref	96	47	347 sec/547 sec	765 sec
-	-	-	-	-	636 sec/685 sec	686 sec
M2	DG-$\mathbb{P}_0$-c	DD-itref	48	27	545 sec/770 sec	1350 sec
-	-	-	96	33	228 sec/322 sec	428 sec
-	-	-	-	-	415 sec/416 sec	417 sec

Mesh	Method	N_s	CPU (min/max)	RAM (min/max)	# dof
M1	DG-$\mathbb{P}_1$-c	96	64 sec/125 sec	640 MB/852 MB	8,684,352
-	DG-$\mathbb{P}_1$-u	96	80 sec/134 sec	633 MB/866 MB	-
M2	DG-$\mathbb{P}_0$-c	48	234 sec/374 sec	1432 MB/1836 MB	11,122,992
-	-	96	53 sec/ 98 sec	519 MB/ 684 MB	-

Some hidden difficulties

- The straightforward formulation of the Schwarz algorithm using a DG discretization for each sudomain leads to a discrete solution which is different from the discrete solution obtained by the DG discretization in the mono-domain.
  This is not the case with the staggered grid strategy and more generally with conforming finite element.
  $\Longrightarrow$ possible deteriotation of the accuracy of the method compared to the mono-domain solution.
- Second order optimized conditions leads to couple some elements wich have no relations in the initial scheme.
  $\Longrightarrow$ possible deterioration of the load balance for factorizing the subdomain problem.

Conclusion and perspectives

- Conclusion
  - A Well-known strategy for time-harmonic Maxwell's system.
  - Some promising results: theory and practice are compatible in 2D and Després conditions gives the first impression for 3D...
- Perpectives
  - ... But a lot of work remains to do: optimized conditions in 3D, a trick to keep the accuracy...
  - Switch from subdomain direct solver to an iterative solver: algebraic multigrid solver?
  - Addition of a coarse grid solver.
  - Equivalent approach in test for time-implicit situation.