Multiscale hybrid methods for time-domain electromagnetics

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Modeling context and challenges

MHM: formulation & algorithm

Numerical Results

Concluding remarks

Modeling context

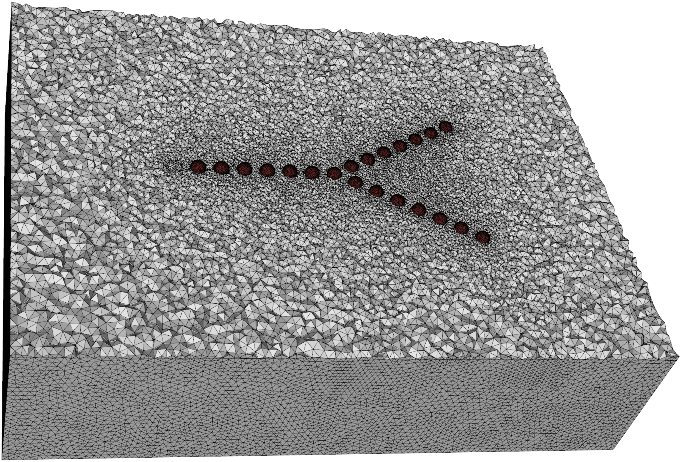
Numerical Nanophotonics

- Interaction of electromagnetic waves in the optical regime with nano-scaled structures
- Nano-Antennas, Nano-scaled optical waveguides ...

Numerical Challenges

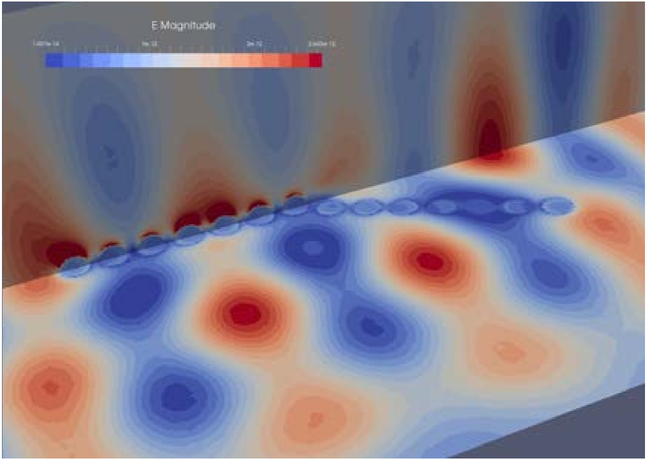
- Complex geometrical structures
- Heterogeneous propagation medium characteristics
- Strong energy concentration phenomena

Modeling context / Example: Y-waveguide



Y-shaped, 21 Au-nanospheres waveguide

Modeling context / Example: Y-waveguide



Snapshot of electric field magnitude

Modeling context

Numerical Nanophotonics

- Interaction of electromagnetic waves in the optical regime with nano-scaled structures
- Nano-Antennas, Nano-scaled optical waveguides ...

Numerical Challenges

- Complex geometrical structures
- Heterogeneous propagation medium characteristics
- Strong energy concentration phenomena

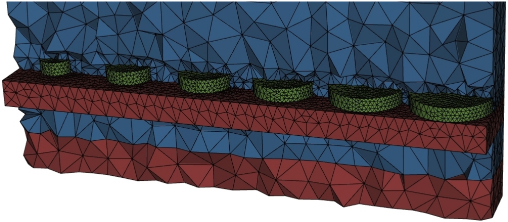
Computational challenge

- Realistic settings yield large problems...
- **We seek good parallelization properties!**

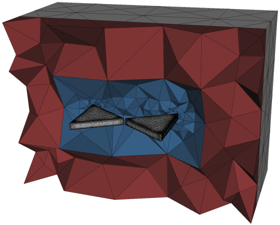
Discontinuous Galerkin Time-Domain Methods @ Nachos

DIOGENeS - DIscOntinuous GalErkin Nano Solver

- 3D Maxwell PDE system + Dispersion Models
- Perfectly-Matched Layers
- Affine & curvilinear elements - Hybrid unstructured/Cartesian meshes
- High-order nodal basis functions - Local order adaptation
- 2nd order / 4th order Leap-Frog - Low Storage Runge-Kutta
- Hybrid MIMD/SIMD parallelization (MPI+OpenMP)



Cylindric Antenna Array



Bow Tie Antenna

MHM for Maxwell

Past & present developments on MHM

- A family of multiscale methods
  - Upscaling of a solution lying on a coarse mesh
  - Intrinsically parallel
- Flows in porous media[3] (Darcy) (@ LNCC)
- Elasticity[4] (@ LNCC)
- Elastodynamics (@ LNCC + INRIA) (M.-H. Lallemand's talk)

Electromagnetics: The Maxwell PDE system

Electromagnetic waves in heterogeneous media $\rightsquigarrow$ Maxwell's equation.

$$\begin{cases} \mu(\mathbf{x})\dfrac{\partial \mathbf{H}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0}, \\ \varepsilon(\mathbf{x})\dfrac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{H} = \mathbf{J} - \sigma(\mathbf{x})\mathbf{E}. \end{cases}$$

$\mathbf{E}$ electric field
$\mathbf{H}$ magnetic field
$\mathbf{J}$ external current
σ conductivity
ε permittivity
μ permeability

[3] Harder, C., et al. " A Family of Multiscale Hybrid-Mixed Finite Element Methods for the Darcy Equation with Rough Coefficients ", JCP, Vol. 245, pp. 107-130, 2013

[4] Harder, C., et al. "New finite elements for elasticity in two and three-dimensions", LNCC

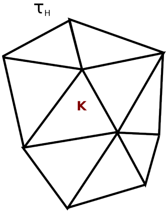
Principle of the method 1/4

Weak-form of Maxwell's equations

$$\begin{cases} (\varepsilon\,\partial_t \mathbf{E}, v) - (\nabla \times \mathbf{H}, v) = (\mathbf{J}, v) & \text{for all } v \in V, \\ (\mu\,\partial_t \mathbf{H}, w) + (\nabla \times \mathbf{E}, w) = 0 & \text{for all } w \in V. \end{cases}$$

$\sim\sim\sim$

$H > 0$, Tessalation $\mathcal{T}_H$ of Ω.



Localization

$$\begin{cases} (\varepsilon\,\partial_t \mathbf{E}, v)_K - (\nabla \times \mathbf{H}, v)_K = (\mathbf{J}, v)_K & \text{for all } v \in V, \\ (\mu\,\partial_t \mathbf{H}, w)_K + (\nabla \times \mathbf{E}, w)_K = 0 & \text{for all } w \in V. \end{cases}$$

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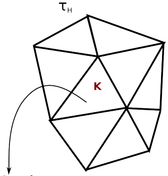

Hybridization and localization

$$\begin{cases} (\varepsilon\,\partial_t \mathbf{E}, v)_K - (\mathbf{H}, \nabla \times v)_K = (\mathbf{J}, v)_K - (\boldsymbol{\lambda}, v)_{\partial K}, \\ (\mu\,\partial_t \mathbf{H}, w)_K + (\nabla \times \mathbf{E}, w)_K = 0. \end{cases}$$

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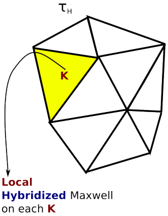

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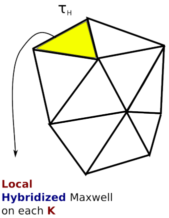

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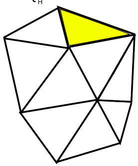

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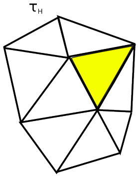

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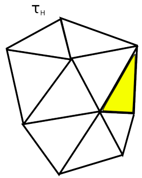

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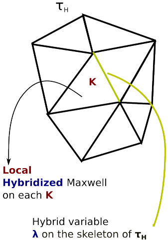

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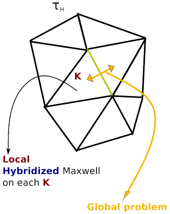

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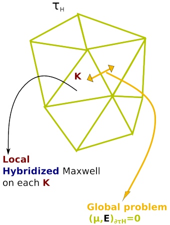

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$$(\mu, \mathbf{E})_{\partial\mathcal{T}_H} = 0 \quad \text{for all } \mu\in\boldsymbol{\Lambda}.$$

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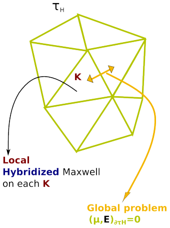

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$$(\mu, \mathbf{E})_{\partial \mathcal{T}_H} = 0 \quad \text{for all } \mu \in \boldsymbol{\Lambda}.$$

$\sim\sim\sim$

2 continuous spaces : $\underbrace{V}_{\mathbf{E},\mathbf{H}}$ and $\underbrace{\boldsymbol{\Lambda}}_{\boldsymbol{\lambda}}$

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$\Updownarrow$ $\rightsquigarrow$ Proved!

Hybridization and localization

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$$(\mu, \mathbf{E})_{\partial \mathcal{T}_H} = 0 \quad \text{for all } \mu \in \boldsymbol{\Lambda}.$$

- Weak form on the skeleton of a coarse mesh $\mathcal{T}_H$ of size H.
- Solution of element-wise ($K \in \mathcal{T}_H$) independent boundary value problems driven by Lagrange multipliers.
- Cell K is deemed a "macro-element".

Principle of the method 2/4

Splitting $\mathbf{E}$ and $\mathbf{H}$

- Unknowns are split between a $\mathbf{J}$ and λ part:

$$\mathbf{E} = \mathbf{E}^{\mathbf{J}} + \mathbf{E}^{\lambda},$$
$$\mathbf{H} = \mathbf{H}^{\mathbf{J}} + \mathbf{H}^{\lambda}.$$

(1) Contribution of the current

$$\begin{cases} (\varepsilon\, \partial_t \mathbf{E}^{\mathbf{J}}, v)_K - (\mathbf{H}^{\mathbf{J}}, \nabla \times v)_K = (\mathbf{J}, v)_K & \text{for all } v \in V, \\ (\mu\, \partial_t \mathbf{H}^{\mathbf{J}}, w)_K + (\nabla \times \mathbf{E}^{\mathbf{J}}, w)_K = 0 & \text{for all } w \in V, \end{cases}$$

(1) + (2)
$\Updownarrow$
initial local weak problem.

(2) Contribution of the hybrid variable

$$\begin{cases} (\varepsilon\, \partial_t \mathbf{E}^{\lambda}, v)_K - (\mathbf{H}^{\lambda}, \nabla \times v)_K = -(\boldsymbol{\lambda}, v)_{\partial K} & \text{for all } v \in V, \\ (\mu\, \partial_t \mathbf{H}^{\lambda}, w)_K + (\nabla \times \mathbf{E}^{\lambda}, w)_K = 0 & \text{for all } w \in V. \end{cases}$$

Principle of the method 3/4

Discretization 1/2 : Discretize the space of $\lambda \rightsquigarrow \boldsymbol{\Lambda}$.

- Choose $\boldsymbol{\Lambda_H} \subset \boldsymbol{\Lambda}$, with $\dim(\boldsymbol{\Lambda_H}) < +\infty \rightsquigarrow$ Seek $\boldsymbol{\lambda_H} \in \boldsymbol{\Lambda_H}$.
- Decompose on a basis $(\boldsymbol{\psi}_i)$

$$\boldsymbol{\lambda}_H = \sum_{i=1}^{\dim \Lambda_{\mathrm{H}}} \beta_i \boldsymbol{\psi}_i.$$

- Seek $\mathbf{E}^{\lambda_H}$ and $\mathbf{H}^{\lambda_H}$ of the form:

$$\mathbf{E}^{\lambda_H} = \sum_{i=1}^{\dim \Lambda_{\mathrm{H}}} \beta_i \boldsymbol{\eta}_i^{\mathbf{E}} \text{ and } \mathbf{H}^{\lambda_H} = \sum_{i=1}^{\dim \Lambda_{\mathrm{H}}} \beta_i \boldsymbol{\eta}_i^{\mathbf{H}},$$

with

$$\begin{cases} (\varepsilon\, \partial_t \boldsymbol{\eta}_i^{\mathbf{E}}, v)_K - (\boldsymbol{\eta}_i^{\mathbf{H}}, \nabla \times v)_K = -(\boldsymbol{\psi}_i \mathbf{n} \cdot \mathbf{n}^K, v)_{\partial K} & \text{for all } v \in V, \\ (\mu\, \partial_t \boldsymbol{\eta}_i^{\mathbf{H}}, w)_K + (\nabla \times \boldsymbol{\eta}_i^{\mathbf{E}}, w)_K = 0 \quad \text{for all } w \in V. \end{cases} \tag{1}$$

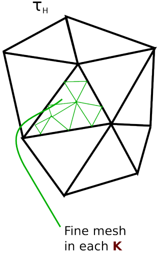
$\sim\sim\sim$

- Finally, in each K, $\mathbf{E} = \sum_{i=1}^{\dim \Lambda_{\mathrm{H}}} \beta_i \boldsymbol{\eta}_i^{\mathbf{E}} + \mathbf{E}^{\mathbf{J}}$ and $\mathbf{H} = \sum_{i=1}^{\dim \Lambda_{\mathrm{H}}} \beta_i \boldsymbol{\eta}_i^{\mathbf{H}} + \mathbf{H}^{\mathbf{J}}$.

Principle of the method 4/4

Discretization 2/2 : Discretizing the space V.

- For each $K \rightsquigarrow V_h(K)$ discretization space of V
  e.g. Discontinuous Galerkin.



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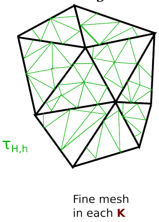

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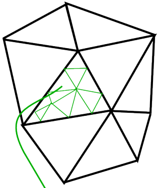

A family of **local**, discrete independent problems stated on macro-elements K:

$$\begin{cases} (\varepsilon\,\partial_t \boldsymbol{\eta}_i^{\mathbf{E}}, v)_K - (\boldsymbol{\eta}_i^{\mathbf{H}}, \nabla\times v)_K = -(\boldsymbol{\psi}_i \mathbf{n}\cdot\mathbf{n}^K, v)_{\partial K} \quad \forall v \in V_h(K), \\ (\mu\,\partial_t \boldsymbol{\eta}_i^{\mathbf{H}}, w)_K + (\nabla\times\boldsymbol{\eta}_i^{\mathbf{E}}, w)_K = 0 \quad \forall w \in V_h(K). \end{cases}$$

$\boldsymbol{\eta}_i^{\mathbf{E}}, \boldsymbol{\eta}_i^{\mathbf{H}} \rightsquigarrow$ are seeked in $V_h(K)$ for each $i \in [1, \dim(\mathrm{V_h(K)})]$

$\looparrowright$ lead to $\mathbf{E}^{\lambda_H}$, $\mathbf{H}^{\lambda_H}$

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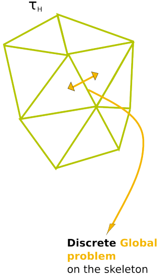
- A family of **local**, discrete independent problems stated on macro-elements K
- A **global, discrete coarse** problem stated on the skeleton of $\mathcal{T}_H$



$$(\mu_H, \mathbf{E}^{\lambda_H})_{\partial\mathcal{T}_{\mathcal{H}}} = -(\mu_H, \mathbf{E}^{\mathbf{J}})_{\partial\mathcal{T}_H} \quad \forall \mu_H \in \mathbf{\Lambda}_{\boldsymbol{H}},$$

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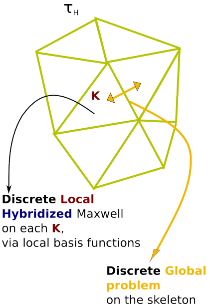


Time Integration: two strategies so far 1/2

Implicit: θ-scheme

- K-locally:

$$\left\{ \begin{aligned} &\left(\varepsilon \frac{\mathbf{E}^n - \mathbf{E}^{n-1}}{\Delta t}, v\right)_K - \theta(\mathbf{H}^n, \nabla \times v)_K - (1-\theta)(\mathbf{H}^{n-1}, \nabla \times v)_K = (\mathbf{J}^n, v)_K \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad - (\boldsymbol{\lambda}^n, v)_{\partial K}, \\ &\left(\mu \frac{\mathbf{H}^n - \mathbf{H}^{n-1}}{\Delta t}, w\right)_K + \theta(\nabla \times \mathbf{E}^n, w)_K + (1-\theta)(\nabla \times \mathbf{E}^{n-1}, w)_K = 0 \end{aligned} \right. \tag{2}$$

Time Integration: two strategies so far 2/2

Explicit: Second order Leap-Frog

- K-locally:

$$\begin{cases} \left(\varepsilon \dfrac{\mathbf{E}^{n+1}-\mathbf{E}^{n}}{\Delta t}, v\right)_K - (\mathbf{H}^{n+1/2}, \nabla\times v)_K = (\mathbf{J}^{n+1/2}, v)_K - (\boldsymbol{\lambda}^{n+1/2}, v)_{\partial K}, \\ \left(\mu \dfrac{\mathbf{H}^{n+3/2}-\mathbf{H}^{n-1/2}}{\Delta t}, w\right)_K + (\nabla\times \mathbf{E}^{n+1}, w)_K = 0 \end{cases} \tag{3}$$

- Writing the time dependencies of splitted unknowns leads, for the lambda part, to:

$$\frac{1}{\Delta t}(\varepsilon \mathbf{E}^{\lambda,n}, v)_K = -(\boldsymbol{\lambda}^{n+1/2}, v)_{\partial K}, \tag{4}$$

- No $\boldsymbol{\eta}^{\mathbf{H}}$ is considered, and we have

$$\frac{1}{\Delta t}(\varepsilon\, \boldsymbol{\eta}_i^{\mathbf{E}}, v)_K = -(\boldsymbol{\psi}_i \mathbf{n}\cdot\mathbf{n}^K, v)_{\partial K} \quad \text{for all } v\in V \tag{5}$$

The Leap-Frog 2 MHM Algorithm

- The MHM-LF2 algorithm:

for $k = 1, N_K$ **do** ! Loop on Macro-elements
    for $j = 1, N_{\lambda_H}$ **do** ! Loop on the edge basis-functions
        Solve (5) for $\boldsymbol{\eta}_j^{\mathbf{E}}\big|_k$ with $\boldsymbol{\psi}_j$
    end for
end for

while $t < T_{\text{end}}$ **do**
    $t = t + \Delta t,$
    for $k = 1, N_K$ **do** ! Loop on Macro-elements
        Determine $\mathbf{E}^{\mathbf{J}}_{n+1}\big|_k$ from $\mathbf{E}_n|_k$, $\mathbf{H}_{n+1/2}\big|_k$ and $\mathbf{J}_{n+1/2}\big|_k$
    end for
    Assemble $\mathbf{E}^{\mathbf{J}}_{n+1}\big|_{k=1\ldots N_k}$ to the right-hand side of the global problem
    Solve the global problem to retrieve $\mathbf{E}^{\boldsymbol{\lambda}}_{n+1}$; $\mathbf{E}_{n+1} = \mathbf{E}^{\boldsymbol{\lambda}}_{n+1} + \mathbf{E}^{\mathbf{J}}_{n+1}$
    for $k = 1, N_K$ **do** ! Loop on Macro-elements
        Determine $\mathbf{H}_{n+3/2}\big|_k$ from $\mathbf{H}_{n+1/2}\big|_k$ and $\mathbf{E}_{n+1}|_k$
    end for
end while

The Leap-Frog 2 MHM Algorithm

- The MHM-LF2 algorithm: "Expensive" loops are parallel!

for $k = 1, N_K$ **do** ! Loop on Macro-elements
    for $j = 1, N_{\lambda_H}$ **do** ! Loop on the edge basis-functions
        Solve (5) for $\boldsymbol{\eta}_j^{\mathbf{E}}\big|_k$ with $\boldsymbol{\psi}_j$
    end for
end for

while $t < T_{\text{end}}$ **do**
    $t = t + \Delta t$,
    for $k = 1, N_K$ **do** ! Loop on Macro-elements
        Determine $\mathbf{E}_{n+1}^{\mathbf{J}}\big|_k$ from $\mathbf{E}_n|_k$, $\mathbf{H}_{n+1/2}\big|_k$ and $\mathbf{J}_{n+1/2}\big|_k$
    end for
    Assemble $\mathbf{E}_{n+1}^{\mathbf{J}}\big|_{k=1\ldots N_k}$ to the right-hand side of the global problem
    Solve the global problem to retrieve $\mathbf{E}_{n+1}^{\boldsymbol{\lambda}}$; $\mathbf{E}_{n+1} = \mathbf{E}_{n+1}^{\boldsymbol{\lambda}} + \mathbf{E}_{n+1}^{\mathbf{J}}$
    for $k = 1, N_K$ **do** ! Loop on Macro-elements
        Determine $\mathbf{H}_{n+3/2}\big|_k$ from $\mathbf{H}_{n+1/2}\big|_k$ and $\mathbf{E}_{n+1}|_k$
    end for
end while

The θ-scheme MHM Algorithm

- The MHM-θ-scheme algorithm: "Expensive" loops are parallel!

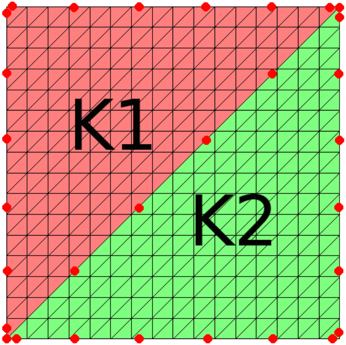
for $k = 1, N_K$ **do** ! Loop on Macro-elements
  for $j = 1, N_{\lambda_H}$ **do** ! Loop on the edge basis-functions
    Solve (1) for $\boldsymbol{\eta}_j^{\mathbf{E},\mathbf{H}}\Big|_k$ with $\boldsymbol{\psi}_j$
  end for
end for

while $t < T_{\text{end}}$ **do**
  $t = t + \Delta t$,
  for $k = 1, N_K$ **do** ! Loop on Macro-elements
    Determine $\mathbf{E}_{n+1}^{\mathbf{J}}\big|_k$ and $\mathbf{H}_{n+1}^{\mathbf{J}}\big|_k$ from $\mathbf{E}_n|_k$, $\mathbf{H}_n|_k$ and $\mathbf{J}_n|_k$
  end for
  Assemble $\mathbf{E}_{n+1}^{\mathbf{J}}\big|_{k=1\dots N_k}$ to the right-hand side of the global problem
  Solve the global problem
  Retrieve $\mathbf{E}_{n+1}^{\boldsymbol{\lambda}}$; $\mathbf{E}_{n+1} = \mathbf{E}_{n+1}^{\boldsymbol{\lambda}} + \mathbf{E}_{n+1}^{\mathbf{J}}$, and
    $\mathbf{H}_{n+1}^{\boldsymbol{\lambda}}$; $\mathbf{H}_{n+1} = \mathbf{H}_{n+1}^{\boldsymbol{\lambda}} + \mathbf{H}_{n+1}^{\mathbf{J}}$,
end while

(2D) Matlab implementation by D. Paredes

Eigenmode of a cavity

- Access to an analytical solution
- Example: 2 macro-elements, $\mathbb{P}_5$ elements for the edges, $\mathbb{P}_2$ for the fields



(2D) Matlab implementation by D. Paredes

Eigenmode of a cavity

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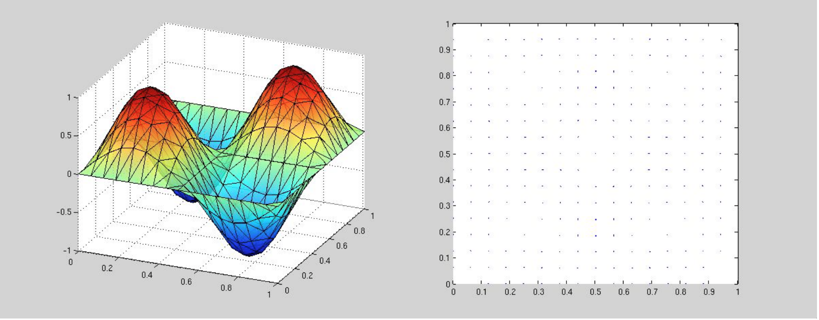
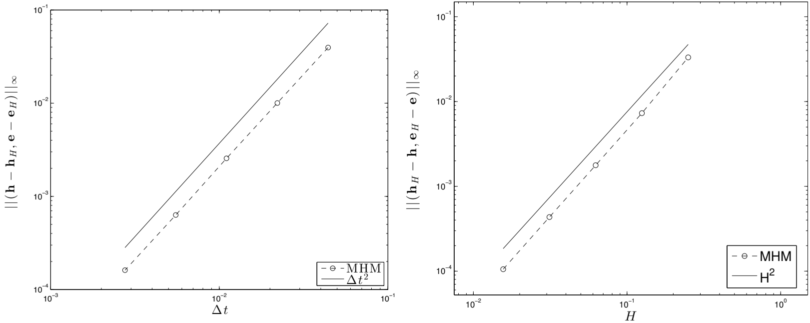


(2D) Matlab implementation by D. Paredes

Eigenmode of a cavity

- Access to an analytical solution
- Convergence results

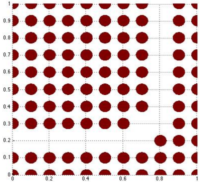


$\mathbb{P}_1$ elements for the edges, $\mathbb{P}_3$ for the electromagnetic field, LF2 time-scheme.

Concluding remarks

Current status

- Writing a 2D Fortran code
- Explicit & implicit time-schemes
  - Moving on to nanophotonics-oriented models & test-cases
  - Experiment with simple parallelism



Longer term objectives: the HOMAR[5] associate team

- Progress on the formulation / theroretical study of MHM-DGTD methods for more complex, Maxwell-based models
- Progress towards implementation of such methods in the 3D case
- Demonstrate their capability to leverage modern HPC architectures

[5] http://www-sop.inria.fr/nachos/index.php/Main/HOMAR