An upscaled DGTD method for time-domain electromagnetics

A Gobé, S. Lanteri, Raphaël Léger, C Scheid, F. Valentin

An upscaled DGTD method for time-domain electromagnetics

Multiscale and multiphysics computation and applications (2P3A)

Alexis Gobé, Stéphane Lanteri, Raphaël Léger and Claire Scheid
Inria Sophia Antipolis - Méditerranée and University Côte d'Azur, France
Diego Paredes
Universidad Católica de Valparaiso, Chile
Frédéric Valentin
LNCC, Petropolis, Brazil

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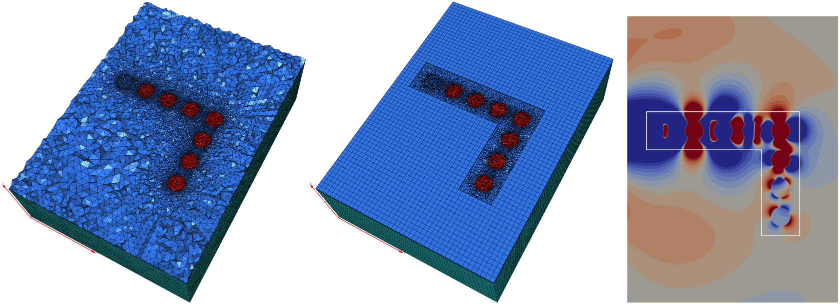
Motivations

Computational nanophotonics: modeling challenges

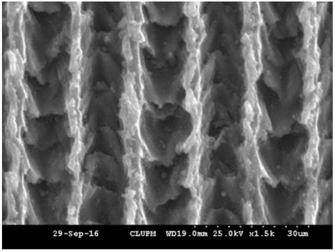
- Material properties:
  - Homogeneous v.s. heterogeneous;
  - Isotropic v.s. anisotropic;
  - Physical dispersion (local v.s. non-local);
  - Linear v.s. non-linear.
- Multiscale problems in space and time

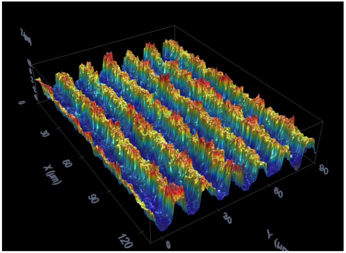


L-shaped waveguide formed of seven 50 nm diameter Au spheres in vacuum, with a 75 nm center-to-center spacing (computational domain: 550 nm $\times$750 nm $\times$400 nm).

A concrete example in photovoltaics

- Collaboration with Division of Renewable Energies, CIEMAT, Spain
- Study of thin-film silicon-heterojunction solar cells
- Texturization technique based on controlled ablation of the surface by laser scanning





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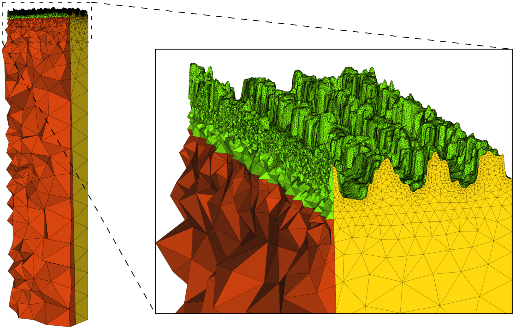
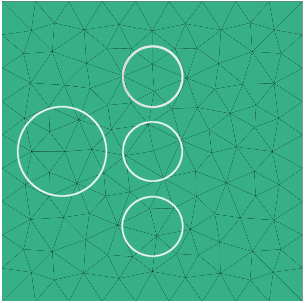


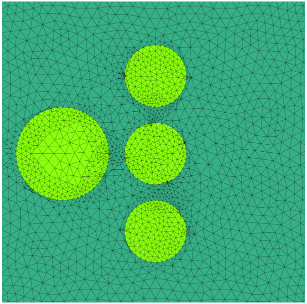
- As-grown TCO: 10 μm
- Crystaline silicon: 510 μm
- Surface: 100 μm x 100 μm

Objectives

Desiging a family of methods which are:

- Highly flexible in the discretization process;
- Well suited to (highly) heterogeneous problems;
- Well suited to multiscale problems;
- Preserving high order convergence;
- Well adapted to massively parallel computing.





Outline

Multiscale Hybrid-Mixed (MHM) method

MHM method in a nutshell

- Finite element type method
- Accurate on general and coarse meshes
- Induce an a posteriori error estimator (to drive mesh adaptivity)
- Locally conservative
- Naturally adapted to HPC

- R. Araya and C. Harder and D. Paredes and F. Valentin
  Multiscale hybrid-mixed method
  SIAM J. Numer. Anal., Vol. 51, No. 6 (2013)
- C. Harder and D. Paredes and F. Valentin
  A family of multiscale hybrid-mixed finite element methods for the Darcy equation with rough coefficients
  J. Comput. Phys., Vol. 245 (2013)

- Our goal: adaptation of the MHM framework to wave propagation contexts

- First target: system of time-domain Maxwell equations

Multiscale Hybrid-Mixed (MHM) method

Basic principles

- One among several solution strategies recently devised for multiscale problems
- A two level method
- First level
  - Discretization based on a very coarse and general mesh
  - The skeleton of this mesh is the support of a hybrid variable
  - Hybrid variable problem discretized by a *classical* finite element formulation based on upscaled basis functions
- Second level
  - Each (macro-)element of the first level mesh is triangulated (second level mesh)
  - Local problems defined on each macro-element of the first level mesh
  - Continuous case: analytical solution for the local problems
  - Discrete case: DGTD[a] method for the local problems

[a] Discontinuous Galerkin Time-Domain

Time-domain Maxwell equations - Initial and boundary value problem

$$\begin{cases} \varepsilon\partial_t\mathbf{E} - \mathbf{curl}\,\mathbf{H} = -\mathbf{J}, \text{ in } \Omega \times [0, T] \\ \mu\partial_t\mathbf{H} + \mathbf{curl}\,\mathbf{E} = 0, \text{ in } \Omega \times [0, T] \\ \mathbf{n} \times \mathbf{E} = 0, \text{ on } \Gamma_m \times [0, T] \\ \mathbf{n} \times \mathbf{E} + \mathbf{n} \times (\mathbf{n} \times \mathbf{H}) = \mathbf{n} \times \mathbf{E}^{\mathrm{inc}} + \mathbf{n} \times (\mathbf{n} \times \mathbf{H}^{\mathrm{inc}}), \text{ on } \Gamma_a \times [0, T] \\ \mathbf{E} = \mathbf{E}_0, \text{ in } \Omega \times \{0\} \text{ and } \mathbf{H} = \mathbf{H}_0, \text{ in } \Omega \times \{0\} \end{cases}$$

Functional space setting

$\mathcal{T}_H$ a simplicial macro-mesh of the computational domain and $\mathcal{T}_{\Delta T} = [0, T] = \bigcup_{n=1}^{N} I_n$

$$\mathbf{V} := \{\mathbf{v} \in \mathbf{L}^2(\Omega) \,:\, \mathbf{v}|_K \in \mathbf{H}^1(K) \text{ for all } K \in \mathcal{T}_H\}$$

$\mathbf{L}$ is the space of the restriction of the tangential component of functions in $\mathbf{H}(curl;\Omega)$ to ∂K

$$\mathbf{L} := \left\{\mathbf{v} \times \mathbf{n}^K|_{\partial K} \in \mathbf{H}^{-1/2}(\partial K) \text{ for all } K \in \mathcal{T}_H \text{ with } \mathbf{v} \in \mathbf{H}(curl;\Omega)\right\}$$

with $\mathbf{n}^K$ being the outward normal vector on ∂K.

Localization: on each I_n, for $K \in \mathcal{T}_h$

find $(\mathbf{E}, \mathbf{H}) \in \mathbf{V} \times \mathbf{V}$ such that

$$\begin{cases} (\varepsilon \partial_t \mathbf{E}, \mathbf{v})_K - (\mathbf{curl}\, \mathbf{H}, \mathbf{v})_K = (\mathbf{J}, \mathbf{v})_K \,, \ \forall \mathbf{v} \in \mathbf{V}, \\ (\mu \partial_t \mathbf{H}, \mathbf{w})_K + (\mathbf{curl}\, \mathbf{E}, \mathbf{w})_K = 0, \ \forall \mathbf{w} \in \mathbf{V}. \end{cases}$$

+ Continuity conditions at the end points of I_n

Localization+hybridization: on each I_n, for $K \in \mathcal{T}_h$

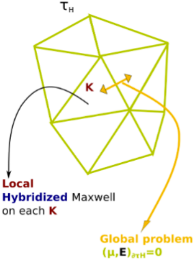
find $(\mathbf{E}, \mathbf{H}, \boldsymbol{\lambda}) \in \mathbf{V} \times \mathbf{V} \times \boldsymbol{\Lambda}$ such that

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

+ Continuity conditions at the end points of I_n

Global problem: $(\boldsymbol{\nu}, \mathbf{E})_{\partial \mathcal{T}_H} = 0, \ \forall \boldsymbol{\nu} \in \boldsymbol{\Lambda}$

It can be shown that $\boldsymbol{\lambda} = -\mathbf{n} \times \mathbf{H}$ on $\partial K \times [0, T]$



Splitting of unknowns: $\mathbf{E} = \mathbf{E}^{\mathbf{J}} + \mathbf{E}^{\boldsymbol{\lambda}}$ and $\mathbf{H} = \mathbf{H}^{\mathbf{J}} + \mathbf{H}^{\boldsymbol{\lambda}}$

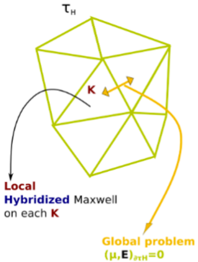
Contribution of the current: on each I_n, for $K \in \mathcal{T}_h$
find $(\mathbf{E}^{\mathbf{J}}, \mathbf{H}^{\mathbf{J}}) \in \mathbf{V} \times \mathbf{V}$ such that

$$\begin{cases} \left(\varepsilon \partial_t \mathbf{E}^{\mathbf{J}}, \mathbf{v}\right)_K - \left(\mathbf{H}^{\mathbf{J}}, \mathbf{curl}\,\mathbf{v}\right)_K = (\mathbf{J}, \mathbf{v})_K \,, \ \forall \mathbf{v} \in \mathbf{V}, \\ \left(\mu \partial_t \mathbf{H}^{\mathbf{J}}, \mathbf{w}\right)_K + \left(\mathbf{curl}\,\mathbf{E}^{\mathbf{J}}, \mathbf{w}\right)_K = 0, \ \forall \mathbf{w} \in \mathbf{V}. \end{cases}$$

Contribution of the hybrid variable: on each I_n, for $K \in \mathcal{T}_h$
find $(\mathbf{E}^{\boldsymbol{\lambda}}, \mathbf{H}^{\boldsymbol{\lambda}}) \in \mathbf{V} \times \mathbf{V}$ such that

$$\begin{cases} \left(\varepsilon \partial_t \mathbf{E}^{\boldsymbol{\lambda}}, \mathbf{v}\right)_K - \left(\mathbf{H}^{\boldsymbol{\lambda}}, \mathbf{curl}\,\mathbf{v}\right)_K = -\,(\boldsymbol{\lambda}, \mathbf{v})_{\partial K} \,, \ \forall \mathbf{v} \in \mathbf{V}, \\ \left(\mu \partial_t \mathbf{H}^{\boldsymbol{\lambda}}, \mathbf{w}\right)_K + \left(\mathbf{curl}\,\mathbf{E}^{\boldsymbol{\lambda}}, \mathbf{w}\right)_K = 0, \ \forall \mathbf{w} \in \mathbf{V}. \end{cases}$$

Global problem: : on each I_n, for $K \in \mathcal{T}_h$
find $\boldsymbol{\lambda} \in \boldsymbol{\Lambda}$ such that $\left(\boldsymbol{\nu}, \mathbf{E}^{\boldsymbol{\lambda}}\right)_{\partial \mathcal{T}_H} = -\left(\boldsymbol{\nu}, \mathbf{E}^{\mathbf{J}}\right)_{\partial \mathcal{T}_H} \,, \ \forall \boldsymbol{\nu} \in \boldsymbol{\Lambda}$



Principle of the method: one-level MHM

- $\boldsymbol{\lambda}_H$ piecewise constant in time on each I_n
- Choose $\boldsymbol{\Lambda}_H$ with $\dim(\boldsymbol{\Lambda}_H) < +\infty$ and seek $\boldsymbol{\lambda}_H \in \boldsymbol{\Lambda}_H$
- Decompose $\boldsymbol{\lambda}_H$ on a basis (Ψ_i) of $\boldsymbol{\Lambda}_H$

$$\boldsymbol{\lambda}_H^n = \sum_{i=1}^{\dim(\boldsymbol{\Lambda}_H)} \beta_i^n \Psi_i$$

Define the set $(\boldsymbol{\eta}_i^{\mathbf{E}}, \boldsymbol{\eta}_i^{\mathbf{H}})$, $i \in [1, \dim(\boldsymbol{\Lambda}_H)]$ solution of

$$\begin{cases} \left(\varepsilon \partial_t \boldsymbol{\eta}_i^{\mathbf{E}}, \mathbf{v}\right)_K - \left(\boldsymbol{\eta}_i^{\mathbf{H}}, \mathbf{curl}\, \mathbf{v}\right)_K = -\left(\Psi_i \mathbf{n}.\mathbf{n}^K, \mathbf{v}\right)_{\partial K}, \ \forall \mathbf{v} \in \mathbf{V}, \\ \left(\mu \partial_t \boldsymbol{\eta}_i^{\mathbf{H}}, \mathbf{w}\right)_K + \left(\mathbf{curl}\, \boldsymbol{\eta}_i^{\mathbf{E}}, \mathbf{w}\right)_K = 0, \ \forall \mathbf{w} \in \mathbf{V}. \end{cases}$$

$(\boldsymbol{\eta}_i^{\mathbf{E}}, \boldsymbol{\eta}_i^{\mathbf{H}})$ are the multiscale basis functions

- On each I_n it can be shown that $\mathbf{E}^{\boldsymbol{\lambda}_H}$ and $\mathbf{H}^{\boldsymbol{\lambda}_H}$ can be defined as

$$\mathbf{E}^{\boldsymbol{\lambda}_H} = \sum_{i=1}^{\dim(\boldsymbol{\Lambda}_H)} \beta_i^n \boldsymbol{\eta}_i^{\mathbf{E}} \ , \quad \mathbf{H}^{\boldsymbol{\lambda}_H} = \sum_{i=1}^{\dim(\boldsymbol{\Lambda}_H)} \beta_i^n \boldsymbol{\eta}_i^{\mathbf{H}}$$

Finally, in each K (and if $\mathbf{J}$ does not depend on time)

$$\mathbf{E}^n = \sum_{i=1}^{\dim(\mathbf{\Lambda}_H)} \beta_i^n \boldsymbol{\eta}_i^{\mathbf{E}} + \mathbf{E}^{\mathbf{J}} \quad , \quad \mathbf{H}^n \sum_{i=1}^{\dim(\mathbf{\Lambda}_H)} \beta_i^n \boldsymbol{\eta}_i^{\mathbf{H}} + \mathbf{H}^{\mathbf{J}}$$

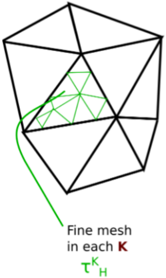
Principle of the method: two-level method

Discretization in the DGTD framework

- For each K, define $\mathbf{V}_h(K)$ as the discretization of $\mathbf{V}$
- In our case, $\mathbf{V}_h(K)$ is the DG discontinuous finite element space
- Formulate a family of local discrete independent problems stated on macro-elements K

$$\begin{cases} \left(\varepsilon \partial_t \boldsymbol{\eta}_i^{\mathbf{E}}, \mathbf{v}\right)_K - \left(\boldsymbol{\eta}_i^{\mathbf{H}}, \mathbf{curl}\,\mathbf{v}\right)_K = -\left(\Psi_i \mathbf{n}.\mathbf{n}^K, \mathbf{v}\right)_{\partial K}, \ \forall \mathbf{v} \in \mathbf{V}_h(K), \\ \left(\mu \partial_t \boldsymbol{\eta}_i^{\mathbf{H}}, \mathbf{w}\right)_K + \left(\mathbf{curl}\,\boldsymbol{\eta}_i^{\mathbf{E}}, \mathbf{w}\right)_K = 0, \ \forall \mathbf{w} \in \mathbf{V}_h(K). \end{cases}$$

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



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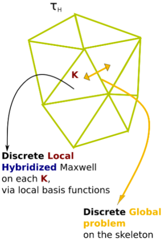
- For each K, define $\mathbf{V}_h(K)$ as the discretization of $\mathbf{V}$
- In our case, $\mathbf{V}_h(K)$ is the DG discontinuous finite element space
- Formulate a family of local discrete independent problems stated on macro-elements K
- Formulate a global discrete coarse problem stated on the skeleton of $\mathcal{T}_h$

$$\left(\boldsymbol{\nu}_H, \mathbf{E}^{\boldsymbol{\lambda}_H}\right)_{\partial\mathcal{T}_H} = -\left(\boldsymbol{\nu}_H, \mathbf{E}^{\mathbf{J}}\right)_{\partial\mathcal{T}_H}, \ \forall \boldsymbol{\nu}_H \in \boldsymbol{\Lambda}_H$$

$\Rightarrow$ leads the β_i^n coefficients



1. Local problem associated to $\mathbf{J}$

Find $(\mathbf{E}^{\mathbf{J}}, \mathbf{H}^{\mathbf{J}}) \in \mathbf{V}_h(K) \times \mathbf{V}_h(K)$ such that

$$\begin{cases} \left(\varepsilon \partial_t \mathbf{E}^{\mathbf{J}}, \mathbf{v}\right)_K - \left(\mathbf{H}^{\mathbf{J}}, \mathbf{curl}\,\mathbf{v}\right)_K = (\mathbf{J}, \mathbf{v})_K\,, \ \forall \mathbf{v} \in \mathbf{V}_h(K), \\ \left(\mu \partial_t \mathbf{H}^{\mathbf{J}}, \mathbf{w}\right)_K + \left(\mathbf{curl}\,\mathbf{E}^{\mathbf{J}}, \mathbf{w}\right)_K = 0, \ \forall \mathbf{w} \in \mathbf{V}_h(K). \end{cases}$$

2. Multiscale basis functions

Find $(\boldsymbol{\eta}_i^{\mathbf{E}}, \boldsymbol{\eta}_i^{\mathbf{H}}) \in \mathbf{V}_h(K) \times \mathbf{V}_h(K)$ such that

$$\begin{cases} \left(\varepsilon \partial_t \boldsymbol{\eta}_i^{\mathbf{E}}, \mathbf{v}\right)_K - \left(\boldsymbol{\eta}_i^{\mathbf{H}}, \mathbf{curl}\,\mathbf{v}\right)_K = -\left(\boldsymbol{\Psi}_i \mathbf{n}.\mathbf{n}^K, \mathbf{v}\right)_{\partial K}\,, \ \forall \mathbf{v} \in \mathbf{V}_h(K), \\ \left(\mu \partial_t \boldsymbol{\eta}_i^{\mathbf{H}}, \mathbf{w}\right)_K + \left(\mathbf{curl}\,\boldsymbol{\eta}_i^{\mathbf{E}}, \mathbf{w}\right)_K = 0, \ \forall \mathbf{w} \in \mathbf{V}_h(K). \end{cases}$$

3. Global problem

Find $(\beta_1^n, \dots, \beta_{\mathrm{dim}(\boldsymbol{\Lambda}_H)}^n) \in \mathbb{R}$ such that

$$\sum_{i=1}^{\mathrm{dim}(\boldsymbol{\Lambda}_H)} \beta_i^n (\boldsymbol{\nu}_H, \boldsymbol{\eta}_i^{\mathbf{E}})_{\partial \mathcal{T}_H} = -(\boldsymbol{\nu}_H, \mathbf{E}^{\mathbf{J}})_{\partial \mathcal{T}_H}, \qquad \forall \boldsymbol{\nu}_H \in \boldsymbol{\Lambda}_H$$

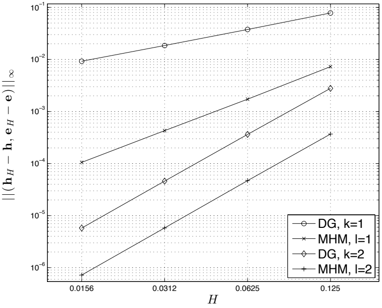
Fully discrete local problem for $(\mathbf{E}^{\mathbf{J}}, \mathbf{H}^{\mathbf{J}})$

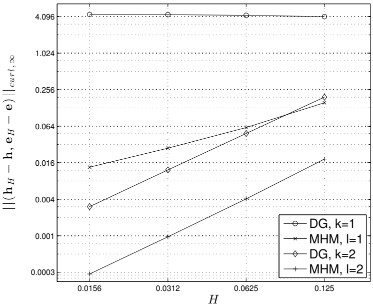
$$\begin{cases} \left(\mu \dfrac{\mathbf{H}^{n,\mathbf{J}} - \mathbf{H}^{n-1,\mathbf{J}}}{\Delta T}, \mathbf{w}_h\right)_K & + \quad \left(\mathbf{E}^{n-\frac{1}{2},\mathbf{J}}, \mathbf{curl}\,\mathbf{w}_h\right)_K = 0 \\ \left(\varepsilon \dfrac{\mathbf{E}^{n+\frac{1}{2},\mathbf{J}} - \mathbf{E}^{n-\frac{1}{2},\mathbf{J}}}{\Delta T}, \mathbf{v}_h\right)_K & - \quad \left(\mathbf{H}^{n,\mathbf{J}}, \mathbf{curl}\,\mathbf{v}_h\right)_K = \left(\mathbf{J}^n, \mathbf{v}_h\right)_K \end{cases}$$

Global problem

$$\sum_{i=1}^{\dim(\mathbf{\Lambda}_H)} \beta_i^n (\boldsymbol{\nu}_H, \boldsymbol{\eta}_i^{\mathbf{E}})_{\partial\mathcal{T}_H} = -(\boldsymbol{\nu}_H, \mathbf{E}^{n+\frac{1}{2},\mathbf{J}})_{\partial\mathcal{T}_H}$$

- S. Lanteri, D. Paredes, C. Scheid and F. Valentin
  SIAM J. Multisc. Model. Simul., 2018
- Second level solver: centered flux DGTD method with explicit LF2 time-stepping
- Formulation and theoretical study in the 3D case
- Numerical study in the 2D case

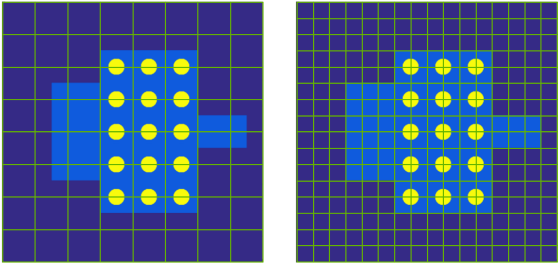




Standing wave in a PEC cavity: comparison between the MHM method and the DG method with respect to the $\|(\mathbf{H}-\mathbf{H}_H, \mathbf{E}-\mathbf{E}_H)\|_\infty$ (left) and $\|(\mathbf{H}-\mathbf{H}_H, \mathbf{E}-\mathbf{E}_H)\|_{\mathrm{curl},\infty}$ (right) norms.

Numerical study in 2D

- Nanophotonic waveguide of photonic crystal type
- Holes of silicium in silica encapsulated in air
- Second level discretization: non-dissipative DGTD method with explicit time-stepping and quadratic elements
- Coarse problem: linear elements



Nanowaveguide problem: coarse quandrangular meshes

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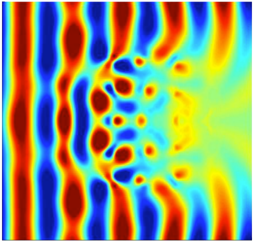
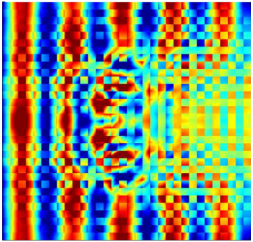
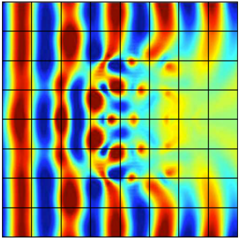


DGTD method
with 589,824 DoF



DGTD method
with 4,608 DoF



MHM-DGTD method
with 9,216 DoF

Nanowaveguide problem: contour lines of the amplitude of the electric field at a given time

Outline

- ΔT: 1st-level (coarse) time step
- Δt^K: 2nd-level (fine) time step verifying the CFL condition for the local problkem in K
- Goal: assess the global stability, accuracy and efficiency of MHM-DGTD method

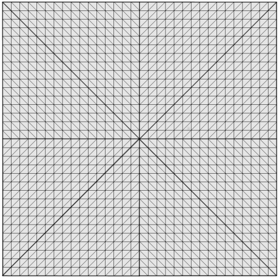
Given $\mathbf{H}^0$ and $\mathbf{E}^{\frac{1}{2}}$;
for $n = 1 \to N$ **do**
  for $k \in \mathcal{T}_H$ **do**
    Set $\mathbf{E}_K^{n,0,} = \mathbf{E}_K^{n-1,M_k}$ and $\mathbf{H}_K^{n,0,} = \mathbf{H}_K^{n-1,M_k}$;
    for $m = 1 \to M_K$ **do**
      if $n = 1$ **then**
        Solve (2) to determine $\eta_{\mathbf{K}}^{\mathbf{m+\frac{1}{2},E}}$ and $\eta_{\mathbf{K}}^{\mathbf{m,H}}$;
      end
      Solve (1) to determine and $\mathbf{E}_K^{n,m+\frac{1}{2},}$ and $\mathbf{H}_K^{n,m,}$;
      Assemble $\mathbf{E}_K^{n,m+\frac{1}{2},}$ to the RHS of (3) ;
    end
  end
  Solve (3) to determine β^n;
  Update $\mathbf{E}_K^{n,M_K+\frac{1}{2}} = \beta^n \eta_{\mathbf{K}}^{\mathbf{E}} + \mathbf{E}^{n+\frac{1}{2},}$
  and $\mathbf{H}_K^{n,M_K} = \beta^n \eta_{\mathbf{K}}^{\mathbf{H}} + \mathbf{H}^{n,}$, $\forall K \in \mathcal{T}_H$;
end

Outline

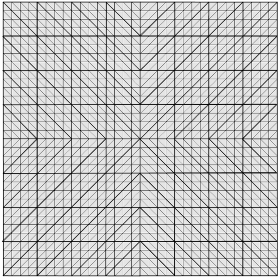
Validation: space refinement

- Standing wave in a PEC cavity
- Macro/micro meshes such that $h = H/2^{\beta}$
- $\mathbb{P}^k - \mathbb{P}^{k}$[a] polynomial order with k in $\{1, 2, 3, 4\}$

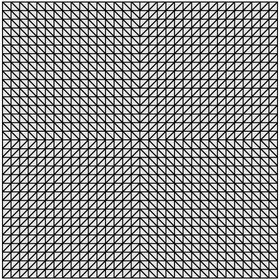
[a] For $\mathbf{V}_h(K)$ and Λ_h respectively.



(a) $H = h \times 2^5$



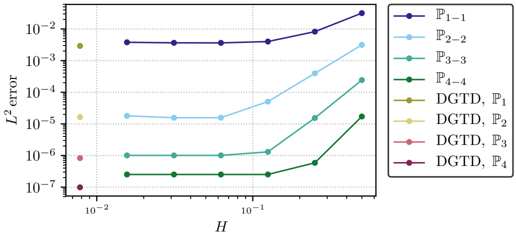
(b) $H = h \times 2^2$



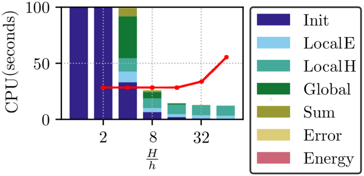
(c) $H = h \times 2^0$

Validation: spatial refinement $(H - h)$

- Standing wave in a PEC cavity
- Macro/micro meshes such that $h = H/2^{\beta}$
- $\mathbb{P}_k - \mathbb{P}_k$ polynomial order with k in $\{1, 2, 3, 4\}$



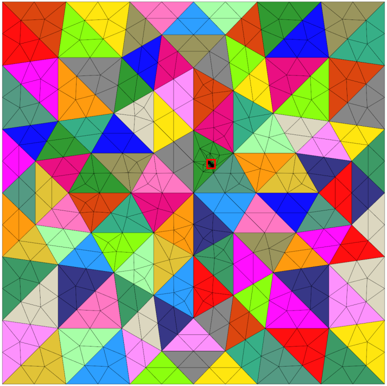
(d) Maximum L_2 error for different H

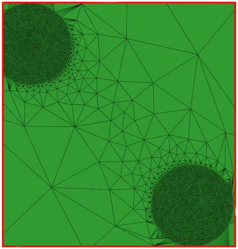


(e) Breakdown of CPU time

Validation: temporal refinement ($\Delta T - \Delta t$)

- Standing wave in a PEC cavity
- Locally refined mesh such that $h_{max}/h_{min} = 1500$





Multiscale mesh with zoom in the refined part

Validation: temporal refinement ($\Delta T - \Delta t$)

- Standing wave in a PEC cavity
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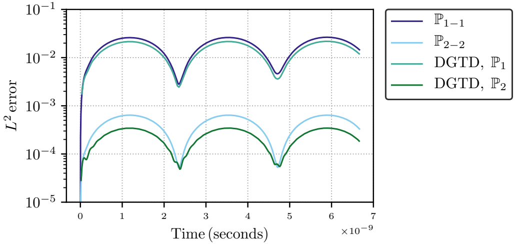

L_2 error without local timestepping

Validation: temporal refinement ($\Delta T - \Delta t$)

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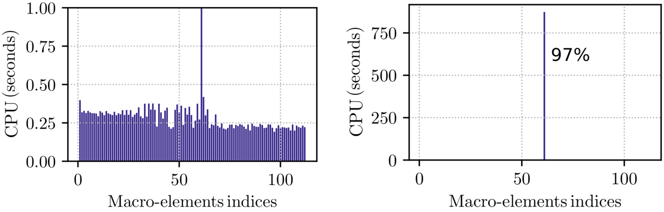
- Interpolation orders: $\mathbb{P}_1 - \mathbb{P}_1$



Computation time for multiscale configuration

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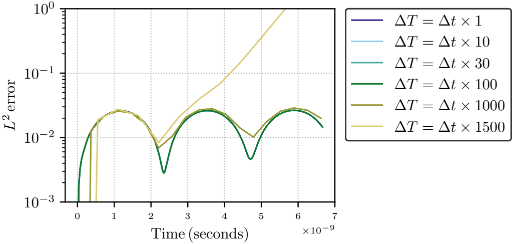

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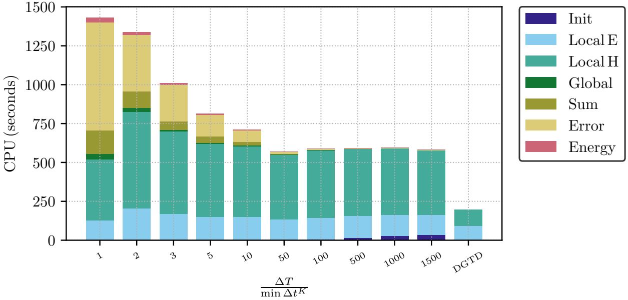

Computation time for multiscale configuration

Outline

Closure

Summary of the main features of the MHM method

- First level elements can be meshed independently to yield the second level mesh
- Non-conformity is naturally allowed
- Local problems are independent i.e. can be solved in parallel
- Local time-stepping is possible i.e. local problems can be time advanced with their own time step (or time scheme)
- In the discrete case, first level problem is a linear system with a symetric positive definite matrix

Open questions and future works

- Stability analysis of the MHM-induced local time stepping method
- A priori convergence analysis (ongoing)
- Implementation in 3D
- High performance computing issues (*data-based* versus *task-based* parallelization)
- Extension to frequency-domain (ongoing)

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Thank you for your attention !

NACHOS project-team

- Numerical methods and high performance algorithms for the numerical modeling of wave interaction with complex geometries/media
- Common project-team with J.A. Dieudonné Mathematics Laboratory UMR CNRS 7351, Côte d'Azur University