

Hybrid Explicit–Implicit Time Integration for Grid-Induced Stiffness in a DGTD Method for Time Domain Electromagnetics

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Abstract In the recent years, there has been an increasing interest in discontinuous Galerkin time domain (DGTD) methods for the numerical modeling of electromagnetic wave propagation. Such methods most often rely on explicit time integration schemes which are constrained by a stability condition that can be very restrictive on highly refined meshes. In this paper, we report on some efforts to design a hybrid explicit–implicit DGTD method for solving the time domain Maxwell equations on locally refined simplicial meshes. The proposed method consists in applying an implicit time integration scheme locally in the refined regions of the mesh while preserving an explicit time scheme in the complementary part.

1 Introduction

Nowadays, a variety of methods exist for the numerical treatment of the time domain Maxwell equations, ranging from the well established and still prominent finite difference time domain (FDTD) methods based on Yee’s scheme to the more recent finite element time domain (FETD) and discontinuous Galerkin time domain (DGTD) methods. The latter are very well adapted to local mesh refinement but at the expense of a restrictive time step in order to preserve the stability of the explicit time integration schemes. In the first one, a local time stepping strategy is combined to an explicit time integration scheme, while the second approach relies on the use of an implicit or a hybrid explicit–implicit time integration scheme. In the present work, we consider the second approach.

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Explicit–implicit methods for the solution of the system of Maxwell equations have been studied by several authors with the shared goal of designing numerical methodologies able to deal with hybrid structured–unstructured meshes. For example, a stable hybrid FDTD–FETD method is considered by Rylander and Bondeson in [8], while Degerfeldt and Rylander [3] propose a FETD method with stable hybrid explicit–implicit time stepping working on brick-tetrahedral meshes that do not require an intermediate layer of pyramidal elements. In [6], the authors study the application of explicit–implicit Runge–Kutta (so-called IMEX-RK) methods in conjunction with high order discontinuous Galerkin discretizations on unstructured triangular meshes, in the framework of unsteady compressible flow problems (i.e., the numerical solution of Euler or Navier–Stokes equations).

This study is concerned with the design of a non-dissipative hybrid explicit–implicit DGTD method for solving the time domain Maxwell equations on unstructured simplicial meshes. The hybrid explicit–implicit DGTD method considered here has been initially introduced by Piperno [7]. However, to our knowledge, this hybrid explicit–implicit DGTD method has not been investigated numerically so far for the simulation of realistic electromagnetic wave propagation problems. The rest of the paper is organized as follows: in Sect. 2, we state the initial and boundary value problem to be solved; the discretization in space by a discontinuous Galerkin method is discussed in Sect. 3 while the integration in time is considered in Sect. 4; numerical results and conclusions are respectively reported in Sect. 5.

2 Continuous Problem

We consider the Maxwell equations in three space dimensions for linear isotropic media with no source. The electric and magnetic fields $\mathbf{E}(\mathbf{x}, t)$ and $\mathbf{H}(\mathbf{x}, t)$ verify:

$$\varepsilon \partial_t \mathbf{E} - \operatorname{curl} \mathbf{H} = -\mathbf{J}, \quad \mu \partial_t \mathbf{H} + \operatorname{curl} \mathbf{E} = 0, \quad (1)$$

where $\mathbf{J}(\mathbf{x}, t)$ is a current source term. These equations are set on a bounded polyhedral domain Ω of \mathbb{R}^3 . The permittivity $\varepsilon(\mathbf{x})$ and the magnetic permeability tensor $\mu(\mathbf{x})$ are varying in space, time-invariant and both positive functions. Our goal is to solve system (1) in a domain Ω with boundary $\partial\Omega = \Gamma_a \cup \Gamma_m$, where we impose the following boundary conditions:

$$\begin{cases} \mathbf{n} \times \mathbf{E} = 0 \text{ on } \Gamma_m, \\ \mathbf{n} \times \mathbf{E} - \sqrt{\frac{\mu}{\varepsilon}} \mathbf{n} \times (\mathbf{H} \times \mathbf{n}) = \mathbf{n} \times \mathbf{E}_{\text{inc}} - \sqrt{\frac{\mu}{\varepsilon}} \mathbf{n} \times (\mathbf{H}_{\text{inc}} \times \mathbf{n}) \text{ on } \Gamma_a. \end{cases} \quad (2)$$

Here \mathbf{n} denotes the unit outward normal to $\partial\Omega$ and $(\mathbf{E}_{\text{inc}}, \mathbf{H}_{\text{inc}})$ is a given incident field. The first boundary condition is called *metallic* (referring to a perfectly conducting surface) while the second condition is called *absorbing* and takes here the

form of the Silver–Müller condition which is a first order approximation of the exact absorbing boundary condition. This absorbing condition is applied on Γ_a which represents an artificial truncation of the computational domain. Finally, system (1) is supplemented with initial conditions: $\mathbf{E}_0(\mathbf{x}) = \mathbf{E}(\mathbf{x}, t)$ and $\mathbf{H}_0(\mathbf{x}) = \mathbf{H}(\mathbf{x}, t)$.

3 Discretization in Space

We consider a partition \mathcal{T}_h of Ω into a set of tetrahedra τ_i of size h_i with boundary $\partial\tau_i$ such that $h = \max_{\tau_i \in \mathcal{T}_h} h_i$. For each τ_i , V_i denotes its volume, and ε_i and μ_i are respectively the local electric permittivity and magnetic permeability of the medium, which are assumed constant inside the element τ_i . For two distinct tetrahedra τ_i and τ_k in \mathcal{T}_h , the intersection $\tau_i \cap \tau_k$ is a triangle a_{ik} which we will call interface. For a given partition \mathcal{T}_h , we seek approximate solutions to (1) in the finite dimensional subspace $V_p(\mathcal{T}_h) = \{\mathbf{v} \in L^2(\Omega)^3 : v_k|_{\tau_i} \in \mathbb{P}_p(\tau_i), \text{ for } k = 1, 3 \text{ and } \forall \tau_i \in \mathcal{T}_h\}$ where $\mathbb{P}_p(\tau_i)$ denotes the space of nodal polynomial functions of degree at most p inside the element τ_i . Following the discontinuous Galerkin approach, the electric and magnetic fields inside each finite element are searched for as linear combinations $(\mathbf{E}_i, \mathbf{H}_i)$ of linearly independent basis vector fields $\boldsymbol{\varphi}_{ij}$, $1 \leq j \leq d$, where d denotes the local number of degrees of freedom inside τ_i . The discretization in space yields the following system of ODEs:

$$M_i^\varepsilon \frac{d\mathbf{E}_i}{dt} = K_i \mathbf{H}_i - \sum_{k \in \mathcal{V}_i} S_{ik} \mathbf{H}_k, \quad M_i^\mu \frac{d\mathbf{H}_i}{dt} = -K_i \mathbf{E}_i + \sum_{k \in \mathcal{V}_i} S_{ik} \mathbf{E}_k, \quad (3)$$

where the symmetric positive definite mass matrices M_i^σ (σ stands for ε or μ), the symmetric stiffness matrix K_i and the symmetric interface matrix S_{ik} (all of size $d \times d$) are given by:

$$(M_i^\sigma)_{jl} = \sigma_i \int_{\tau_i} {}^t \boldsymbol{\varphi}_{ij} \cdot \boldsymbol{\varphi}_{il}, \quad (S_{ik})_{jl} = \frac{1}{2} \int_{a_{ik}} {}^t \boldsymbol{\varphi}_{ij} \cdot (\boldsymbol{\varphi}_{kl} \times \mathbf{n}_{ik}), \\ (K_i)_{jl} = \frac{1}{2} \int_{\tau_i} {}^t \boldsymbol{\varphi}_{ij} \cdot \text{curl} \boldsymbol{\varphi}_{il} + {}^t \boldsymbol{\varphi}_{il} \cdot \text{curl} \boldsymbol{\varphi}_{ij}.$$

4 Time Discretization

The choice of the time discretization method is a crucial step for the global efficiency of the numerical method. Then, a possible alternative is to combine the strengths of explicit (easy to implement, greater accuracy with less computational effort) and implicit schemes (unconditional stability) applying an implicit time integration scheme locally in the refined regions of the mesh while preserving an explicit time scheme in the complementary part, resulting in an hybrid explicit–implicit

(or locally implicit) time integration strategy. The set of local system of ordinary differential equations for each τ_i (3) can be formally transformed in a global system. To this end, we suppose that all electric (resp. magnetic) unknowns are gathered in a column vector \mathbb{E} (resp. \mathbb{H}) of size $d_g = N_{\mathcal{T}_h} d$ where $N_{\mathcal{T}_h}$ stands for the number of elements in \mathcal{T}_h . Then system (3) can be rewritten as (we set $\mathbb{S} = \mathbb{K} - \mathbb{A} - \mathbb{B}$):

$$\mathbb{M}^\varepsilon \frac{d\mathbb{E}}{dt} = \mathbb{K}\mathbb{H} - \mathbb{A}\mathbb{H} - \mathbb{B}\mathbb{H} = \mathbb{S}\mathbb{H}, \quad \mathbb{M}^\mu \frac{d\mathbb{H}}{dt} = -\mathbb{K}\mathbb{E} + \mathbb{A}\mathbb{E} - \mathbb{B}\mathbb{E} = -{}^t\mathbb{S}\mathbb{E}. \quad (4)$$

where we have the following definitions and properties:

- $\mathbb{M}^\varepsilon, \mathbb{M}^\mu$ and \mathbb{K} are $d_g \times d_g$ block diagonal matrices with diagonal blocks equal to M_i^ε, M_i^μ and K_i respectively.
- \mathbb{A} is also a $d_g \times d_g$ block sparse matrix, whose non-zero blocks are equal to S_{ik} when a_{ik} is an internal interface of the mesh.
- \mathbb{B} is a $d_g \times d_g$ block diagonal matrix, whose non-zero blocks are associated to the numerical treatment of the boundary conditions (2).

4.1 Explicit and Implicit Time Schemes

The system (4) can be time integrated using a second-order Leap–Frog scheme as:

$$\mathbb{M}^\varepsilon \left(\frac{\mathbb{E}^{n+1} - \mathbb{E}^n}{\Delta t} \right) = \mathbb{S}\mathbb{H}^{n+\frac{1}{2}}, \quad \mathbb{M}^\mu \left(\frac{\mathbb{H}^{n+\frac{3}{2}} - \mathbb{H}^{n+\frac{1}{2}}}{\Delta t} \right) = -{}^t\mathbb{S}\mathbb{E}^{n+1}. \quad (5)$$

The resulting fully explicit DGTD- \mathbb{P}_p method is analyzed in [5] where it is shown that the method is non-dissipative, conserves a discrete form of the electromagnetic energy and is stable under the CFL-like condition:

$$\Delta t \leq \frac{2}{d_2}, \quad \text{with } d_2 = \| (\mathbb{M}^{-\mu})^{\frac{1}{2}} {}^t\mathbb{S} (\mathbb{M}^{-\varepsilon})^{\frac{1}{2}} \|, \quad (6)$$

where $\|\cdot\|$ denote the canonical norm of a matrix ($\forall X, \|AX\| \leq \|A\| \|X\|$), and the matrix $(\mathbb{M}^{-\sigma})^{\frac{1}{2}}$ is the inverse square root of \mathbb{M}^σ . Alternatively, (4) can be time integrated using a second-order Crank–Nicolson scheme as:

$$\begin{cases} \mathbb{M}^\varepsilon \left(\frac{\mathbb{E}^{n+1} - \mathbb{E}^n}{\Delta t} \right) = \mathbb{S} \left(\frac{\mathbb{H}^n + \mathbb{H}^{n+1}}{2} \right), \\ \mathbb{M}^\mu \left(\frac{\mathbb{H}^{n+1} - \mathbb{H}^n}{\Delta t} \right) = -{}^t\mathbb{S} \left(\frac{\mathbb{E}^n + \mathbb{E}^{n+1}}{2} \right). \end{cases} \quad (7)$$

Such a fully implicit DGTD- \mathbb{P}_p method is considered in [2] for the solution of the 2D Maxwell equations. In particular, the resulting method is unconditionally stable.

4.2 Hybrid Explicit–Implicit Time Scheme

We consider here a method of this kind that was recently proposed by Piperno in [7]. The set of elements τ_i of the mesh is now assumed to be partitioned into two subsets: one made of the smallest elements and the other one gathering the remaining elements. In the following, these two subsets are respectively referred as \mathcal{S}_i and \mathcal{S}_e . In the proposed hybrid time scheme, the small elements are handled using a Crank–Nicolson scheme while all other elements are time advanced using a variant of the classical Leap–Frog scheme known as the Verlet method. Then, starting from the values of the fields at time $t^n = n\Delta t$, the proposed hybrid explicit–implicit time integration scheme consists in three sub-steps:

1. The components of \mathbb{H} and \mathbb{E} associated to the set \mathcal{S}_e are time advanced from t^n to $t^{n+\frac{1}{2}}$ with time step $\Delta t/2$ using a pseudo-forward Euler scheme,
2. The components of \mathbb{H} and \mathbb{E} associated to the set \mathcal{S}_i are time advanced from t^n to t^{n+1} with time step Δt using the Crank–Nicolson scheme,
3. The components of \mathbb{H} and \mathbb{E} associated to the set \mathcal{S}_e are time advanced from $t^{n+\frac{1}{2}}$ to t^{n+1} with time step $\Delta t/2$ using the reversed pseudo-forward Euler scheme.

In order to further describe this scheme, the problem unknowns are reordered such that sub-vectors with an e subscript (respectively, an i subscript) are associated to the elements of the set \mathcal{S}_e (respectively, the set \mathcal{S}_i). Thus, the global system of ordinary differential equations (4) can be split into two systems:

$$\begin{cases} \mathbb{M}_e^\varepsilon \frac{d\mathbb{E}_e}{dt} = \mathbb{S}_e \mathbb{H}_e - \mathbb{A}_{ei} \mathbb{H}_i, \\ \mathbb{M}_e^\mu \frac{d\mathbb{H}_e}{dt} = -{}^t\mathbb{S}_e \mathbb{E}_e + \mathbb{A}_{ei} \mathbb{E}_i, \end{cases} \quad \begin{cases} \mathbb{M}_i^\varepsilon \frac{d\mathbb{E}_i}{dt} = \mathbb{S}_i \mathbb{H}_i - \mathbb{A}_{ie} \mathbb{H}_e, \\ \mathbb{M}_i^\mu \frac{d\mathbb{H}_i}{dt} = -{}^t\mathbb{S}_i \mathbb{E}_i + \mathbb{A}_{ie} \mathbb{E}_e. \end{cases} \quad (8)$$

Then, the proposed hybrid explicit–implicit algorithm consists in the following steps:

$$\text{Step 1 : } \begin{cases} \mathbb{M}_e^\mu \left(\frac{\mathbb{H}_e^{n+\frac{1}{2}} - \mathbb{H}_e^n}{\Delta t/2} \right) = -{}^t\mathbb{S}_e \mathbb{E}_e^n + \mathbb{A}_{ei} \mathbb{E}_i^n, \\ \mathbb{M}_e^\varepsilon \left(\frac{\mathbb{E}_e^{n+\frac{1}{2}} - \mathbb{E}_e^n}{\Delta t/2} \right) = \mathbb{S}_e \mathbb{H}_e^{n+\frac{1}{2}} - \mathbb{A}_{ei} \mathbb{H}_i^n. \end{cases} \quad (9)$$

$$\text{Step 2 : } \begin{cases} \mathbb{M}_i^\varepsilon \left(\frac{\mathbb{E}_i^{n+1} - \mathbb{E}_i^n}{\Delta t} \right) = \mathbb{S}_i \left(\frac{\mathbb{H}_i^{n+1} + \mathbb{H}_i^n}{2} \right) - \mathbb{A}_{ie} \mathbb{H}_e^{n+\frac{1}{2}}, \\ \mathbb{M}_i^\mu \left(\frac{\mathbb{H}_i^{n+1} - \mathbb{H}_i^n}{\Delta t} \right) = -{}^t\mathbb{S}_i \left(\frac{\mathbb{E}_i^{n+1} + \mathbb{E}_i^n}{2} \right) + \mathbb{A}_{ie} \mathbb{E}_e^{n+\frac{1}{2}}. \end{cases} \quad (10)$$

$$\text{Step 3 : } \begin{cases} \mathbb{M}_e^\varepsilon \left(\frac{\mathbb{E}_e^{n+1} - \mathbb{E}_e^{n+\frac{1}{2}}}{\Delta t/2} \right) = \mathbb{S}_e \mathbb{H}_e^{n+\frac{1}{2}} - \mathbb{A}_{ei} \mathbb{H}_i^{n+1}, \\ \mathbb{M}_e^\mu \left(\frac{\mathbb{H}_e^{n+1} - \mathbb{H}_e^{n+\frac{1}{2}}}{\Delta t/2} \right) = -{}^t \mathbb{S}_e \mathbb{E}_e^{n+1} + \mathbb{A}_{ei} \mathbb{E}_i^{n+1}. \end{cases} \quad (11)$$

In [7], the author shows that the hybrid explicit–implicit scheme (9)–(11) for time integration of the semi-discrete system (4) associated to the DGTD- \mathbb{P}_p method exactly conserves the following quadratic form of the numerical unknowns \mathbb{E}_e^n , \mathbb{E}_i^n , \mathbb{H}_e^n and \mathbb{H}_i^n :

$$\mathcal{E}^n = \mathcal{E}_e^n + \mathcal{E}_i^n + \mathcal{E}_h^n \quad \text{with} \quad \begin{cases} \mathcal{E}_e^n = {}^t \mathbb{E}_e^n \mathbb{M}_e^\varepsilon \mathbb{E}_e^n + {}^t \mathbb{H}_e^{n+\frac{1}{2}} \mathbb{M}_e^\mu \mathbb{H}_e^{n-\frac{1}{2}}, \\ \mathcal{E}_i^n = {}^t \mathbb{E}_i^n \mathbb{M}_i^\varepsilon \mathbb{E}_i^n + {}^t \mathbb{H}_i^n \mathbb{M}_i^\mu \mathbb{H}_i^n, \\ \mathcal{E}_h^n = -\frac{\Delta t^2}{4} {}^t \mathbb{H}_i^n {}^t \mathbb{A}_{ei} (\mathbb{M}_e^\varepsilon)^{-1} \mathbb{A}_{ei} \mathbb{H}_i^n, \end{cases} \quad (12)$$

as far as $\Gamma_a = \emptyset$. However, the condition under which \mathcal{E}^n is a positive definite quadratic form and thus represents a discrete form of the electromagnetic energy is not given. In the following we state such a condition on the global time step Δt .

Lemma 1. *The discrete electromagnetic energy \mathcal{E}^n given by (12) is a positive definite quadratic form of the numerical unknowns \mathbb{E}_e^n , \mathbb{E}_i^n , \mathbb{H}_e^n and \mathbb{H}_i^n if:*

$$\Delta t \leq \frac{2}{\alpha_e + \max(\beta_{ei}, \gamma_{ei})} \quad \text{with} \quad \begin{cases} \alpha_e = \| (\mathbb{M}_e^\varepsilon)^{-\frac{1}{2}} \mathbb{S}_e (\mathbb{M}_e^\mu)^{-\frac{1}{2}} \|, \\ \beta_{ei} = \| (\mathbb{M}_e^\varepsilon)^{-\frac{1}{2}} \mathbb{A}_{ei} (\mathbb{M}_i^\mu)^{-\frac{1}{2}} \|, \\ \gamma_{ei} = \| (\mathbb{M}_e^\mu)^{-\frac{1}{2}} \mathbb{A}_{ei} (\mathbb{M}_i^\varepsilon)^{-\frac{1}{2}} \|, \end{cases} \quad (13)$$

where $\| \cdot \|$ denotes a matrix norm and the matrix $(\mathbb{M}_{e/i}^\sigma)^{-\frac{1}{2}}$ is the inverse of the square root of the matrix $\mathbb{M}_{e/i}^\sigma$ (σ stands for ε or μ).

The proof can be found in [4]. In summary, (13) states that the stability of the hybrid explicit–implicit DGTD- \mathbb{P}_p method is deduced from a criterion which is essentially the one obtained for the fully explicit method here restricted to the subset of explicit elements \mathcal{S}_e , augmented by two terms involving elements of the implicit subset \mathcal{S}_i associated to hybrid internal interfaces (i.e., interfaces a_{ik} such that $\tau_i \in \mathcal{S}_e$ and $\tau_k \in \mathcal{S}_i$).

5 Numerical Results

In this section we apply the proposed hybrid explicit–implicit DGTD- \mathbb{P}_p method to the simulation of a 3D problem involving the scattering of a plane wave ($F = 1$ GHz) by a perfectly conducting sphere with wall thickness $e = 5 \cdot 10^{-3}$ m and radius

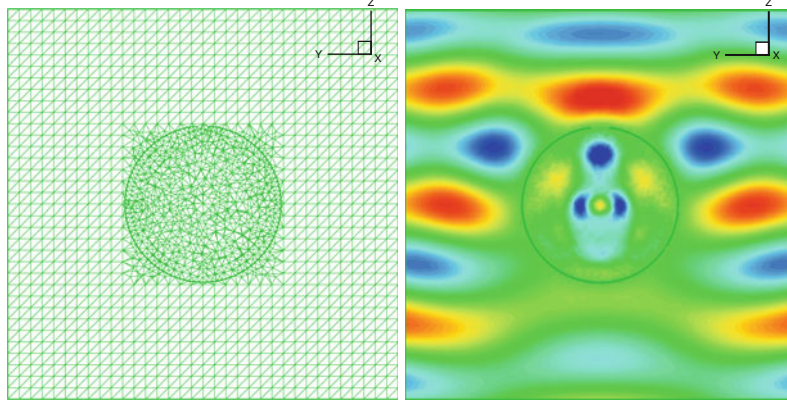


Fig. 1 Scattering of plane wave by a spherical mesh cavity with a hole. Geometry setting and unstructured mesh (*left*), contour lines of E_x for the hybrid explicit–implicit DGTD- \mathbb{P}_2 method (*right*)

$R = 0.2$ m with a hole of radius $r = 2.5 \cdot 10^{-2}$ m at one of its pole (see Fig. 1 left for a view of the geometry and the unstructured mesh in a selected plane). The computational domain is artificially bounded by a cubic surface on which the Silver–Müller boundary condition is applied. The underlying tetrahedral mesh consists of 56,482 vertices and 301,116 tetrahedra. The contour lines of E_x for a physical simulation time corresponding to 10 periods of the incident wave are shown on Fig. 1 right. The definition of the subsets \mathcal{S}_i and \mathcal{S}_e relies on the geometric criterion $c_g(\tau_i) = 4 \min_{j \in \mathcal{V}_i} \frac{V_i V_j}{P_i P_j}$. In the present case, the threshold value $2.5 \cdot 10^{-3}$ m has been selected resulting in $|\mathcal{S}_e| = 300,526$ and $|\mathcal{S}_i| = 590$ (i.e., only 0.2% of the mesh elements are treated implicitly). The time steps used in the simulations are the following: 0.34 (2.8) picosec for the explicit (hybrid) DGTD- \mathbb{P}_1 method and 0.17 (1.4) picosec for the explicit (hybrid) DGTD- \mathbb{P}_2 method. Numerical simulations have been conducted on a cluster of Intel Xeon 2.33 GHz based nodes interconnected by a high performance Myrinet network. Each node consists of a dual processor quad core board sharing 16 GB of RAM memory. The parallelization of the hybrid explicit–implicit DGTD- \mathbb{P}_p method relies on a SPMD (Single Program Multiple Data) strategy which combines a partitioning of the tetrahedral mesh with a message passing programming using the MPI interface. Performance results for the simulations based on the DGTD- \mathbb{P}_1 and DGTD- \mathbb{P}_2 methods are summarized in Table 1 where “RAM (LU)” is the maximum per-processor memory overhead for computing and storing the sparse L and U factors (after an AMD reordering for the minimization of the bandwidth), while “Time (LU)” gives the maximum factors construction time. The direct solver used is MUMPS (see [1]) The results of Table 1 show that the memory overhead associated to the construction and the storage of the L and U factors of the implicit matrix is acceptable while the gain in computing time is roughly equal to 4.4 for both the \mathbb{P}_1 and \mathbb{P}_2 interpolation methods.

Table 1 Scattering of plane wave by a spherical mesh cavity. Performance results ($N_s = 8$ processing units)

Method	RAM (LU)	Time (LU)	Total time
Explicit DGTD- \mathbb{P}_1	–	–	44 mn
Hybrid explicit–implicit DGTD- \mathbb{P}_1	2 MB	<1 s	10 mn
Explicit DGTD- \mathbb{P}_2	–	–	4 h 24 mn
Hybrid explicit–implicit DGTD- \mathbb{P}_2	8 MB	<1 s	56 mn

6 Conclusions

We have presented some preliminary results of the development of a hybrid explicit–implicit DGTD method for overcoming the grid-induced stiffness in time domain electromagnetics. The proposed method allows to reduce notably the overall computing time as compared to a fully explicit method, when a rather small number of the mesh elements are treated implicitly (typically a few percent) which is often the case in practical situations involving locally refined simplicial meshes. Future works will follow several directions: (a) improvement of the temporal accuracy by studying the combination of a high order Leap-Frog scheme with a high order implicit time scheme, (b) design of an auto-adaptive solution strategy for the selection of the reference time step minimizing dispersion error and, (c) treatment of load balancing issues raised by the separation of mesh elements into two subsets in order to obtain a scalable hybrid explicit–implicit DGTD method.

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