

On a Finite-Element Method for Solving the Three-Dimensional Maxwell Equations

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The aim of this paper is to present a method for solving the time-domain three-dimensional Maxwell equations, which can be coupled with a particle solver. For this purpose, Maxwell's equations are reformulated as a constrained wave equation system, with Lagrange multipliers associated to the conditions $\nabla \cdot B = 0$ and $\nabla \cdot E = \rho/\epsilon_0$. We approximate both the fields and the Lagrange multipliers with a finite element method using a Taylor-Hood element. © 1993 Academic Press, Inc.

1. INTRODUCTION

The numerical modeling in plasma physics as well as in hyperfrequency devices or vacuum diode technology, requires to develop three-dimensional Vlasov-Maxwell solvers in the time domain, which can deal with arbitrary geometries. In this context, a Maxwell solver has to fulfill, if possible, the following requirements:

1. The electromagnetic fields have to be continuous, which is a stability condition for the classical Vlasov solvers.
2. The electric field must satisfy Gauss law and the magnetic field must be divergence free.
3. The space and time discretizations have to lead to an explicit scheme in order to avoid the solution of a linear system at each time-step.

Most of the numerical codes which are currently developed are based on finite difference approximations of Maxwell's equations on structured meshes. Such an approach is more straightforward to implement in the simple cases. However, as soon as the domain geometry becomes too complex or when local refinements are necessary, the structured mesh strategy requires a lot of skill, such as domain decomposition [1] or boundary fitting [2]. On the other hand,

unstructured meshes provide more flexibility to approximate complex geometries, to achieve local refinements, and to eventually implement adaptive strategies. But they require a finite volume or finite element resolution of the Maxwell equations, which means some kind of integral or variational formulation, together with the choice of appropriate spaces of approximation functions.

Up to now, very few finite volume or finite element methods have been developed for the numerical resolution of the Maxwell equations on unstructured meshes. On the one hand, the finite volume technique, described and analyzed in [3, 4], does not fulfill condition 1 and needs Delaunay-Voronoi meshes, which is a severe drawback in 3D. On the other hand, finite edge-element methods, such as conforming $H(\text{curl})$ or $H(\text{div})$ element in a "standard" [5] or "modified" form [6], implicitly satisfy condition 2, but they do not satisfy conditions 1 and 3.

The method we shall describe in this paper is close to [7], in the sense that we use decoupled second-order wave equation formulations of the Maxwell equations, and a $P1$ conforming finite element discretization. However, in [7], no control on the divergence of the fields can be obtained. In the context of scattering calculations, where no external charges and currents are present, this may not be a major drawback. The situation is opposite in our case. We thus cope with the condition 2 by reformulating the Maxwell equations as a constrained problem, with associated Lagrange multipliers (which are close to the "correcting potentials" in the usual methods [8]). We approximate both the fields and the Lagrange multipliers by using a modified Taylor-Hood element, which is standard in incompressible fluid dynamics [9].

2. A CONSTRAINED VARIATIONAL FORMULATION FOR THE MAXWELL EQUATIONS

2.1. Classical Form of Maxwell's Equations

In this paper, we consider a homogeneous three-dimensional bounded domain Ω without any symmetry. We will

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therefore use cartesian coordinates (x, y, z) . We denote by Γ the boundary of Ω . We introduce the Maxwell equations

$$\frac{1}{c^2} \frac{\partial E}{\partial t} - \nabla \times B = -\mu_0 J, \quad (2.1)$$

$$\frac{\partial B}{\partial t} + \nabla \times E = 0, \quad (2.2)$$

$$\nabla \cdot E = \frac{\rho}{\epsilon_0}, \quad (2.3)$$

$$\nabla \cdot B = 0, \quad (2.4)$$

where

c is the speed of the light in the vacuum

μ_0 is the magnetic permeability in the vacuum

ϵ_0 is the dielectric permittivity in the vacuum

and they satisfy

$$\epsilon_0 \mu_0 c^2 = 1.$$

It is well known that the constraint $\nabla \cdot B = 0$ is satisfied at any time t if it is satisfied at the initial time $t = 0$. Indeed, $\nabla \cdot (\nabla \times E) = 0$ with (2.2) implies $(\partial/\partial t)(\nabla \cdot B) = 0$ and $\nabla \cdot B = \nabla \cdot B(t = 0)$.

Similarly, the constraint $\nabla \cdot E = \rho/\epsilon_0$ is satisfied at any time t , provided it is satisfied at the initial time $t = 0$ and if the charge conservation equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot J = 0 \quad (2.5)$$

holds. Recall that Eqs. (2.1), (2.5) and $\nabla \cdot (\nabla \times B) = 0$ imply $(1/c^2)(\partial/\partial t)(\nabla \cdot E) + \mu_0(\nabla \cdot J) = 0$ and $(\partial/\partial t)(\nabla \cdot E - \rho/\epsilon_0) = 0$ which leads to $\nabla \cdot E - \rho/\epsilon_0 = (\nabla \cdot E - \rho/\epsilon_0)|_{t=0}$.

However, in the discrete case it may very well happen that these properties do not pass to the numerical approximation either because

$$\frac{\partial \rho_h}{\partial t} + \nabla_h \cdot J_h \neq 0, \quad (2.6)$$

where ρ_h, J_h , and ∇_h are the discrete charge density, current density, and divergence operator, respectively, or because the discrete divergence and curl operators do not satisfy

$$\nabla_h \cdot (\nabla_h \times) = 0. \quad (2.7)$$

Therefore a convenient way to deal with this problem is to introduce the Lagrange multipliers of the constraints (2.3) and (2.4).

2.2. The Maxwell Equations as a Constrained Problem

We now introduce the Lagrange multipliers $\varphi(x, t)$ and $p(x, t)$ of the constraints (2.3), (2.4), which can be viewed as some sort of electric and magnetic correcting potentials [8]. We may impose homogeneous Dirichlet boundary conditions on φ and p :

$$\varphi = 0 \quad \text{on } \Gamma, \quad (2.8)$$

$$p = 0 \quad \text{on } \Gamma. \quad (2.9)$$

The Maxwell equations (2.1)–(2.4) can be written as

$$\frac{1}{c^2} \left(\frac{\partial E}{\partial t} - \nabla \varphi \right) - \nabla \times B = -\mu_0 J, \quad (2.10)$$

$$\frac{\partial B}{\partial t} - \nabla p + \nabla \times E = 0, \quad (2.11)$$

$$\nabla \cdot E = \rho/\epsilon_0, \quad (2.12)$$

$$\nabla \cdot B = 0. \quad (2.13)$$

We supplement this system with appropriate boundary conditions. For the sake of simplicity, we will only consider perfectly conducting boundaries in Sections 2 and 3, whereas the case of the Silver–Müller absorbing boundary condition will be treated in a special section (Section 4). For the time being, we suppose that

$$E \times n = 0 \quad \text{on } \Gamma. \quad (2.14)$$

Finally, we are given initial conditions

$$E(t = 0) = E_0, \quad (2.15)$$

$$B(t = 0) = B_0, \quad (2.16)$$

with the following constraints:

$$\nabla \cdot E_0 = \rho/\epsilon_0, \quad (2.17)$$

$$\nabla \cdot B_0 = 0, \quad (2.18)$$

$$E_0 \times n = 0 \quad \text{on } \Gamma. \quad (2.19)$$

Obviously, p is identically zero and so is φ if ρ and J satisfy the charge conservation equation (2.5). Hence, the system of equations (2.8)–(2.19) is an equivalent formulation of the classical Maxwell equations.

2.3. Formulation in Terms of Two Second-Order Wave Equations

The finite element discretization of the Maxwell equations leads to a very unstable numerical algorithm [10]. Indeed, in [11], Lesaint shows why it is impossible to

control the oscillations which may appear in such a formulation. The L^2 -type control on the solutions via the energy functional $\int_{\Omega} (|E|^2 + (1/c^2) |B|^2) dx$ does not enable us to control the gradients of the solutions. On the other hand, a formulation of the Maxwell equations as a second-order wave equation leads to a H^1 control on the solution [12] with an energy functional of the form

$$\int_{\Omega} \left(\left| \frac{\partial E}{\partial t} \right|^2 + |\nabla E|^2 + \frac{1}{c^2} \left(\left| \frac{\partial B}{\partial t} \right|^2 + |\nabla B|^2 \right) \right) dx.$$

For these reasons, we prefer to work with second-order wave equations for both the electric and magnetic fields, i.e., for Eqs. (2.10) and (2.11).

Differentiating (2.10) with respect to t gives

$$\frac{1}{c^2} \left(\frac{\partial^2 E}{\partial t^2} - \nabla \frac{\partial \phi}{\partial t} \right) - \nabla \times \frac{\partial B}{\partial t} = -\mu_0 \frac{\partial J}{\partial t}$$

and, using (2.11), we obtain, by setting $\partial \phi / \partial t = \phi$,

$$\frac{\partial^2 E}{\partial t^2} + c^2 \nabla \times (\nabla \times E) - \nabla \phi = -\frac{1}{\varepsilon_0} \frac{\partial J}{\partial t}. \quad (2.20)$$

In the same way, differentiating (2.11) with respect to t gives

$$\frac{\partial^2 B}{\partial t^2} - \nabla \left(\frac{\partial p}{\partial t} \right) + \nabla \times \frac{\partial E}{\partial t} = 0$$

and, using (2.10), we obtain by setting $\partial p / \partial t = P$,

$$\frac{\partial^2 B}{\partial t^2} + c^2 \nabla \times (\nabla \times B) - \nabla P = \frac{1}{\varepsilon_0} \nabla \times J. \quad (2.21)$$

The two vector wave equations (2.20) and (2.21) are supplemented with the constraints

$$\nabla \cdot E = \rho / \varepsilon_0, \quad (2.22)$$

$$\nabla \cdot B = 0, \quad (2.23)$$

with the initial conditions

$$E(t=0) = 0, \quad B(t=0) = 0, \quad (2.24)$$

and with the boundary conditions

$$\phi = 0, \quad P = 0 \quad \text{on } \Gamma, \quad (2.25)$$

$$E \times n = 0, \quad (\nabla \times B) \times n = \mu_0 J \times n \quad \text{on } \Gamma. \quad (2.26)$$

Moreover, we have to add initial conditions for $\partial E / \partial t$ and

$\partial B / \partial t$, since we are dealing with a second-order problem. We obtain them in a direct way from (2.10) and (2.11) as

$$\frac{\partial B}{\partial t}(t=0) = \nabla p(t=0) - \nabla \times E_0, \quad (2.27)$$

$$\frac{\partial E}{\partial t}(t=0) = \nabla \phi(t=0) + c^2 \nabla \times B_0 - \frac{1}{\varepsilon_0} J(t=0). \quad (2.28)$$

Observe that the coupling between the fields E and B is preserved due to these initial conditions (and due to ρ and J with (2.5), but in an implicit way). Let us also remark that the boundary condition $(\nabla \times B) \times n = \mu_0 J \times n$ on Γ is a consequence of the condition $E \times n|_{\Gamma} = 0$. The former is a Neuman boundary condition, whereas the latter is a Dirichlet boundary condition. It is an easy matter to show the equivalence between the formulations (2.8)–(2.19) and (2.20)–(2.28).

2.4. Variational Formulation

Let us now introduce the variational formulation of the problem (2.20)–(2.28), which will be the basis of the finite element method (cf. Section 3). Observe first that for given charge density ρ and current density J , and for given initial conditions, the problem (2.20)–(2.28) reduces to a set of two uncoupled initial boundary value problems for the vector wave equation. Since these two problems are of the same mathematical nature, we will concentrate on one of them, namely the B -constrained wave equation.

Now, let C be a sufficiently smooth vector test function. Taking the dot product of (2.21) by C and integrating over Ω yields

$$\int_{\Omega} \frac{\partial^2 B}{\partial t^2} \cdot C \, dx + c^2 \int_{\Omega} (\nabla \times (\nabla \times B)) \cdot C \, dx - \int_{\Omega} \nabla P \cdot C \, dx = \frac{1}{\varepsilon_0} \int_{\Omega} (\nabla \times J) \cdot C \, dx.$$

By using the Green formulae

$$\int_{\Omega} (\nabla \times (\nabla \times B)) \cdot C \, dx = \int_{\Omega} (\nabla \times B) \cdot (\nabla \times C) \, dx - \int_{\Gamma} ((\nabla \times B) \times n) \cdot C \, dy \quad (2.29)$$

and

$$\int_{\Omega} (\nabla \times J) \cdot C \, dx = \int_{\Omega} J \cdot (\nabla \times C) \, dx - \int_{\Gamma} (J \times n) \cdot C \, dy, \quad (2.30)$$

together with the boundary condition (2.26), we obtain

$$\int_{\Omega} \frac{\partial^2 B}{\partial t^2} \cdot C \, dx + c^2 \int_{\Omega} (\nabla \times B) \cdot (\nabla \times C) \, dx - \int_{\Omega} \nabla P \cdot C \, dx = \frac{1}{\epsilon_0} \int_{\Omega} J \cdot (\nabla \times C) \, dx.$$

Then, by using the Green formula

$$\int_{\Omega} \nabla P \cdot C \, dx = - \int_{\Omega} P \nabla \cdot C \, dx + \int_{\Gamma} P(C \cdot n) \, d\gamma \quad (2.31)$$

and the boundary condition (2.25), we have

$$\int_{\Omega} \frac{\partial^2 B}{\partial t^2} \cdot C \, dx + c^2 \int_{\Omega} (\nabla \times B) \cdot (\nabla \times C) \, dx + \int_{\Omega} P \nabla \cdot C \, dx = \frac{1}{\epsilon_0} \int_{\Omega} J \cdot (\nabla \times C) \, dx.$$

Let us next turn to Eq. (2.23). For any sufficiently smooth function q , we can write

$$\int_{\Omega} \nabla \cdot Bq \, dx = 0.$$

We now introduce the functional spaces, with the classical notations

$$\begin{aligned} H(\text{curl}, \Omega) &= \{v \in L^2(\Omega)^3, \nabla \times v \in L^2(\Omega)^3\}, \\ H(\text{div}, \Omega) &= \{v \in L^2(\Omega)^3, \nabla \cdot v \in L^2(\Omega)\}, \\ H^1(\Omega) &= \{p \in L^2(\Omega), \nabla p \in L^2(\Omega)\}. \end{aligned}$$

Then, we define

$$\begin{aligned} Y &= H(\text{curl}, \Omega) \cap H(\text{div}, \Omega), \\ Y_0 &= \{F \in Y, F \times n = 0 \text{ on } \Gamma\} \end{aligned}$$

and

$$\begin{aligned} Z &= H^1(\Omega)^3, \\ Z_0 &= \{F \in Z, F \times n = 0 \text{ on } \Gamma\}. \end{aligned}$$

Hence, a variational formulation of the problem is to find $(B(t), P(t)) \in Y \in L^2(\Omega)$ as the solution of the problem

$$\int_{\Omega} \frac{\partial^2 B}{\partial t^2} \cdot C \, dx + c^2 \int_{\Omega} (\nabla \times B) \cdot (\nabla \times C) \, dx + \int_{\Omega} P \nabla \cdot C \, dx = \frac{1}{\epsilon_0} \int_{\Omega} J \cdot (\nabla \times C) \, dx, \quad \forall C \in Y, \quad (2.32)$$

$$\int_{\Omega} \nabla \cdot Bq \, dx = 0, \quad \forall q \in L^2(\Omega), \quad (2.33)$$

$$B(0) = B_0, \quad (2.34)$$

$$\frac{\partial B}{\partial t}(t=0) = \nabla p(t=0) - \nabla \times E_0. \quad (2.35)$$

Observe that we do not require any boundary condition on Γ for the Lagrange multiplier P anymore. This will make the numerical approximation easier.

We formally show that any sufficiently smooth solution of the formulation (2.32)–(2.35) is a solution of the initial boundary value problem. It follows from (2.32), (2.33) that we have, first in the distributional sense, and then in the classical sense since the fields are smooth,

$$\begin{aligned} \frac{\partial^2 B}{\partial t^2} + c^2 \nabla \times (\nabla \times B) - \nabla P &= \frac{1}{\epsilon_0} \nabla \times J, \quad \text{in } \Omega, \\ \nabla \cdot B &= 0, \quad \text{in } \Omega. \end{aligned}$$

Then, by using Green's formulae (2.29), (2.30), (2.31), we obtain, for any $C \in Y$,

$$\begin{aligned} c^2 \int_{\Gamma} ((\nabla \times B) \times n) \cdot C \, d\gamma - \int_{\Gamma} P(C \cdot n) \, d\gamma &= \frac{1}{\epsilon_0} \int_{\Gamma} (J \times n) \cdot C \, d\gamma. \end{aligned} \quad (2.36)$$

By choosing test functions C such that either $C \cdot n_{|\Gamma}$ or $C \times n_{|\Gamma}$ vanish, we easily conclude from (2.36) that

$$c^2(\nabla \times B) \times n = \frac{1}{\epsilon_0} J \times n, \quad P = 0 \quad \text{on } \Gamma.$$

The stationary problem associated with the variational formulation (2.32)–(2.35) can be seen as a standard mixed formulation for a constrained problem. It is well known [9] that such a problem is well posed, if the pair of spaces $(Y, L^2(\Omega))$ are compatible in a sense expressed by the following inf-sup condition [9]:

$$\begin{aligned} \exists \beta > 0: \sup_{C \in Y} \frac{\int_{\Omega} \nabla \cdot Cq \, dx}{\|C\|_Y} &\geq \beta \|q\|_{L^2(\Omega)} \quad \forall q \in L^2(\Omega). \end{aligned} \quad (2.37)$$

This condition is indeed fulfilled in our case (see [13]). The classical semi-group theory allows us to conclude that the time dependent problem (2.32)–(2.35) is also well posed.

Furthermore, since $P \in L^2(\Omega)$, there exists a unique $\xi \in H_0^1(\Omega)$ such that $\Delta \xi = P$. Thus, $C = \nabla \xi$ belongs to Y and may be chosen as test function in (2.32). This yields

$$\frac{\partial^2}{\partial t^2} \int_{\Omega} B \nabla \xi \, dx + \int_{\Omega} |P|^2 \, dx = 0.$$

By using Green's formula (2.31) and Eq. (2.33), we obtain

$$\int_{\Omega} |P|^2 \, dx = 0.$$

This variational formulation indeed preserves the property that the Lagrange multiplier is identically zero.

Let us now introduce a second variational formulation whose form will appear more appropriate for the numerical computation: The augmented Lagrangian formulation. By using the property that $\nabla \cdot B = 0$, one can equivalently add in (2.32) the term

$$\int_{\Omega} \nabla \cdot B \nabla \cdot C \, dx, \quad \forall C \in Y.$$

Then, taking into account the property [14]: For any $B, C \in H^1(\Omega)^3 = Z$, we have

$$\begin{aligned} & \int_{\Omega} (\nabla \times B) \cdot (\nabla \times C) \, dx + \int_{\Omega} \nabla \cdot B \nabla \cdot C \, dx \\ &= \int_{\Omega} \nabla B : \nabla C \, dx + \sum_{\alpha=1}^3 \int_{\Gamma} (\nabla B_{\alpha} \times n) \cdot (u_{\alpha} \times C) \, d\gamma, \end{aligned} \quad (2.38)$$

where u_{α} , $1 \leq \alpha \leq 3$, denote the canonical basis of \mathbb{R}^3 , and the double dots $:$, the contracted product of two tensors.

We find

$$\begin{aligned} & \int_{\Omega} \frac{\partial^2 B}{\partial t^2} \cdot C \, dx + c^2 \int_{\Omega} \nabla B : \nabla C \, dx \\ &+ c^2 \sum_{\alpha=1}^3 \int_{\Gamma} (\nabla B_{\alpha} \times n) \cdot (u_{\alpha} \times C) \, d\gamma + \int_{\Omega} P \nabla \cdot C \, dx \\ &= \frac{1}{\varepsilon_0} \int_{\Omega} J \cdot (\nabla \times C) \, dx. \end{aligned} \quad (2.39)$$

Note that, in Eq. (2.39), the field B and the vector test function C have to be in the space Z , whereas in the formulation (2.32), it is sufficient that they be in the space $Y = H(\text{div}, \Omega) \cap H(\text{rot}, \Omega)$. Hence, in case that the two

spaces are different, in particular when Ω is a non-convex polyhedron, the solutions of the Z -formulation differ from the solutions of Maxwell's equations because they do not include singularities at corners pointing inside the domain. Nevertheless, we shall rather use this formulation which presents some advantages that we will see in a next section. For a similar purpose, we equivalently replace in (2.39) $\int_{\Omega} J \cdot (\nabla \times C) \, dx$ by $\int_{\Omega} (\nabla \times J) \cdot C \, dx + \int_{\Gamma} (J \times n) \cdot C \, d\gamma$.

For the inf-sup condition of this formulation, we have one that is analogous to condition (2.37) (cf. [13]). Hence, the associated time dependent problem is also well posed.

We cannot choose a vector test function C according to

$$C = \nabla \xi, \quad \Delta \xi = P,$$

as in the preceding case because the fact that such a C belongs to Z is not guaranteed. We cannot ensure that the Lagrange multiplier P is identically zero. Indeed, the Z -formulation can be seen as leading to a projection of the solution of the Maxwell equations onto the H^1 vector fields in which singularities due to the reentrant corners are projected.

We now turn to the second constrained wave equation for the electric field E . Using similar arguments as above, we obtain also an augmented Lagrangian formulation. However, we need to work with the subspace Z_0 of Z of vector fields which satisfy the condition $E \times n|_{\Gamma} = 0$. This remark will play an important role for the finite element approximation.

Let us now conclude this section by summarizing the various variational formulations that we shall approximate. We are looking for $(B(t), P(t)) \in Z \in L^2(\Omega)$, solutions of the equations

$$\begin{aligned} & \int_{\Omega} \frac{\partial^2 B}{\partial t^2} \cdot C \, dx + c^2 \int_{\Omega} \nabla B : \nabla C \, dx \\ &+ c^2 \sum_{\alpha=1}^3 \int_{\Gamma} (\nabla B_{\alpha} \times n) \cdot (u_{\alpha} \times C) \, d\gamma + \int_{\Omega} P \nabla \cdot C \, dx \\ &= \frac{1}{\varepsilon_0} \int_{\Omega} (\nabla \times J) \cdot C \, dx \\ &+ \frac{1}{\varepsilon_0} \int_{\Gamma} (J \times n) \cdot C \, d\gamma, \quad \forall C \in Z, \end{aligned} \quad (2.40)$$

$$\int_{\Omega} \nabla \cdot B q \, dx = 0, \quad \forall q \in L^2(\Omega), \quad (2.41)$$

$$B(0) = B_0, \quad (2.42)$$

$$\frac{\partial B}{\partial t}(t=0) = \nabla p(t=0) - \nabla \times E_0, \quad (2.43)$$

and $(E(t), \phi(t)) \in Z_0 \times L^2(\Omega)$, solutions of the equations

$$\begin{aligned} & \int_{\Omega} \frac{\partial^2 E}{\partial t^2} \cdot F \, dx + c^2 \int_{\Omega} \nabla E : \nabla F \, dx \\ & + c^2 \sum_{\alpha=1}^3 \int_{\Gamma} (\nabla E_{\alpha} \times n) \cdot (u_{\alpha} \times F) \, d\gamma + \int_{\Omega} -\nabla \cdot F \, dx \\ & = \frac{c^2}{\varepsilon_0} \int_{\Omega} \rho \nabla \cdot F \, dx - \frac{1}{\varepsilon_0} \int_{\Omega} \frac{\partial J}{\partial t} \cdot F \, dx, \quad \forall F \in Z_0, \end{aligned} \quad (2.44)$$

$$\int_{\Omega} \nabla \cdot E \psi \, dx = \frac{1}{\varepsilon_0} \int_{\Omega} \rho \psi \, dx, \quad \forall \psi \in L^2(\Omega), \quad (2.45)$$

$$E(0) = E_0, \quad (2.46)$$

$$\frac{\partial E}{\partial t}(t=0) = \nabla \varphi(t=0) + c^2 \nabla \times B_0 - \frac{1}{\varepsilon_0} J_0. \quad (2.47)$$

3. A TAYLOR-HOOD FINITE ELEMENT DISCRETIZATION OF THE FORMULATIONS (2.40)–(2.43) AND (2.44)–(2.47)

Starting from the variational formulation (2.40)–(2.47), we are now ready to derive a finite element approximation of Maxwell's equations expressed in terms of two constrained wave equations. As in the continuous case, the finite element discretization requires the choice of a pair of compatible approximation subspaces such that the discrete analogy of the inf-sup condition (2.37) is verified, with a constant β that is independent of the mesh size h . The fulfillment of this condition ensures that the discrete problem is well posed and converges to a solution of the continuous problem when the mesh size h tends to zero.

The problem of finding such a pair of compatible approximation spaces has been well studied in fluid dynamics [9]. But among the possible choices, the Taylor-Hood element retained our attention, because by using an appropriate quadrature formula, it leads to a diagonal mass matrix without any lumping. It is thus very well suited to an explicit time discretization.

We actually used the modified Taylor-Hood element (or " P_2 iso P_1 "), which first requires the definition of two levels of meshes. A coarser tetrahedrization \mathcal{T}_{2h} is first defined, and then, a finer one \mathcal{T}_h is defined by dividing each tetrahedron K_{2h} into eight subtetrahedra. Therefore, the nodes $\{a_i, i \in I_h\}$ of the finer tetrahedrization, consist of the vertices and of the middle of the edges of the tetrahedra of the coarser one. Then, the approximation spaces for the vector fields contain functions which are P_1 -conforming componentwise on the finer tetrahedrization. More precisely, they are continuous and their restriction to each

tetrahedron K_h of the finer mesh is a polynomial of degree one. At the same time, the approximation space for the Lagrange multipliers consists of the P_1 -conforming finite element on the coarser grid. Therefore, much fewer degrees of freedom are needed for the Lagrange multipliers (only defined on the nodes $\{a_l, l \in I_{2h}\}$ of \mathcal{T}_{2h}), which are not interesting physical quantities anyway, than for the magnetic and electric fields B and E .

Let us now introduce the approximation of the variational problem (2.40)–(2.47) for each field separately. We begin with

3.1. The Formulation (2.40)–(2.43)

We introduce the finite element subspaces of the spaces Z and $L^2(\Omega)$ respectively defined by

$$Z_h = \{F_h \in \mathcal{C}^0(\bar{\Omega})^3, \forall K_h \in \mathcal{T}_h, F_{h|K_h} \in P_1^3\}, \quad (3.1)$$

$$L_{2h} = \{\phi_{2h} \in \mathcal{C}^0(\bar{\Omega}), \forall K_{2h} \in \mathcal{T}_{2h}, \phi_{2h|K_{2h}} \in P_1\}. \quad (3.2)$$

For any function $F \in Z_h$, we may write

$$F(x) = \sum_{\alpha=1}^3 \sum_{i \in I_h} F_{\alpha}^i \phi_{\alpha}^i(x), \quad (3.3)$$

where $\{\phi_{\alpha}^i\}_{i \in I_h}$ is a basis of Z_h , with

$$\begin{aligned} \phi_{\alpha}^i &= \phi^i u_{\alpha}, & \phi^i(a_j) &= \delta_{ij}, \\ & i, j \in I_h & (u_{\alpha} \text{ defined in (2.38)}). \end{aligned} \quad (3.4)$$

Similarly, we may write for all function $q \in L_{2h}$,

$$q(x) = \sum_{l \in I_{2h}} q^l \psi^l(x), \quad (3.5)$$

where $\{\psi^l\}_{l \in I_{2h}}$ is a basis of L_{2h} , with

$$\psi^l(a_m) = \delta_{lm}, \quad l, m \in I_{2h}.$$

Hence, we look for approximation of B and P defined by

$$B_h(x, t) = \sum_{\alpha=1}^3 \sum_{i \in I_h} B_{\alpha}^i(t) \phi_{\alpha}^i(x), \quad (3.6)$$

$$P_{2h}(x, t) = \sum_{l \in I_{2h}} P^l(t) \psi^l(x). \quad (3.7)$$

So the finite-element method associated with the variational

formulation (2.40)–(2.43) amounts to finding $(B_h(t), P_{2h}(t)) \in Z_h \times L_{2h}$, solutions of the equations

$$\begin{aligned} & \int_{\Omega} \frac{\partial^2 B_h}{\partial t^2} \cdot C_h \, dx + c^2 \int_{\Omega} \nabla B_h : \nabla C_h \, dx \\ & + c^2 \sum_{\alpha=1}^3 \int_{\Gamma} (\nabla B_{h\alpha} \times n) \cdot (u_{\alpha} \times C_h) \, d\gamma + \int_{\Omega} P_{2h} \nabla \cdot C_h \, dx \\ & = \frac{1}{\varepsilon_0} \int_{\Omega} (\nabla \times J_h) \cdot C_h \, dx \\ & + \frac{1}{\varepsilon_0} \int_{\Gamma} (J_h \times n) \cdot C_h \, d\gamma, \quad \forall C_h \in Z_h, \end{aligned} \quad (3.8)$$

$$\int_{\Omega} \nabla \cdot B_h q_{2h} \, dx = 0, \quad \forall q_{2h} \in L_{2h}(\Omega). \quad (3.9)$$

We supplement these equations with fairly natural initial conditions. We take

$$B_h(0) = \Pi_h(B_0), \quad (3.10)$$

$$\frac{\partial B_h}{\partial t}(0) = \nabla \Pi_h(p_0) - \nabla \times \Pi_h(E_0), \quad (3.11)$$

where Π_h is a suitably defined projector from continuous to discrete fields. For instance, we take for all nodes a_i of \mathcal{T}_h ,

$$\Pi_h(B_0) = B_0(a_i), \quad \Pi_h(B) \in Z_h. \quad (3.12)$$

3.2. The Formulation (2.44)–(2.47)

We look for an approximation E_h of the electric field E which belongs to a finite element subspace of Z_h for which the boundary condition $(E_h \times n)|_{\Gamma} = 0$ is satisfied in an approximate way. We choose to deal with this condition by dualizing the constraint $(E \times n)|_{\Gamma} = 0$ in the continuous problem. For the sake of simplicity, we assume that Ω is a polyedron and that the exact and approximate boundaries Γ and Γ_h coincide. We then introduce the Lagrange multiplier λ , $\lambda \in H^{-1/2}(\Gamma)^3$ such that (2.44), (2.45) amounts to finding $(E(t), \phi(t), \lambda) \in Z \in L^2(\Omega) \times H^{-1/2}(\Gamma)^3$ solutions of

$$\begin{aligned} & \int_{\Omega} \frac{\partial^2 E}{\partial t^2} \cdot F \, dx + c^2 \int_{\Omega} \nabla E : \nabla F \, dx \\ & + c^2 \sum_{\alpha=1}^3 \int_{\Gamma} (\nabla E_{\alpha} \times n) \cdot (u_{\alpha} \times F) \, d\gamma \\ & + \int_{\Omega} \phi \nabla \cdot F \, dx + \int_{\Gamma} (\lambda \times n) \cdot (F \times n) \, d\gamma \\ & = \frac{c^2}{\varepsilon_0} \int_{\Omega} \rho \nabla \cdot F \, dx \\ & - \frac{1}{\varepsilon_0} \int_{\Omega} \frac{\partial J}{\partial t} \cdot F \, dx, \quad \forall F \in Z, \end{aligned} \quad (3.13)$$

$$\begin{aligned} & \int_{\Omega} \nabla \cdot E \psi \, dx \\ & = \frac{1}{\varepsilon_0} \int_{\Omega} \rho \psi \, dx, \quad \forall \psi \in L^2(\Omega), \end{aligned} \quad (3.14)$$

$$\begin{aligned} & \int_{\Gamma} (v \times n) \cdot (E \times n) \, d\gamma \\ & = 0, \quad \forall v \in H^{-1/2}(\Gamma)^3, \end{aligned} \quad (3.15)$$

$$\begin{aligned} & \int_{\Gamma} (\lambda \cdot n) \theta \, d\gamma \\ & = 0, \quad \forall \theta \in H^{1/2}(\Gamma). \end{aligned} \quad (3.16)$$

We then introduce the finite element subspace of the space $H^{-1/2}(\Gamma)^3$ according to

$$M_h = \{ \lambda \in \mathcal{C}^0(\Gamma)^3, \forall K_h^{\Gamma} \in \mathcal{T}_h^{\Gamma}, \lambda|_{K_h^{\Gamma}} \in P_1(K_h^{\Gamma})^3 \}, \quad (3.17)$$

where \mathcal{T}_h^{Γ} denotes the triangulation of Γ deduced from \mathcal{T}_h and the triangles K_h^{Γ} are the faces of the tetrahedra element of Γ . We also denote by I_h^{Γ} ($I_h^{\Gamma} \subset I_h$), the set of indices of the nodes $a_i \in \Gamma$. For any function $\lambda_h \in M_h$, we may write

$$\lambda_h(x) = \sum_{i \in I_h^{\Gamma}} \lambda_i \phi^i(x), \quad (3.18)$$

where $\phi^i(x)$ is the trace on Γ of the basis function ϕ^i defined by (3.4).

Now, we set

$$\begin{aligned} b(F, \lambda) &= \int_{\Gamma} (\lambda \times n) \cdot (F \times n) \, d\gamma, \\ & \forall F \in Z, \quad \forall \lambda \in H^{-1/2}(\Gamma)^3. \end{aligned}$$

Applying this bilinear form $b(\cdot, \cdot)$ to approximate fields yields

$$\begin{aligned} b(F_h, \lambda_h) &= \sum_{i, i' \in I_h^{\Gamma}} \int_{\Gamma} (\lambda_i \times n) \cdot (F_{i'} \times n) \phi^i \phi^{i'} \, d\gamma, \\ & \forall F_h \in Z_h, \quad \forall \lambda_h \in M_h. \end{aligned} \quad (3.19)$$

By splitting the integral over Γ into integrals over all $K_h^{\Gamma} \in \mathcal{T}_h^{\Gamma}$, and by using the property that $\phi^i \phi^{i'} \neq 0$ if and only if a_i and $a_{i'}$ are nodes of the same triangle K_h^{Γ} of \mathcal{T}_h^{Γ} , we obtain

$$\begin{aligned} b(F_h, \lambda_h) &= \sum_{i, i' \in I_h^{\Gamma}} \sum_{\substack{K_h^{\Gamma} \text{ s.t. } a_i, a_{i'} \\ \text{are nodes of } K_h^{\Gamma}}} (\lambda_i \times n_K) \cdot (F_{i'} \times n_K) \\ & \times \int_{K_h^{\Gamma}} \phi^i \phi^{i'} \, d\gamma, \end{aligned} \quad (3.20)$$

where n_K denotes the constant outside unit normal of Γ on K_h^r .

It remains to evaluate the integral of formula (3.20) by using the following quadrature formula (see Section 5 for more details)

$$\int_{K_h^r} v \, d\gamma \simeq \frac{|K_h^r|}{3} \sum_{a_i \text{ nodes of } K_h^r} v(a_i), \quad (3.21)$$

which is exact for any polynomial $v \in P^1$. We then obtain a first expression for an approximate bilinear form $\bar{b}_h(\cdot, \cdot)$ of $b(\cdot, \cdot)$ by

$$\begin{aligned} \bar{b}_h(F_h, \lambda_h) &= \sum_{i \in I_h^r} \sum_{\substack{K_h^r \text{ s.t. } a_i \\ \text{is a node of } K_h^r}} (\lambda_i \times n_K) \\ &\quad \times (F_i \times n_K) \frac{|K_h^r|}{3}. \end{aligned} \quad (3.22)$$

However, it leads to easier and cheaper computations if we replace the outside unit normal n_K in (3.22) by a normal n_i defined on each node a_i , $i \in I_h^r$, of \mathcal{T}_h^r . For instance, in the elementary case where all the triangles K_h^r , one of the vertices of which is a_i , are coplanar, all the normals, n_K 's, are equal and may be denoted by n_i . We thus can equivalently replace the expression (3.22) by

$$\bar{b}_h(F_h, \lambda_h) = \sum_{i \in I_h^r} (\lambda_i \times n_i) \cdot (F_i \times n_i) \sum_{K_h^r} \frac{|K_h^r|}{3}. \quad (3.23)$$

Let us now construct such a normal in the general case. Consider first the second sum of (3.22), which can be written according to (for a fixed $i \in I_h^r$)

$$\sum_{K_h^r} (\lambda_i \times n_K) \cdot (F_i \times n_K) \frac{|K_h^r|}{3} \frac{\sum_{K_h^r \in \mathcal{T}_h^r} |K_h^r|}{\sum_{K_h^r \in \mathcal{T}_h^r} |K_h^r|}. \quad (3.24)$$

Then, by using an appropriate averaging formula [15], the expression (3.24) can be approximated by

$$\begin{aligned} &\left(\sum_{K_h^r} \lambda_i \times \frac{n_K |K_h^r|}{\sum_{K_h^r \in \mathcal{T}_h^r} |K_h^r|} \right) \cdot \left(\sum_{K_h^r} F_i \times \frac{n_K |K_h^r|}{\sum_{K_h^r \in \mathcal{T}_h^r} |K_h^r|} \right) \\ &\quad \times \sum_{K_h^r} \frac{|K_h^r|}{3}. \end{aligned} \quad (3.25)$$

Finally, by setting

$$n_i = \frac{\sum_{K_h^r} n_K |K_h^r|}{\sum_{K_h^r} |K_h^r|}, \quad (3.26)$$

we obtain a second approximation $b_h(\cdot, \cdot)$ of the bilinear form $b(\cdot, \cdot)$ on $Z_h \times M_h$ by

$$b_h(F_h, \lambda_h) = \sum_{i \in I_h^r} (\lambda_i \times n_i) \cdot (F_i \times n_i) \alpha_i, \quad (3.27)$$

where

$$\alpha_i = \sum_{\substack{K_h^r \in \mathcal{T}_h^r \text{ s.t. } a_i \\ \text{is a node of } K_h^r}} \frac{|K_h^r|}{3}.$$

Of course, the straighter the angles between consecutive faces are, the more precise the approximation is.

The same work can be done with the bilinear form

$$\begin{aligned} c(\lambda, \theta) &= \int_{\Gamma} (\lambda \cdot n) \theta \, d\gamma, \\ &\quad \forall \lambda \in H^{-1/2}(\Gamma)^3, \quad \forall \theta \in H^{1/2}(\Gamma). \end{aligned}$$

Introducing the subspace Θ_h of $H^{1/2}(\Gamma)$ defined by

$$\Theta_h = \{\theta \in \mathcal{C}^0(\Gamma), \forall K_h^r \in \mathcal{T}_h^r, \theta|_{K_h^r} \in P_1(K_h^r)\}, \quad (3.28)$$

we can write for $\theta \in \Theta_h$,

$$\theta_h(x) = \sum_{i \in I_h^r} \theta_i \phi^i(x), \quad (3.29)$$

and for $\lambda_h \in M_h$, $\theta_h \in \Theta_h$,

$$\begin{aligned} c(\lambda_h, \theta_h) &= \sum_{i, i' \in I_h^r} \sum_{\substack{K_h^r \text{ s.t. } a_i, a_{i'} \\ \text{are nodes of } K_h^r}} (\lambda_i \cdot n_K) \theta_{i'} \\ &\quad \times \int_{K_h^r} \phi^i \phi^{i'} \, d\gamma. \end{aligned} \quad (3.30)$$

By using the same integration formula (3.21), we are led to the approximate bilinear form

$$c_h(\lambda_h, \theta_h) = \sum_{i \in I_h^r} \sum_{\substack{K_h^r \text{ s.t. } a_i \\ \text{is a node of } K_h^r}} (\lambda_i \cdot n_K) \theta_i \frac{|K_h^r|}{3}, \quad (3.31)$$

which can be rewritten, using the definition (3.27) for the node-normal,

$$c_h(\lambda_h, \theta_h) = \sum_{i \in I_h^r} (\lambda_i \cdot n_i) \theta_i \alpha_i. \quad (3.32)$$

Let us first introduce the subspace M_h^0 of M_h defined by

$$M_h^0 = \{\lambda_h \in M_h, c_h(\lambda_h, \theta_h) = 0, \forall \theta_h \in \Theta_h\}. \quad (3.33)$$

It is a simple matter to check that, thanks to (3.32), we have

$$M_h^0 = \{\lambda_h \in M_h, \lambda_i \cdot n_i = 0, \forall a_i \in \Gamma\}. \quad (3.34)$$

Let us now introduce the finite element subspace of Z_h ,

$$Z_h^0 = \{F_h \in Z_h, b_h(F_h, v_h) = 0, \forall v_h \in M_h^0\}, \quad (3.35)$$

which is not a subspace of Z_0 .

Again, it is a simple matter to check that, thanks to the expression (3.27), we have

$$Z_h^0 = \{F_h \in Z_h, F_i \times n_i = 0, \forall a_i \in \Gamma\}. \quad (3.36)$$

Hence, the elimination of the approximate Lagrange multipliers λ_h and θ_h in the formulation is obvious and leads us to find $(E_h(t), \phi_h(t)) \in Z_h^0 \times L_{2h}$, solution of the equations

$$\begin{aligned} & \int_{\Omega} \frac{\partial^2 E_h}{\partial t^2} \cdot F_h \, dx + c^2 \int_{\Omega} \nabla E_h : \nabla F_h \, dx \\ & + c^2 \sum_{x=1}^3 \int_{\Gamma} (\nabla E_{hx} \times n) \cdot (u_x \times F_h) \, dy \\ & + \int_{\Omega} \phi_{2h} \nabla \cdot F_h \, dx \\ & = \frac{c^2}{\varepsilon_0} \int_{\Omega} \rho_{2h} \nabla \cdot F_h \, dx \\ & - \frac{1}{\varepsilon_0} \int_{\Omega} \frac{\partial J_h}{\partial t} F_h \, dx, \quad \forall F_h \in Z_h^0, \end{aligned} \quad (3.37)$$

$$\begin{aligned} & \int_{\Omega} \nabla \cdot E_h \psi_{2h} \, dx \\ & = \frac{1}{\varepsilon_0} \int_{\Omega} \rho_{2h} \psi_{2h} \, dx, \quad \forall \psi_{2h} \in L_{2h}. \end{aligned} \quad (3.38)$$

Like in the formulation (3.8)–(3.9), we supplement these equations with the initial conditions (see (3.12) for the definition of Π_h),

$$E_h(0) = \Pi_h(E_0), \quad (3.39)$$

$$\frac{\partial E_h}{\partial t}(0) = \nabla \Pi_h(\varphi_0) + c^2 \nabla \times \Pi_h(B_0) - \frac{1}{\varepsilon_0} \Pi_h(J_0). \quad (3.40)$$

In Section 6, we shall see how we numerically take into account the condition $E_i \times n_i = 0, \forall a_i \in \Gamma$, by a projection algorithm in the spirit of [16].

4. THE CASE OF THE SILVER-MÜLLER BOUNDARY CONDITION

We suppose that a part Γ_1 of the boundary Γ of Ω behaves as a perfect conductor (i.e., $E \times n|_{\Gamma_1} = 0$). On the

other part, $\Gamma_2 = \Gamma \setminus \Gamma_1$, we have to model the electromagnetic interactions between the domain Ω and the exterior. We have chosen the following model: We locally approximate the boundary Γ_2 by its tangent plane, and we assume that

- Outgoing electromagnetic plane waves which propagate normally to the boundary Γ of the domain Ω can leave freely Ω , without being reflected at the boundary: They are absorbed at the boundary.

- Ingoing plane waves are allowed to enter normally the domain Ω and are imposed by either giving functions $e(x, t)$ or $b(x, t)$ according to:

$$(E - cB \times n) \times n = (e - cb \times n) \times n \quad \text{on } \Gamma_2 \text{ for the magnetic field,} \quad (4.1)$$

or

$$(cB + E \times n) \times n = (cb + e \times n) \times n \quad \text{on } \Gamma_2 \text{ for the electric field.} \quad (4.2)$$

These conditions are known as the Silver–Müller conditions [17]. These conditions are designed in the same spirit as the ones given in [8, pp. 370–371].

We now turn to the wave equation formulation of the initial problem, in order to see how the conditions (4.1), (4.2) can be introduced.

From (2.10), we obtain on Γ

$$\frac{\partial}{\partial t} (E \times n) - c^2 (\nabla \times B) \times n = -\frac{1}{\varepsilon_0} J \times n. \quad (4.3)$$

By differentiating (4.1) with respect to time, we obtain on Γ_2

$$\begin{aligned} & c \frac{\partial}{\partial t} ((B \times n) \times n) - c^2 (\nabla \times B) \times n \\ & = -\frac{1}{\varepsilon_0} J \times n - \frac{\partial}{\partial t} (e - cb \times n) \times n. \end{aligned} \quad (4.4)$$

Similarly for the electric field, from (2.11) and (4.2), we obtain

$$\begin{aligned} & \frac{\partial}{\partial t} ((E \times n) \times n) - c (\nabla \times E) \times n \\ & = \frac{\partial}{\partial t} (cb + e \times n) \times n \quad \text{on } \Gamma_2. \end{aligned} \quad (4.5)$$

Let us next deal with the variational formulation (2.40)–(2.43). By using the Green formulae (2.29) and

(2.30), together with the boundary condition (4.4), we obtain the additional integrals on Γ_2 ,

$$\begin{aligned} & c \int_{\Gamma_2} \left(\frac{\partial B}{\partial t} \times n \right) \cdot (C \times n) \, d\gamma \\ & - \int_{\Gamma_2} \left[\frac{\partial}{\partial t} (e - cb \times n) \times n \right] \cdot C \, d\gamma, \quad (4.6) \end{aligned}$$

so that (2.40) transforms into

$$\begin{aligned} & \int_{\Omega} \frac{\partial^2 B}{\partial t^2} \cdot C \, dx + c \int_{\Gamma_2} \left(\frac{\partial B}{\partial t} \times n \right) \cdot (C \times n) \, d\gamma \\ & + c^2 \int_{\Omega} \nabla B : \nabla C \, dx \\ & + c^2 \sum_{\alpha=1}^3 \int_{\Gamma} (\nabla B_{\alpha} \times n) \cdot (u_{\alpha} \times C) \, d\gamma \\ & + \int_{\Omega} P \nabla \cdot C \, dx \\ & = \frac{1}{\varepsilon_0} \int_{\Omega} (\nabla \times J) \cdot C \, dx + \frac{1}{\varepsilon_0} \int_{\Gamma} (J \times n) \cdot C \, d\gamma \\ & + \int_{\Gamma_2} \left[\frac{\partial}{\partial t} (e - cb \times n) \times n \right] \cdot C \, d\gamma, \quad \forall C \in Z. \quad (4.7) \end{aligned}$$

Concerning the variational formulation (2.44)–(2.47), we use similar arguments as above, so that (2.44) is transformed into

$$\begin{aligned} & \int_{\Omega} \frac{\partial^2 E}{\partial t^2} \cdot F \, dx + c \int_{\Gamma_2} \left(\frac{\partial E}{\partial t} \times n \right) \cdot (F \times n) \, d\gamma \\ & + c^2 \int_{\Omega} \nabla E : \nabla F \, dx \\ & + c^2 \sum_{\alpha=1}^3 \int_{\Gamma} (\nabla E_{\alpha} \times n) \cdot (u_{\alpha} \times F) \, d\gamma \\ & + \int_{\Omega} \phi \nabla \cdot F \, dx \\ & = \frac{c^2}{\varepsilon_0} \int_{\Omega} \rho \nabla \cdot F \, dx - \frac{1}{\varepsilon_0} \int_{\Omega} \frac{\partial J}{\partial t} \cdot F \, dx \\ & - c \int_{\Gamma_2} \left[\frac{\partial}{\partial t} (cb + e \times n) \times n \right] \cdot F \, d\gamma, \quad \forall F \in Z_0. \quad (4.8) \end{aligned}$$

Finally, it remains to deal with the finite element discretization of these variational formulations. The discrete formulation corresponding to the B field is directly obtained by adding an approximation of the integral term (4.6) to the formulation (3.8), which becomes

$$\begin{aligned} & \int_{\Omega} \frac{\partial^2 B_h}{\partial t^2} \cdot C_h \, dx + c \int_{\Gamma_2} \left(\frac{\partial B_h}{\partial t} \times n \right) \cdot (C_h \times n) \, d\gamma \\ & + c^2 \int_{\Omega} \nabla B_h : \nabla C_h \, dx \\ & + c^2 \sum_{\alpha=1}^3 \int_{\Gamma} (\nabla B_{h\alpha} \times n) \cdot (u_{\alpha} \times C_h) \, d\gamma \\ & + \int_{\Omega} P_{2h} \nabla \cdot C_h \, dx \\ & = \frac{1}{\varepsilon_0} \int_{\Omega} (\nabla \times J_h) \cdot C_h \, dx + \frac{1}{\varepsilon_0} \int_{\Gamma} (J_h \times n) \cdot C_h \, d\gamma \\ & + \int_{\Gamma_2} \left[\frac{\partial}{\partial t} (e_h - cb_h \times n) \times n \right] \cdot C_h \, d\gamma, \quad \forall C_h \in Z_h, \quad (4.9) \end{aligned}$$

where e_h and b_h are suitably defined approximations of e and b on Γ_2 .

The discretization of the formulation for the E field deserves special attention, particularly because of the boundary condition $E \times n|_{\Gamma_1} = 0$. As in the previous section, we introduce the normal n_i^1 , defined by (3.26) for each node a_i^1 of $\mathcal{T}_h^{\Gamma_1}$ ($\mathcal{T}_h^{\Gamma_1} = \mathcal{T}_h^{\Gamma} \cap \Gamma_1$). Observe that, even for the nodes $a_i^1 \in \Gamma_1 \cap \Gamma_2$, we define a normal n_i^1 , which only takes into account the faces of the tetrahedra which belong to Γ_1 . We also construct a normal n_i^2 of Γ_2 at each node a_i^2 of $\mathcal{T}_h^{\Gamma_2}$ ($\mathcal{T}_h^{\Gamma_2} = \mathcal{T}_h^{\Gamma} \cap \Gamma_2$), so that the nodes of $\Gamma_1 \cap \Gamma_2$ will be provided with two independent normals n_i^1 and n_i^2 (this choice is due to the fact that the physical boundary conditions associated to Γ_1 and Γ_2 are independent).

Let us now introduce the finite element subspace (without changing the notations)

$$Z_h^0 = \{F_h \in Z_h, F_i \times n_i^1 = 0, \forall a_i \in \mathcal{T}_h^{\Gamma_1}\}. \quad (4.10)$$

Hence we obtain the formulation for the E field by replacing (3.36) by (4.10) and the equation (3.37) by

$$\begin{aligned} & \int_{\Omega} \frac{\partial^2 E_h}{\partial t^2} \cdot F_h \, dx + c \int_{\Gamma_2} \left(\frac{\partial E_h}{\partial t} \times n \right) \cdot (F_h \times n) \, d\gamma \\ & + c^2 \int_{\Omega} \nabla E_h : \nabla F_h \, dx \\ & + c^2 \sum_{\alpha=1}^3 \int_{\Gamma} (\nabla E_{h\alpha} \times n) \cdot (u_{\alpha} \times F_h) \, d\gamma \\ & + \int_{\Omega} \phi_{2h} \nabla \cdot F_h \, dx \\ & = \frac{c^2}{\varepsilon_0} \int_{\Omega} \rho_{2h} \nabla \cdot F_h \, dx - \frac{1}{\varepsilon_0} \int_{\Omega} \frac{\partial J_h}{\partial t} \cdot F_h \, dx \\ & - \int_{\Gamma_2} \left[\frac{\partial}{\partial t} (cb_h + e_h \times n) \times n \right] \cdot F_h \, d\gamma, \quad \forall F_h \in Z_h^0. \quad (4.11) \end{aligned}$$

The above boundary conditions are first-order absorbing conditions. Following the ideas developed in [18, 19], we can improve our model by introducing higher order absorbing boundary conditions. This point will be addressed in a forthcoming paper.

5. THE QUADRATURE FORMULAE

In order to precisely specify the finite element approximation of the E and B fields formulations, we now have to evaluate the various integrals which are occurring in these formulations. We choose to perform an exact computation for almost all of them. However, it is convenient to use a quadrature formula to evaluate the ones which need to be inverted, namely the mass matrices, in order to lead to easier and cheaper computations, provided it does not deteriorate the accuracy of the method. First consider terms of the form (with the notations introduced in (3.3))

$$\int_{\Omega} F_h \cdot G_h \, dx = \sum_{\alpha=1}^3 \sum_{i,j \in I_h} \left(\int_{\Omega} \phi_{\alpha}^i \cdot \phi_{\alpha}^j \, dx \right) F_{\alpha}^i G_{\alpha}^j, \quad F_h, G_h \in Z_h,$$

which appear in (4.9) and also in (4.11). In order to use an explicit finite difference scheme in time (of leap-frog type) and to avoid solving a linear system of equations at each time-step, we need to diagonalize the mass matrix (for each component)

$$\left(\int_{\Omega} \phi^i \phi^j \, dx \right)_{i,j \in I_h}. \tag{5.1}$$

This is achieved by using the following quadrature formula on each tetrahedron K_h with vertices a_k , $1 \leq k \leq 4$:

$$\int_{K_h} f(x) \, dx \simeq \frac{|K_h|}{4} \sum_{k=1}^4 f(a_k). \tag{5.2}$$

This formula is exact if $f \in P_1(K_h)$.

Hence, by using the properties of the basis functions $\{\phi_{\alpha}^i\}_{i \in I_h}$ and formula (5.2), we approximate (5.1) by

$$\int_{\Omega} \phi^i \phi^j \, dx \simeq \sum_{K_h \in \text{supp}(\phi^i)} \frac{|K_h|}{4} \delta_{ij}, \tag{5.3}$$

where $\text{supp}(\phi^i)$ denotes the support of the function ϕ^i . Formula (5.3), indeed, leads to a diagonal mass matrix.

Next consider terms of the form

$$\begin{aligned} & \int_{\Gamma_2} (F_h \times n) \cdot (G_h \times n) \, d\gamma \\ &= \sum_{\alpha, \beta=1}^3 \sum_{i,j \in I_h^{\Gamma_2}} \left(\int_{\Gamma_2} (\phi_{\alpha}^i \times n) \cdot (\phi_{\beta}^j \times n) \, d\gamma \right) \\ & \quad \times F_{\alpha}^i G_{\beta}^j, \quad F_h, G_h \in Z_h, \end{aligned}$$

which can be found in (4.9) and also in (4.11). We have now to evaluate the boundary mass matrix

$$\left(\int_{\Gamma_2} (\phi_{\alpha}^i \times n) \cdot (\phi_{\beta}^j \times n) \, d\gamma \right)_{i,j \in I_h^{\Gamma_2}}^{\alpha, \beta \in \{1,2,3\}}. \tag{5.4}$$

An exact computation of (5.4) involves terms of the form

$$\int_{\Gamma_2} \phi^i \phi^j n^{\alpha} n^{\beta} \, d\gamma. \tag{5.5}$$

For the same reason as in (5.1), it is convenient, on each side of $K_h^{\Gamma_2} = (a_1^2, a_2^2, a_3^2)$ of $\mathcal{T}_h^{\Gamma_2}$, to use the quadrature formula

$$\int_{K_h^{\Gamma_2}} f(x) \, dx \simeq \frac{|K_h^{\Gamma_2}|}{3} \sum_{k=1}^3 f(a_k^2). \tag{5.6}$$

This formula is exact if $f \in P_1(K_h^{\Gamma_2})$. By using (5.6) on each $K_h^{\Gamma_2}$ in (5.5), we obtain

$$\begin{aligned} & \int_{\Gamma_2} \phi^i \phi^j n^{\alpha} n^{\beta} \, d\gamma \\ & \simeq \sum_{K_h^{\Gamma_2} \in \text{supp}(\phi^i)} n_{K_h^{\Gamma_2}}^{\alpha} n_{K_h^{\Gamma_2}}^{\beta} \frac{|K_h^{\Gamma_2}|}{3} \delta_{ij}, \end{aligned} \tag{5.7}$$

where n_K^{α} denotes the α th component of the constant outside unit normal of Γ_2 on $K_h^{\Gamma_2} \in \mathcal{T}_h^{\Gamma_2}$. Then following the idea introduced in Section 3, we define a normal n_i^2 at each node a_i^2 , $i \in I_h^{\Gamma_2}$ (see (3.26)), and we use the following approximation, which coincides with (5.7) if Γ_2 is a plane:

$$\begin{aligned} & \int_{\Gamma_2} \phi^i \phi^j n^{\alpha} n^{\beta} \, d\gamma \\ & \simeq \sum_{K_h^{\Gamma_2} \in \text{supp}(\phi^i)} \frac{|K_h^{\Gamma_2}|}{3} n_{i,\alpha}^2 n_{i,\beta}^2. \end{aligned} \tag{5.8}$$

By using this procedure, we obtain a boundary mass matrix on Γ_2 , which is block diagonal, each block being an easily invertible 3×3 matrix.

6. TIME MARCHING AND COMPUTATION OF THE LAGRANGE MULTIPLIERS

So far, we have only derived a semi-discrete in space approximation of the Maxwell system of equations. In order to obtain an effective method of solution, it remains to introduce a suitable time-stepping method: we have adopted a classical leap-frog scheme. For the sake of simplicity, we turn back to the formulation of Section 3, in which we have only considered perfectly conducting boundary conditions, namely $E \times n|_F = 0$.

Given a constant time step Δt , we set $t_n = n \Delta t$, $t_{n+1/2} = (n + \frac{1}{2}) \Delta t$. The electric field E^n is defined at time t_n while the magnetic field $B^{n+1/2}$ is evaluated at time $t_{n+1/2}$. We also denote by (\cdot, \cdot) the classical L^2 inner product, so that a fully discrete approximation of Maxwell's equation is defined as follows.

6.1. The B Field Formulation

Starting from (3.8), (3.9), for any integer $n \geq 1$, we look for $(B^{n+1/2}, P^{n+1/2}) \in Z_h \times L_{2h}$, solutions of the equations

$$\begin{aligned} (B^{n+1/2}, C_h) + \Delta t^2 (\nabla \cdot C_h, P^{n+1/2}) \\ = (G_B^n, C_h), \quad \forall C_h \in Z_h, \end{aligned} \quad (6.1)$$

$$(\nabla \cdot B^{n+1/2}, q_{2h}) = 0, \quad \forall q_{2h} \in L_{2h}, \quad (6.2)$$

where the right-hand side G_B^n contains all the other known terms coming from the data and the previous time steps. The initial conditions are also derived from a variational formulation. We set (see (3.11))

$$p_{2h}(0) = \Pi_h(p_0), \quad (6.3)$$

$$E_h(0) = \Pi_h(E_0). \quad (6.4)$$

We need to define $B^{1/2}$ and $B^{-1/2}$ from these data. We begin by writing a semi-discrete (in space) variational formulation of Eq. (2.11), and we look for $(B_h(t), p_{2h}(t)) \in Z_h \times L_{2h}$, solution of the equations,

$$\begin{aligned} \int_{\Omega} \frac{\partial B_h}{\partial t} \cdot C_h \, dx = - \int_{\Omega} p_{2h} \nabla \cdot C_h \, dx - \int_{\Omega} (\nabla \times E_h) \cdot C_h \, dx, \\ \forall C_h \in Z_h, \end{aligned} \quad (6.5)$$

$$\int_{\Omega} \nabla \cdot B_h q_{2h} \, dx = 0, \quad \forall q_{2h} \in L_{2h}. \quad (6.6)$$

We then take the time approximation

$$\begin{aligned} (B^{\pm 1/2}, C_h) \pm \frac{\Delta t}{2} (\nabla \cdot P^{\pm 1/2}) \\ = (G_B^0, C_h), \quad \forall C_h \in Z_h, \end{aligned} \quad (6.7)$$

$$(\nabla \cdot B^{\pm 1/2}, q_{2h}) = 0, \quad \forall q_{2h} \in L_{2h}, \quad (6.8)$$

where G_B^0 again contains terms coming from the data, as given by the right-hand side of (6.5). It remains now to invert the system of equations (6.7), (6.8) and (6.1), (6.2). This is achieved by the aid of an Uzawa algorithm [20].

6.2. The E Field Formulation

Starting from (3.37), (3.38), for any integer $n \geq 1$, we look for $(E^{n+1}, \phi^{n+1}) \in Z_h^0 \times L_{2h}$ solutions of

$$\begin{aligned} (E^{n+1}, F_h) + \Delta t^2 (\nabla \cdot F_h, \phi^{n+1}) \\ = (G_E^{n+1/2}, F_h), \quad \forall F_h \in Z_h^0, \end{aligned} \quad (6.9)$$

$$\begin{aligned} (\nabla \cdot E^{n+1}, \psi_{2h}) \\ = \frac{1}{\varepsilon_0} (\rho_{2h}, \psi_{2h}), \quad \forall \psi_{2h} \in L_{2h}. \end{aligned} \quad (6.10)$$

Here again, the right-hand side $G_E^{n+1/2}$ contains all the known terms at time $t_{n+1/2}$, from the data and the previous time steps. For the initial conditions, using similar arguments as above, we obtain E^1 by solving the following system:

$$\begin{aligned} (E^1, F_h) + \Delta t (\nabla \cdot F_h, \varphi_{2h}) \\ = (G_E^{1/2}, F_h), \quad \forall F_h \in Z_h^0, \end{aligned} \quad (6.11)$$

$$\begin{aligned} (\nabla \cdot E^1, \psi_{2h}) \\ = \frac{1}{\varepsilon_0} (\rho_{2h}^1, \psi_{2h}), \quad \forall \psi_{2h} \in L_{2h}. \end{aligned} \quad (6.12)$$

We numerically take into account the discrete boundary condition on E_h , $E_{hi} \times n_i|_F = 0$, by a projection algorithm. Namely we introduce the orthogonal projection Q from Z_h to Z_h^0 , defined for any $E_h \in Z_h$ by

$$QE_h \in Z_h^0, \quad (6.13)$$

$$(QE_h - E_h, F_h) = 0, \quad \forall F_h \in Z_h^0. \quad (6.14)$$

The projection Q does not affect the values of E_h at the interior nodes to Ω . For any node a_i on the boundary, it consists in an orthogonal projection of $E_h(a_i)$ onto the node-normal n_i . We then replace the problem (6.9), (6.10) (or (6.11), (6.12)) by the equivalent problem, which consists of finding $(E^{n+1}, \phi^{n+1}) \in Z_h \times L_{2h}$ solution of

$$\begin{aligned} (QE^{n+1}, QF_h) + \Delta t^2 (\nabla \cdot QF_h, \phi^{n+1}) \\ = (G_E^{n+1/2}, QF_h), \quad \forall F_h \in Z_h, \end{aligned} \quad (6.15)$$

$$\begin{aligned} (\nabla \cdot QE^{n+1}, \psi_{2h}) \\ = \frac{1}{\varepsilon_0} (\rho_{2h}, \psi_{2h}), \quad \forall \psi_{2h} \in L_{2h}. \end{aligned} \quad (6.16)$$

Since the matrix of the projector Q can be computed directly, the inversion of the system (6.15), (6.16) is easily achieved numerically by the aid of an Uzawa algorithm. We refer to [16] for more details.

Remark. When some part of the boundary is absorbing (i.e., $\Gamma_2 \neq \emptyset$) and intersects the perfectly conducting boundary (i.e., $\Gamma_1 \cap \Gamma_2 \neq \emptyset$), the determination of the projection Q requires some special care, but is easily found after some (tedious) elementary calculations.

7. NUMERICAL RESULTS

We now give two numerical examples as a first attempt to show the validity of the proposed method. A more complete study about the performance measurements for our Maxwell solver will be presented in a forthcoming paper.

As a first case, we study a cubic resonant cavity. At time $t=0$, we initialize the three components of E and B randomly in the domain, except at the boundary where we impose the conditions $E \times n = 0$ and $B \cdot n = 0$. Then the simulation is run during 8192 time steps with a Courant

number of approximately 0.5 (calculated on the finer mesh). A Fourier analysis is performed on the last 4096 time steps for different field components in several points of the cube. Figure 1 shows the spectrum obtained for E_x at the center of the cube. With the mesh we used (constituted by irregular tetrahedra), the fundamental mode is discretized with about 30 points per wavelength, whereas the last depicted mode is discretized with about six points per wavelength. As one can see there is a very good agreement between the theoretical 3D resonant mode frequencies of the cube (depicted with vertical arrows in Fig. 1) and the numerical values deduced from this spectrum.

As a second case, we study the propagation of the TEM mode in a coaxial cylindrical waveguide, which is of interest because an analytic expression of the solution is known. Moreover, this test is a validation of the complete formulation (4.9), (4.11), since it requires the different kinds of boundary conditions, especially the Silver-Müller conditions. At time $t=0$, we first initialize the electromagnetic fields $E(0)$ and $B(0)$ in the whole domain with a discretization of the exact solution (at the initial time). The coax (also discretized by irregular tetrahedra) is then illuminated by

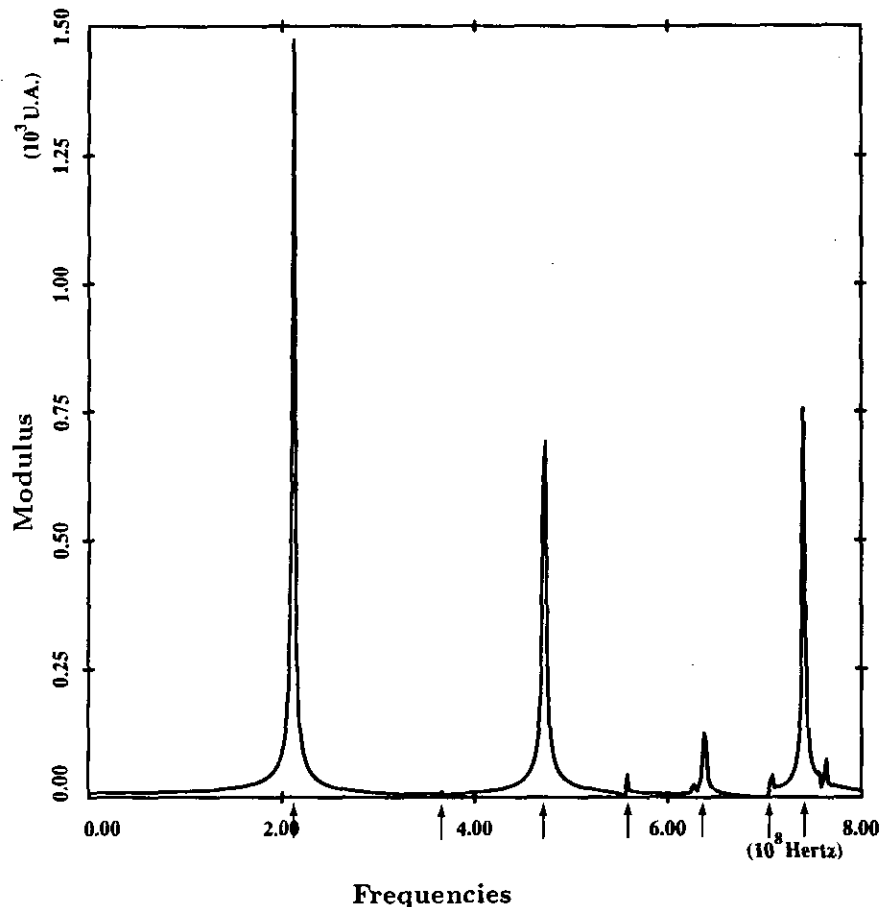


FIG. 1. E_x spectrum in a cubic resonant cavity.

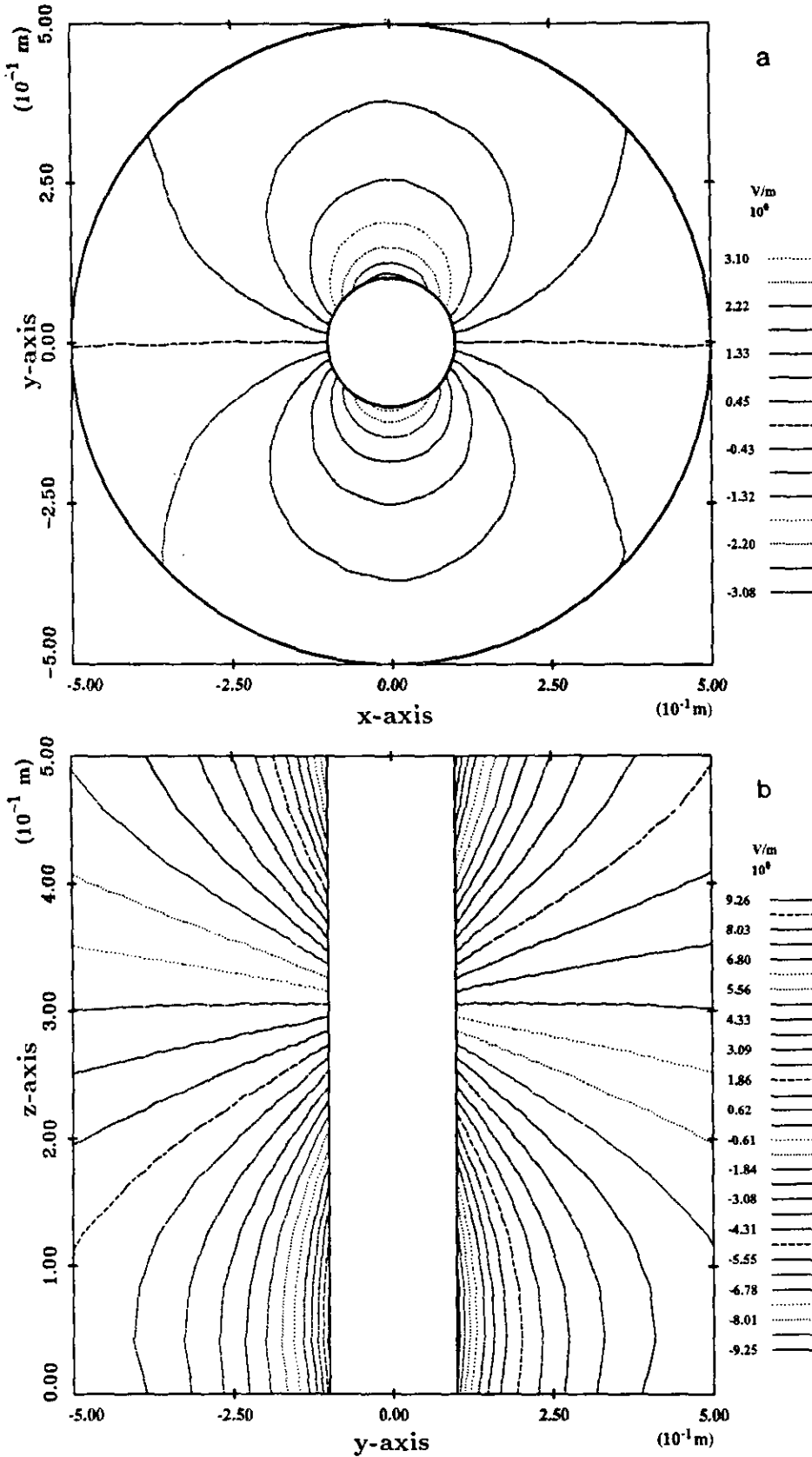


FIG. 2. Computed solution: (a) E_y in the (x, y) -plane, for $z = 0.25$; (b) E_y in the (y, z) -plane, for $x = 0$.

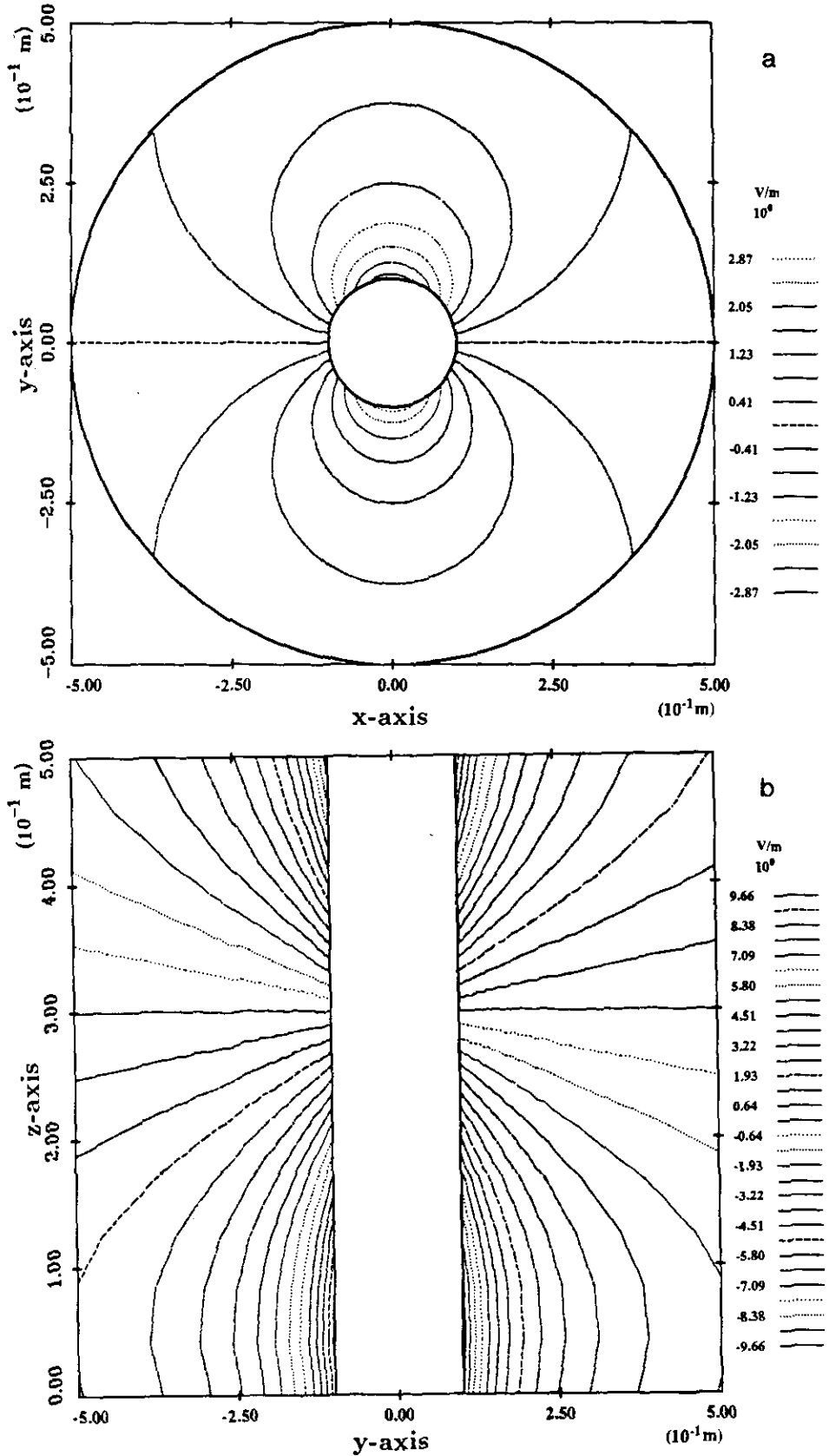


FIG. 3. Analytical solution: (a) E_y in the (x, y) -plane, for $z = 0.25$; (b) E_y in the (y, z) -plane, for $x = 0$.

ingoing plane waves which enter normally to the bottom, according to the relations (4.1) and (4.2). Figures 2a and b show respectively the transverse and longitudinal sections of E_z , obtained after 100 time steps of simulation, with a Courant number of approximately 0.3. The number of points per wavelength is of about 24 in the propagation direction. These figures have to be compared with the corresponding exact solutions, depicted in Figs. 3a and b. One can see that there is a good agreement between the analytic and computed solutions, even if the problem we deal with is stiff, the exact solutions varying as $1/r$ (r being the radius of the transverse section of the coax).

8. CONCLUSION

In this paper, we proposed a constrained formulation of 3D Maxwell's equations in terms of second-order wave equations. We then developed a numerical approximation for both the fields and the Lagrange multipliers, based on the modified Taylor–Hood finite element. Preliminary results on unstructured meshes have been presented in the cases of resonant cavities and coaxial TEM modes, showing the validity and the accuracy of the method. A more complete study on various examples for measuring precisely the performances of the method is actually in progress.

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