

The Origin of Spurious Solutions in Computational Electromagnetics

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It is commonly believed that the divergence equations in the Maxwell equations are “redundant” for transient and time-harmonic problems, therefore most of the numerical methods in computational electromagnetics solve only two first-order curl equations or the second-order curl–curl equations. This misconception is the true origin of spurious modes and inaccurate solutions in computational electromagnetics. By studying the div–curl system this paper clarifies that the first-order Maxwell equations are not “overdetermined,” and the divergence equations must always be included to maintain the ellipticity of the system in the space domain, to guarantee the uniqueness of the solution and the accuracy of the numerical methods, and to eliminate the infinitely degenerate eigenvalue. This paper shows that the common derivation and usage of the second-order curl–curl equations are incorrect and that the solution of Helmholtz equations needs the divergence condition to be enforced on an associated part of the boundary. The div–curl method and the least-squares method introduced in this paper provide rigorous derivation of the equivalent second-order Maxwell equations and their boundary conditions. The node-based least-squares finite element method (LSFEM) is recommended for solving the first-order full Maxwell equations directly. Examples of the numerical solutions by LSFEM are given to demonstrate that the LSFEM is free of spurious solutions. © 1996 Academic Press, Inc.

1. INTRODUCTION

The occurrence of spurious solutions in computational electromagnetics has been known for more than two decades, and elimination of such non-physical solutions is still a subject of great interest. The noted feature of these fictitious solutions has been their violating the divergence-free conditions in cases where the physical solution is completely solenoidal. It is commonly believed that the erroneous solutions are caused by numerical process; see, e.g., Jin [27, p. 164]. In our opinion, the trouble with spurious solutions in computational electromagnetics is deeply rooted in a misconception of the first-order Maxwell equations and in an incorrect derivation and use of the second-order curl–curl equations. We agree with Mur [43, 44] that spurious solutions can only be avoided by a correct formulation of the problem to be solved.

In terms of the type of differential equations to be solved, conventional numerical methods for general vector field

problems in computational electromagnetics may be classified mainly into four categories: (1) those based on the vector potentials; (2) those based on the first-order curl equations; (3) those based on the second-order curl–curl equations; (4) those based on the Helmholtz equations.

The potential approach is widely used in the computation of static fields and eddy currents. It also can be used for time-harmonic problems; see, e.g., Boyse *et al.* [4]. The potential approach does not give rise to spurious modes, since the divergence-free equations are automatically satisfied by introducing the vector potentials. It also makes material discontinuities easy to model. However, this approach involves difficulties related to the appropriate gauging method and the loss of accuracy and continuity (in homogeneous media) of the calculated field intensity from the potentials by the numerical differentiation.

The most widely used numerical method for the solution of time-dependent electromagnetic problems has been the finite-difference time-domain (FD-TD) scheme developed by Yee [70] and extensively utilized and refined by Taflov and Umashankar [62], Kunz and Luebbers [32], as well as others. In the Yee scheme, only two Maxwell curl equations are solved. Some other time-domain methods are also based on two Maxwell curl equations, such as the finite volume method developed by Shankar *et al.* [57], the finite difference and finite volume methods by Shang [58] and Shang and Gaitonde [59], and the finite element methods by Mei and his colleagues [5], Madsen and his colleagues [36, 33], Noack and Anderson [46], and Ambrosiano *et al.* [1].

In the original full Maxwell equations, when the constitutive relations are specified, for three-dimensional cases there are eight first-order equations but with only six unknown vector components, and for two-dimensional TE and TM cases, four equations with only three unknowns. That is, the number of equations is larger than the number of the unknown functions. It is also well known that by taking the divergence of the Faraday and Ampere laws one can see that these divergence-free conditions will be satisfied for all time if they are satisfied initially. For these two reasons, it is traditionally believed that the full first-

order Maxwell equations are “overdetermined” or “over-specified,” and the two divergence equations are thus regarded as “auxiliary” or “dependent” and are often neglected in numerical computation (see, e.g., Taflove and Umashankar [62, p. 38], Chew [9, p. 5], Kunz and Luebbers [32, p. 11], and Jin [27, p. 2]).

In the past, no one was even concerned about whether the divergence-free conditions were satisfied or not in these time-domain solutions, except Shang and Gaitonde [59] who seriously examined the value of divergence of the computed magnetic field. Recently, Wu and Jiang [69] gave some evidence that clearly shows the significant violation of the divergence-free condition near the boundary of scatterers in the solutions of the curl equations only. Morgan [42] also found that in some cases ignoring the divergence-free conditions leads to incorrect radar cross sections.

The first-order full Maxwell equations have a mathematical structure in which the fundamental ingredient is the div–curl system that looks “overdetermined.” A similar situation exists in fluid dynamics; see Jiang *et al.* [25]. By introducing a dummy variable (Chang and Gunzburger [8]), however, it can be shown that the div–curl system is not “overdetermined.” In this paper, we use this technique to study the full Maxwell equations and show that they are properly determined; that is, the two divergence equations should not be ignored regardless, either in the static or in the time-varying cases.

In electromagnetics, there are mainly two reasons why the second-order curl–curl equations are often employed. First, it is hard for conventional numerical methods to deal with the non-self-adjoint first-order derivatives. Second, in the curl–curl equations the electric field and the magnetic field are decoupled. There is a vast body of reports about spurious solutions associated with the numerical solution of the curl–curl equations in the context of the finite element method, (see, e.g., Cendes and Silvester [7], Bird [3], Ikeuchi *et al.* [20], Mabaya *et al.* [35], Davies *et al.* [12], Rahman and Davies [51, 52], Winkler and Davies [66], Webb [64], Welt and Webb [65], Koshiba *et al.* [29, 30], Ise *et al.* [19], Rahman *et al.* [53], and Schroeder and Wolff [55]). The majority of spurious solutions has been found in the eigenvalue analysis. A spurious mode does not correspond to the physical modes which the waveguide or resonator under consideration actually supports. The spurious mode problem is severe and often renders the numerical solution useless. The spurious solutions have been also revealed in boundary-value problems; see, e.g., Crowley *et al.* [11], Pinchuk *et al.* [49], Wong and Cendes [67, 68], and Paulsen and Lynch [48]. The phenomenon of spurious solutions for the curl–curl equations is not exclusive with the finite element method. This phenomenon has been also reported in the context of the finite difference method (see, e.g., Corr and Davies [10], Schweg and Bridges [56], and Su [60]), the boundary element method (see, e.g.,

Ganguly and Spielman [15] and Swaminathan *et al.* [61]), and the spectral method (see Farrar and Adams [13]). This fact itself undermines the common belief that the spurious solution is a result of the numerical process.

The popular engineering approach to removing spurious vector modes in the curl–curl equations is to modify the variational functional by penalizing the non-zero divergence. The key to success with this so-called penalty method, first used by Hara *et al.* [18] and Rahman and Davies [52], depends on the choice of the correct penalty factor—values too small or too large do not eliminate spurious solutions. Unfortunately, this is an ad hoc and problem-dependent treatment and there has been a lack of systematic study of the rationale for selecting this parameter for general problems.

Recently, the edge element method of Nedelec [45] (see, e.g., Jin [27] and the references therein) has been advocated, because it is believed to be a cure for many difficulties that are encountered when attempting to solve electromagnetic field problems by using conventional node-based finite elements. Apart from the fact that such an approach can only be used in the simple divergence-free case, edge elements violate the normal field continuity between adjacent elements in the homogeneous material domain; see Mur [44] for comments and an example. The accuracy of edge elements is lower than that of the nodal elements for the same number of unknowns, or the computational cost of edge elements is much higher than that of nodal elements for the same accuracy; see Mur [44] and Monk [41]. The edge element method also needs non-conventional meshing and postprocessing which are not normally available. Moreover, Ross *et al.* [54] reported that the edge element method broke down for large-scale computations due to the fact that edge elements cannot represent purely TE fields.

The curl–curl equations are derived from the first-order Maxwell curl equations by applying the curl operator. There is a very important issue: the curl–curl equations obtained by simple differentiation without additional equations and boundary conditions admit more solutions than do its progenitors. In order to derive an equivalent higher-order system from a system of vector partial differential equations, one should use the div–curl method that is based on the theorem: if a vector is divergence-free and curl-free in a domain, and its normal component or tangential components on the boundary are zero, then this vector is identically zero. In other words, the curl and the divergence operators must act together with appropriate boundary conditions to guarantee that there are no spurious solutions in the resulting higher-order equations. In this paper, this div–curl method originally developed by Jiang *et al.* [25] is employed to derive the second-order system of time-dependent Maxwell equations and their boundary conditions and to show that the divergence equa-

tions and additional boundary conditions must be supplemented to the curl–curl equations.

We remark that in the past only Assous *et al.* [2] completely realized the importance of the divergence equations in the time-domain Maxwell equations and correctly worked with second-order wave equations. For a special case, they supplemented two divergence equations and an additional boundary condition to the curl–curl equations. They introduced the Lagrange multipliers (which are identically equal to our dummy variables introduced for other reasons; see Sections 2.2 and 3.2) associated to the divergence constraints and reformulated the full Maxwell equations as a constrained variational problem. Then they used the well-developed mixed Galerkin finite element method in fluid mechanics to solve the problem. The importance of their work is obvious: it was the first mathematically rigorous approach to deal with the time-domain Maxwell equations.

It is well known that the solution of the Helmholtz equations with proper boundary conditions is free of spurious modes; see Mayergoyz and D’Angelo [37]. The key issue in the Helmholtz method is how to specify proper boundary conditions. In this paper, we use the div–curl method and the least-squares method to derive the Helmholtz equations and their boundary conditions and to show that the divergence equations need to be enforced only on the corresponding part of boundary and they will be implicitly satisfied in the domain. We also give a Galerkin variational formulation which corresponds to the Helmholtz equations. This theoretically justifies that the penalty parameter s in the penalty method should be equal to one.

This paper emphasizes that in any case the divergence equations must be included explicitly or implicitly as a part of the formulation for electromagnetic problems. However, it is not so easy to combine the divergence equations in conventional methods. In the method proposed by Assous *et al.* [2], inconvenient non-equal order elements must be employed. Attempts to satisfy the divergence-free equations by using edge elements merely complicates the situation by introducing the need to impose an additional condition of normal field continuity.

This paper shows that the satisfaction of the divergence equations and the elimination of spurious solutions can be achieved easily by the application of the node-based least-squares finite element method (LSFEM). We believe that the LSFEM is the best choice among the available methods for numerical solution of many problems in electromagnetics, since it is simple, universal, robust, efficient, and often optimal. The LSFEM is based on the minimization of the residuals in first-order partial differential equations. The LSFEM has been successfully applied to various fluid dynamics problems (see, e.g., Jiang *et al.* [22, 24], Tang and Tsang [63], and Lefebvre *et al.* [34]). The LSFEM is naturally suitable for the first-order full Maxwell equations.

The results of LSFEM for time-domain scattering wave problems can be found in Wu and Jiang [69]. The div–curl theory and the corresponding least-squares method discussed in this paper can be employed to directly solve static electric or magnetic fields without introducing the potentials and gauging. In the last section of this paper we briefly discuss the general formulation of the LSFEM and apply it to time-harmonic problems. Numerical examples are given to demonstrate that the LSFEM is free of spurious solutions.

2. THE DIV–CURL SYSTEM

In this section we study the div–curl system. We shall show that the three dimensional div–curl system is not “overdetermined.” We shall introduce the div–curl method to derive a second-order system equivalent to the div–curl system. We shall show why the least-squares method is the best method for the solution of the div–curl system. The technique and the procedure developed here will be applied to dealing with the Maxwell equations. Since the static Maxwell equations are typical div–curl systems, the least-squares method introduced in this section can be applied to the direct solution of static electric or magnetic fields.

2.1. Basic Theorems

Let $\Omega \subset \mathbb{R}^3$ be a bounded, simply connected, convex, and open domain with a piecewise smooth boundary $\Gamma = \Gamma_1 \cup \Gamma_2$. Either Γ_1 or Γ_2 , not both, may be empty. Also Γ_1 and Γ_2 must have at least one common point. Let $\mathbf{x} = (x, y, z)$ be a point in Ω , let \mathbf{n} be a unit outward normal vector. Let (\cdot, \cdot) and $\langle \cdot, \cdot \rangle$ denote the inner products defined in the domain and on the boundary, respectively. Throughout the paper C denotes a positive constant dependent on Ω with possibly different values in each appearance.

The following theorems are essential in this paper.

THEOREM 1. *If $\mathbf{u} \in H^1(\Omega)^3$ and $\mathbf{n} \times \mathbf{u} = \mathbf{0}$ on $\Gamma_2 \neq \emptyset$, then $\mathbf{n} \cdot \nabla \times \mathbf{u} = 0$ on Γ_2 .*

The proof of Theorem 1 is straightforward by using the Stokes theorem; see Pironneau [50, p. 53] or Jiang *et al.* [25].

THEOREM 2 (Friedrichs’ div–curl inequality). *Every function \mathbf{u} of $H^1(\Omega)^3$ with $\mathbf{n} \cdot \mathbf{u} = 0$ on Γ_1 and $\mathbf{n} \times \mathbf{u} = \mathbf{0}$ on Γ_2 satisfies*

$$\|\mathbf{u}\|_1^2 \leq C(\|\nabla \cdot \mathbf{u}\|_0^2 + \|\nabla \times \mathbf{u}\|_0^2), \quad (2.1)$$

where the constant $C > 0$ depends only on Ω .

For the proof we refer to Girault and Raviart [16], Krizek and Neittaanmäki [31] and Jiang *et al.* [25]. This theorem implies that the div–curl norm appearing in the right-hand side of (2.1) is equivalent to the H^1 norm. This theorem plays a key role in the analysis of the least-squares method. From Theorem 2, we can immediately obtain the following theorem which is the basis of the div–curl method for deriving higher-order vector equations:

THEOREM 3 (The div–curl theorem). *If $\mathbf{u} \in H^1(\Omega)^3$ satisfies*

$$\begin{aligned}\nabla \cdot \mathbf{u} &= 0 & \text{in } \Omega, \\ \nabla \times \mathbf{u} &= \mathbf{0} & \text{in } \Omega, \\ \mathbf{n} \cdot \mathbf{u} &= 0 & \text{on } \Gamma_1, \\ \mathbf{n} \times \mathbf{u} &= \mathbf{0} & \text{on } \Gamma_2,\end{aligned}$$

then

$$\mathbf{u} \equiv \mathbf{0} \quad \text{in } \Omega.$$

THEOREM 4 (The gradient theorem). *If $g \in H^1(\Omega)$ satisfies*

$$\begin{aligned}\nabla g &= \mathbf{0} & \text{in } \Omega, \\ g &= 0 & \text{on } \Gamma_1 \neq \emptyset \text{ (or on } \Gamma_2 \neq \emptyset),\end{aligned}$$

then

$$g \equiv 0 \quad \text{in } \Omega.$$

The validation of Theorem 4 is obvious. In fact, $g = 0$ needs to be specified only at any point in the domain or on the boundary. This theorem will be used to derive the higher-order equations which are equivalent to a scalar equation.

2.2. The Div–Curl System

Let us consider the following three-dimensional div–curl system:

$$\nabla \times \mathbf{u} = \boldsymbol{\omega} \quad \text{in } \Omega, \quad (2.2a)$$

$$\nabla \cdot \mathbf{u} = \rho \quad \text{in } \Omega, \quad (2.2b)$$

$$\mathbf{n} \cdot \mathbf{u} = 0 \quad \text{on } \Gamma_1, \quad (2.2c)$$

$$\mathbf{n} \times \mathbf{u} = \mathbf{0} \quad \text{on } \Gamma_2, \quad (2.2d)$$

where the given vector function $\boldsymbol{\omega} \in L_2(\Omega)^3$ must satisfy the following compatibility conditions:

$$\nabla \cdot \boldsymbol{\omega} = 0 \quad \text{in } \Omega, \quad (2.3a)$$

$$\mathbf{n} \cdot \boldsymbol{\omega} = 0 \quad \text{on } \Gamma_2, \quad (2.3b)$$

$$\int_{\Gamma} \mathbf{n} \cdot \boldsymbol{\omega} \, ds = 0. \quad (2.3c)$$

If Γ_2 is empty, then the given scalar function $\rho \in L_2(\Omega)$ must satisfy the compatibility condition:

$$\int_{\Omega} \rho \, d\Omega = 0. \quad (2.3d)$$

At first glance, system (2.2) seems “overdetermined” or “overspecified,” since there are four equations and three unknowns. For this reason, indeed, solving (2.2) is not trivial by conventional finite difference or finite element methods. However, after careful investigation we shall find that system (2.2) is properly determined and elliptic.

By introducing a dummy variable ϑ , system (2.2) can be written as

$$\nabla \vartheta + \nabla \times \mathbf{u} = \boldsymbol{\omega} \quad \text{in } \Omega, \quad (2.4a)$$

$$\nabla \cdot \mathbf{u} = \rho \quad \text{in } \Omega, \quad (2.4b)$$

$$\mathbf{n} \cdot \mathbf{u} = 0 \quad \text{on } \Gamma_1, \quad (2.4c)$$

$$\vartheta = 0 \quad \text{on } \Gamma_1, \quad (2.4d)$$

$$\mathbf{n} \times \mathbf{u} = \mathbf{0} \quad \text{on } \Gamma_2. \quad (2.4e)$$

Notice that we impose $\vartheta = 0$ on Γ_1 , and we do not specify any boundary condition for the dummy variable ϑ on Γ_2 .

By virtue of Theorem 3, Eq. (2.4a) is equivalent to the following equations and boundary conditions:

$$\nabla \times (\nabla \vartheta + \nabla \times \mathbf{u} - \boldsymbol{\omega}) = \mathbf{0} \quad \text{in } \Omega, \quad (2.5a)$$

$$\nabla \cdot (\nabla \vartheta + \nabla \times \mathbf{u} - \boldsymbol{\omega}) = 0 \quad \text{in } \Omega, \quad (2.5b)$$

$$\mathbf{n} \times (\nabla \vartheta + \nabla \times \mathbf{u} - \boldsymbol{\omega}) = \mathbf{0} \quad \text{on } \Gamma_1, \quad (2.5c)$$

$$\mathbf{n} \cdot (\nabla \vartheta + \nabla \times \mathbf{u} - \boldsymbol{\omega}) = 0 \quad \text{on } \Gamma_2. \quad (2.5d)$$

Taking into account the compatibility conditions (2.3a) and (2.3b), the boundary condition (2.4e), and Theorem 1, Eqs. (2.5b), (2.4d), and (2.5d) lead to

$$\Delta \vartheta = 0 \quad \text{in } \Omega, \quad (2.6a)$$

$$\vartheta = 0 \quad \text{on } \Gamma_1, \quad (2.6b)$$

$$\frac{\partial \vartheta}{\partial n} = 0 \quad \text{on } \Gamma_2. \quad (2.6c)$$

From (2.6) we know that $\vartheta \equiv 0$ in Ω . That is, the introduction of ϑ into (2.2) does not change anything, and thus system (2.4) with four equations and four unknowns is indeed equivalent to system (2.2).

Now let us classify system (2.4). In Cartesian coordinates the equations in system (2.4) are given as

$$\begin{aligned}
\frac{\partial \vartheta}{\partial x} + \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} &= \omega_x, \\
\frac{\partial \vartheta}{\partial y} + \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} &= \omega_y, \\
\frac{\partial \vartheta}{\partial z} + \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} &= \omega_z, \\
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} &= \rho.
\end{aligned} \tag{2.7}$$

We may write system (2.7) in the standard matrix form,

$$\mathbf{A}_1 \frac{\partial \bar{\mathbf{u}}}{\partial x} + \mathbf{A}_2 \frac{\partial \bar{\mathbf{u}}}{\partial y} + \mathbf{A}_3 \frac{\partial \bar{\mathbf{u}}}{\partial z} + \mathbf{A}_0 \bar{\mathbf{u}} = \mathbf{f}, \tag{2.8}$$

in which

$$\begin{aligned}
\mathbf{A}_1 &= \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, & \mathbf{A}_2 &= \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \\
\mathbf{A}_3 &= \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, & \mathbf{A}_0 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \\
\mathbf{f} &= \begin{pmatrix} \omega_x \\ \omega_y \\ \omega_z \\ \rho \end{pmatrix}, & \bar{\mathbf{u}} &= \begin{pmatrix} u \\ v \\ w \\ \vartheta \end{pmatrix}.
\end{aligned}$$

The characteristic polynomial associated with system (2.7) is

$$\begin{aligned}
\det(\mathbf{A}_1 \xi + \mathbf{A}_2 \eta + \mathbf{A}_3 \zeta) &= \det \begin{pmatrix} 0 & -\zeta & \eta & \xi \\ \zeta & 0 & -\xi & \eta \\ -\eta & \xi & 0 & \zeta \\ \xi & \eta & \zeta & 0 \end{pmatrix} \\
&= (\xi^2 + \eta^2 + \zeta^2)^2 \neq 0
\end{aligned}$$

for all nonzero real triplets (ξ, η, ζ) , system (2.4) is thus elliptic and properly determined.

The first-order elliptic system (2.4) has four equations and four unknowns, so two boundary conditions on each boundary are needed to make system (2.4) well-posed. Here $\vartheta = 0$ and $\mathbf{n} \cdot \mathbf{u} = 0$ serve as two boundary conditions on Γ_1 , while $\mathbf{n} \times \mathbf{u} = \mathbf{0}$ implies that two tangential components of \mathbf{u} are zero on Γ_2 .

Since system (2.2) is equivalent to system (2.4), and System (2.4) is elliptic and properly determined, so is system (2.2).

Remark. In fact, the compatibility conditions (2.3a), (2.3b) can be obtained by applying the div-curl method to Eq. (2.2a).

2.3. The Div-Curl Method

Let us derive a higher-order system which is equivalent to the div-curl system (2.2). By virtue of Theorem 3, system (2.2) is equivalent to the following system:

$$\nabla \times (\nabla \times \mathbf{u} - \boldsymbol{\omega}) = \mathbf{0} \quad \text{in } \Omega, \tag{2.9a}$$

$$\nabla \cdot (\nabla \times \mathbf{u} - \boldsymbol{\omega}) = 0 \quad \text{in } \Omega, \tag{2.9b}$$

$$\mathbf{n} \times (\nabla \times \mathbf{u} - \boldsymbol{\omega}) = \mathbf{0} \quad \text{on } \Gamma_1, \tag{2.9c}$$

$$\mathbf{n} \cdot (\nabla \times \mathbf{u} - \boldsymbol{\omega}) = 0 \quad \text{on } \Gamma_2, \tag{2.9d}$$

$$\nabla \cdot \mathbf{u} = \rho \quad \text{in } \Omega, \tag{2.9e}$$

$$\mathbf{n} \cdot \mathbf{u} = 0 \quad \text{on } \Gamma_1, \tag{2.9f}$$

$$\mathbf{n} \times \mathbf{u} = \mathbf{0} \quad \text{on } \Gamma_2. \tag{2.9g}$$

(2.9b) and (2.9d) are satisfied due to the compatibility conditions (2.3a), (2.3b), the boundary condition (2.9g) and Theorem 1. Therefore, system (2.9) can be simplified as

$$\nabla \times (\nabla \times \mathbf{u}) = \nabla \times \boldsymbol{\omega} \quad \text{in } \Omega, \tag{2.10a}$$

$$\nabla \cdot \mathbf{u} = \rho \quad \text{in } \Omega, \tag{2.10b}$$

$$\mathbf{n} \cdot \mathbf{u} = 0 \quad \text{on } \Gamma_1, \tag{2.10c}$$

$$\mathbf{n} \times (\nabla \times \mathbf{u}) = \mathbf{n} \times \boldsymbol{\omega} \quad \text{on } \Gamma_1, \tag{2.10d}$$

$$\mathbf{n} \times \mathbf{u} = \mathbf{0} \quad \text{on } \Gamma_2. \tag{2.10e}$$

Now at least one thing is made clear by the div-curl method. That is, the curl-curl equation (2.10a) cannot stand alone; it must go with the divergence equation (2.10b) and the additional Neumann boundary condition (2.10d).

System (2.10) can be further simplified. By virtue of Theorem 4, Eq. (2.10b) is equivalent to the following system of equations and boundary condition (assuming that $\Gamma_2 \neq \emptyset$):

$$\nabla(\nabla \cdot \mathbf{u} - \rho) = \mathbf{0} \quad \text{in } \Omega, \tag{2.11a}$$

$$\nabla \cdot \mathbf{u} = \rho \quad \text{on } \Gamma_2. \quad (2.11b)$$

Taking into account (2.11) and the vector identity,

$$\nabla \times \nabla \times \mathbf{u} = \nabla(\nabla \cdot \mathbf{u}) - \Delta \mathbf{u}, \quad (2.12)$$

system (2.10) can be reduced as

$$\Delta \mathbf{u} = -\nabla \times \boldsymbol{\omega} + \nabla \rho \quad \text{in } \Omega, \quad (2.13a)$$

$$\nabla(\nabla \cdot \mathbf{u} - \rho) = \mathbf{0} \quad \text{in } \Omega, \quad (2.13b)$$

$$\mathbf{n} \cdot \mathbf{u} = 0 \quad \text{on } \Gamma_1, \quad (2.13c)$$

$$\mathbf{n} \times (\nabla \times \mathbf{u}) = \mathbf{n} \times \boldsymbol{\omega} \quad \text{on } \Gamma_1, \quad (2.13d)$$

$$\mathbf{n} \times \mathbf{u} = \mathbf{0} \quad \text{on } \Gamma_2, \quad (2.13e)$$

$$\nabla \cdot \mathbf{u} = \rho \quad \text{on } \Gamma_2. \quad (2.13f)$$

The solution of the derived second-order system (2.10) or (2.13) is completely identical to the solution of the original div–curl system (2.2), therefore no spurious solution will be produced by the system (2.10) or (2.13). Moreover, the divergence equation (2.13b) in system (2.13) can be deleted. That is, the divergence equation is implicitly satisfied by Eq. (2.13a) and boundary conditions (2.13c)–(2.13f). The rigorous proof of this statement will be given by using the least-squares method in the next section. Here we give a simple explanation adopted from Mayergoyz and D’Angelo [37]. Let us consider a slightly different problem:

$$\Delta \mathbf{u} = -\nabla \times \boldsymbol{\omega} + \nabla \rho \quad \text{in } \Omega, \quad (2.14a)$$

$$\mathbf{n} \cdot \mathbf{u} = 0 \quad \text{on } \Gamma_1, \quad (2.14b)$$

$$\mathbf{n} \times (\nabla \times \mathbf{u}) = \mathbf{n} \times \boldsymbol{\omega} \quad \text{on } \Gamma_1, \quad (2.14c)$$

$$\mathbf{n} \times \mathbf{u} = \mathbf{0} \quad \text{on } \Gamma_2, \quad (2.14d)$$

$$\nabla \cdot \mathbf{u} - \rho = 0 \quad \text{on } \Gamma. \quad (2.14e)$$

That is, we let the divergence equation be satisfied on the whole boundary. Although this condition needs to be specified only on Γ_2 , it is not wrong for it to be enforced on Γ . By taking the divergence of (2.14a) we obtain a Poisson equation of $\phi = \nabla \cdot \mathbf{u} - \rho$:

$$\Delta \phi = 0 \quad \text{in } \Omega. \quad (2.15)$$

Since $\phi = 0$ on the whole boundary, ϕ must be equal to zero in the whole domain, i.e., the divergence equation is implicitly satisfied in the system (2.14).

2.4. The Least-Squares Method

Let us introduce a more powerful and systematic method, the least-squares method, to solve system (2.2)

and to derive a higher-order system without spurious solutions. We construct the following quadratic functional:

$$I: \mathcal{H} \rightarrow \mathbb{R},$$

$$I(\mathbf{u}) = \|\nabla \times \mathbf{u} - \boldsymbol{\omega}\|_0^2 + \|\nabla \cdot \mathbf{u} - \rho\|_0^2,$$

where $\mathcal{H} = \{\mathbf{u} \in H^1(\Omega)^3 \mid \mathbf{n} \cdot \mathbf{u} = 0 \text{ on } \Gamma_1, \mathbf{n} \times \mathbf{u} = 0 \text{ on } \Gamma_2\}$. We note that the introduction of a dummy variable ϑ in Section 2.2 is only for the verification of the determination, and it is not required in the least-squares functional I . Taking the variation of I with respect to \mathbf{u} , and letting $\delta \mathbf{u} = \mathbf{v}$ and $\delta I = 0$, we obtain a least-squares variational formulation of the following type: find $\mathbf{u} \in \mathcal{H}$ such that

$$B(\mathbf{u}, \mathbf{v}) = L(\mathbf{v}) \quad \forall \mathbf{v} \in \mathcal{H}, \quad (2.16)$$

where $B(\cdot, \cdot)$ is a bilinear form of the type

$$B(\mathbf{u}, \mathbf{v}) = (\nabla \times \mathbf{u}, \nabla \times \mathbf{v}) + (\nabla \cdot \mathbf{u}, \nabla \cdot \mathbf{v})$$

and $L(\cdot)$ is a linear form of the type

$$L(\mathbf{v}) = (\boldsymbol{\omega}, \nabla \times \mathbf{v}) + (\rho, \nabla \cdot \mathbf{v}).$$

Obviously the bilinear form $B(\mathbf{u}, \mathbf{v})$ is symmetric and continuous. The coerciveness of $B(\mathbf{u}, \mathbf{v})$ is due to Theorem 2. Therefore, we immediately have

$$\frac{1}{C} \|\mathbf{u}\|_1^2 \leq B(\mathbf{u}, \mathbf{u}) = L(\mathbf{u}) \leq \|\mathbf{u}\|_1 (\|\boldsymbol{\omega}\|_0 + \|\rho\|_0).$$

By virtue of the Lax–Milgram theorem, (see, e.g., Oden and Reddy [47] or Johnson [28]), in fact, we have proved the following theorem.

THEOREM 5. *The solution of (2.16) uniquely exists and satisfies*

$$\|\mathbf{u}\|_1 \leq C(\|\boldsymbol{\omega}\|_0 + \|\rho\|_0). \quad (2.17)$$

The following theorem about the error estimate is also a direct consequence of the above results.

THEOREM 6. *The LSFEM based on (2.16) has an optimal rate of convergence and an optimal satisfaction of the divergence condition:*

$$\|\mathbf{u} - \mathbf{u}_h\|_0 \leq Ch^{k+1} \|\mathbf{u}\|_{k+1}, \quad (2.18a)$$

$$\|\nabla \cdot (\mathbf{u}_h - \rho)\|_0 \leq Ch^k \|\mathbf{u}\|_{k+1}, \quad (2.18b)$$

where \mathbf{u}_h is the finite element solution and k is the order of complete polynomials used in the finite element interpolation.

The error estimate (2.18a) is not totally new. The early results were obtained by Fix and Rose [14] for the case $\Gamma_2 = 0$ and by Krizek and Neittaanmäki [31] for the case $\Gamma_1 = 0$. The two-dimensional numerical results and a preliminary analysis can also be found in Jiang and Chai [21] and Carey and Jiang [6].

The advantages of the LSFEM over the potential method for solving the div–curl system is obvious: the trouble of selecting a proper gauging method is avoided; the electric or magnetic fields are obtained directly without numerical differentiation and thus have a higher accuracy; and the electric or magnetic fields are continuous across the element boundaries.

In order to further understand the least-squares method, we derive the Euler–Lagrange equations associated with the least-squares variational formulation (2.16) which can be rewritten as: find $\mathbf{u} \in \mathcal{H}$ such that

$$(\nabla \times \mathbf{u} - \boldsymbol{\omega}, \nabla \times \mathbf{v}) + (\nabla \cdot \mathbf{u} - \rho, \nabla \cdot \mathbf{v}) = 0 \quad \forall \mathbf{v} \in \mathcal{H}. \quad (2.19)$$

Suppose that \mathbf{u} , $\boldsymbol{\omega}$, and ρ are sufficiently smooth. By using Green’s formulae, Eq. (2.19) can be written as

$$\begin{aligned} & (\nabla \times (\nabla \times \mathbf{u} - \boldsymbol{\omega}), \mathbf{v}) + \langle (\nabla \times \mathbf{u} - \boldsymbol{\omega}), \mathbf{n} \times \mathbf{v} \rangle_{\Gamma} \\ & + (-\nabla(\nabla \cdot \mathbf{u} - \rho), \mathbf{v}) \\ & + \langle (\nabla \cdot \mathbf{u} - \rho), \mathbf{n} \cdot \mathbf{v} \rangle_{\Gamma} = 0 \quad \forall \mathbf{v} \in \mathcal{H}. \end{aligned} \quad (2.20)$$

Taking into account (2.12) and that \mathbf{v} satisfies $\mathbf{n} \cdot \mathbf{v} = 0$ on Γ_1 and $\mathbf{n} \times \mathbf{v} = \mathbf{0}$ on Γ_2 , from (2.20) we obtain

$$\begin{aligned} & (-\Delta \mathbf{u} - \nabla \times \boldsymbol{\omega} + \nabla \rho, \mathbf{v}) - \langle \mathbf{n} \times (\nabla \times \mathbf{u} - \boldsymbol{\omega}), \mathbf{v} \rangle_{\Gamma_1} \\ & + \langle (\nabla \cdot \mathbf{u} - \rho), \mathbf{n} \cdot \mathbf{v} \rangle_{\Gamma_2} = 0 \end{aligned} \quad (2.21)$$

for all admissible $\mathbf{v} \in \mathcal{H}$, hence we have the Euler–Lagrange equation and boundary conditions:

$$\Delta \mathbf{u} = -\nabla \times \boldsymbol{\omega} + \nabla \rho \quad \text{in } \Omega, \quad (2.22a)$$

$$\mathbf{n} \cdot \mathbf{u} = 0 \quad \text{on } \Gamma_1, \quad (2.22b)$$

$$\mathbf{n} \times (\nabla \times \mathbf{u}) = \mathbf{n} \times \boldsymbol{\omega} \quad \text{on } \Gamma_1, \quad (2.22c)$$

$$\mathbf{n} \times \mathbf{u} = \mathbf{0} \quad \text{on } \Gamma_2, \quad (2.22d)$$

$$\nabla \cdot \mathbf{u} = \rho \quad \text{on } \Gamma_2. \quad (2.22e)$$

We note that in system (2.22) the divergence equation does not appear in the domain. In fact, we have rigorously proved that under additional boundary conditions (2.22c) and (2.22e) the solution of the Helmholtz-type system (2.22a) automatically satisfies the divergence equation. We also remark that if Γ_2 is empty, the divergence equation does not even appear on the boundary. The attraction of using the higher-order system (2.22) now becomes apparent: one

avoids dealing with the divergence condition (2.2b) which is implicitly satisfied; instead, one deals with three Poisson equations that everyone would rather solve. However, we should mention that if one chooses the finite difference method to solve (2.22a), the additional natural boundary conditions (2.22c), (2.22e) must be supplemented.

Now it is clear that the following four formulations are equivalent to each other: (1) the first-order div–curl system (2.2); (2) the least-squares variational formulation (2.16); (3) the Helmholtz-type system (2.22); and (4) the Galerkin formulation (2.21). It turns out that the least-squares method (2.16) for the div–curl equations (2.2) corresponds to using the Galerkin method (2.21) to solve system (2.22) which consists of three independent second-order Poisson equations (2.22a) and three coupled boundary conditions on each boundary, where the original first-order equations (2.22c) and (2.22e) serve as the natural boundary conditions and (2.22b) and (2.22d) serve as the essential boundary conditions.

Obviously, the least-squares problem is formally equivalent to a higher-order problem with additional natural boundary conditions provided by the original first-order differential equations. The least-squares method (2.16) is the simplest approach among these equivalent methods, because it does not need any additional boundary conditions. The trial function \mathbf{u} and the test function \mathbf{v} need to satisfy only the original essential boundary conditions. This is one of the reasons why we strongly recommend the least-squares method.

Now we have shown that the three-dimensional div–curl system can have three equivalent differential forms: (1) the first-order system (2.2); (2) the curl–curl equation (2.10a) which must be accompanied by the divergence equation (2.10b) and the additional Neumann boundary condition (2.10d); (3) three uncoupled Poisson equations (2.22a) with additional Neumann boundary conditions (2.22c) and (2.22e) provided by the original first-order system.

In the following sections, we will show that the Maxwell equations have similar equivalent forms.

3. THE FIRST-ORDER MAXWELL EQUATIONS

In this section we shall show that the first-order full Maxwell equations are not “overdetermined,” and the divergence equations are not “redundant” and thus should not be ignored.

3.1. The Basic Equations

For general time-varying fields, the original first-order full Maxwell equations can be written as

$$\begin{aligned} \nabla \times \mathbf{E} + \frac{\partial(\boldsymbol{\mu}\mathbf{H})}{\partial t} = -\mathbf{K}^{imp} \quad \text{in } \Omega, \\ \text{(Faraday's law)} \end{aligned} \quad (3.1a)$$

$$\nabla \times \mathbf{H} - \frac{\partial(\varepsilon \mathbf{E})}{\partial t} - \sigma \mathbf{E} = \mathbf{J}^{imp} \quad \text{in } \Omega, \quad \int_{\Gamma} \mathbf{n} \cdot \mathbf{K}^{imp} d\Gamma = 0, \quad (3.2c)$$

(Maxwell–Ampere’s law) (3.1b)

$$\nabla \cdot (\varepsilon \mathbf{E}) = \rho^{imp} \quad \text{in } \Omega, \quad (3.1c)$$

(Gauss’s law—electric)

$$\nabla \cdot (\mu \mathbf{H}) = 0 \quad \text{in } \Omega, \quad (3.1d)$$

(Gauss’s law—magnetic),

where \mathbf{E} and \mathbf{H} are the electric and magnetic field intensities, respectively, ρ^{imp} is the imposed source of electric charge density, and \mathbf{J}^{imp} and \mathbf{K}^{imp} are imposed sources of electric and magnetic current density. All imposed sources are given functions of the space and time coordinates.

In system (3.1) we have already made use of the constitutive relations

$$\mathbf{D} = \varepsilon \mathbf{E},$$

$$\mathbf{B} = \mu \mathbf{H},$$

$$\mathbf{J} = \sigma \mathbf{E},$$

where \mathbf{D} is the electric flux density, \mathbf{B} is the magnetic flux density, and \mathbf{J} is the electric (eddy) current density; the constitutive parameters ε , μ , and σ denote, respectively, the permittivity, permeability, and conductivity of the medium. These parameters are tensors for anisotropic media. They may be functions of position and time, and may depend on the field intensities. For simplicity, we consider isotropic and homogeneous media, therefore they are constant scalars.

The field equations are supplemented by the boundary conditions

$$\mathbf{n} \times \mathbf{E} = \mathbf{0} \quad \text{on } \Gamma_1, \quad (3.1e)$$

$$\mathbf{n} \cdot (\mu \mathbf{H}) = 0 \quad \text{on } \Gamma_1, \quad (3.1f)$$

$$\mathbf{n} \times \mathbf{H} = \mathbf{0} \quad \text{on } \Gamma_2, \quad (3.1g)$$

$$\mathbf{n} \cdot (\varepsilon \mathbf{E}) = 0 \quad \text{on } \Gamma_2, \quad (3.1h)$$

where Γ_1 is an electric wall and Γ_2 is a magnetic symmetry wall. Here we consider only homogeneous boundary conditions, since inhomogeneous boundary terms can always be converted into source terms.

For transient problems, the initial conditions on \mathbf{E} and \mathbf{H} should also be provided.

To allow system (3.1) to have a solution, the source terms must satisfy the following compatibility conditions:

$$\nabla \cdot \mathbf{K}^{imp} = 0 \quad \text{in } \Omega, \quad (3.2a)$$

$$\mathbf{n} \cdot \mathbf{K}^{imp} = 0 \quad \text{on } \Gamma_1, \quad (3.2b)$$

$$\nabla \cdot \mathbf{J}^{imp} + \frac{\partial \rho^{imp}}{\partial t} + (\sigma/\varepsilon)\rho^{imp} = 0 \quad \text{in } \Omega, \quad (3.2d)$$

$$\mathbf{n} \cdot \mathbf{J}^{imp} = 0 \quad \text{on } \Gamma_2. \quad (3.2e)$$

We remark that the compatibility conditions (3.2a), (3.2b), (3.2d), (3.2e) can be obtained by applying the div–curl method to the Maxwell’s curl equations (3.1a), (3.1b).

3.2. The Determination

Consider the following system augmented by the variables φ and χ :

$$\nabla \varphi + \nabla \times \mathbf{E} + \frac{\partial(\mu \mathbf{H})}{\partial t} = -\mathbf{K}^{imp} \quad \text{in } \Omega, \quad (3.3a)$$

$$\nabla \chi + \nabla \times \mathbf{H} - \frac{\partial(\varepsilon \mathbf{E})}{\partial t} - \sigma \mathbf{E} = \mathbf{J}^{imp} \quad \text{in } \Omega, \quad (3.3b)$$

$$\nabla \cdot (\varepsilon \mathbf{E}) = \rho^{imp} \quad \text{in } \Omega, \quad (3.3c)$$

$$\nabla \cdot (\mu \mathbf{H}) = 0 \quad \text{in } \Omega, \quad (3.3d)$$

$$\mathbf{n} \times \mathbf{E} = \mathbf{0} \quad \text{on } \Gamma_1, \quad (3.3e)$$

$$\chi = 0, \quad \mathbf{n} \cdot (\mu \mathbf{H}) = 0 \quad \text{on } \Gamma_1, \quad (3.3f)$$

$$\mathbf{n} \times \mathbf{H} = \mathbf{0} \quad \text{on } \Gamma_2, \quad (3.3g)$$

$$\varphi = 0, \quad \mathbf{n} \cdot (\varepsilon \mathbf{E}) = 0 \quad \text{on } \Gamma_2. \quad (3.3h)$$

We emphasize that the introduction of the variables φ and χ is purely for showing that the Maxwell equations are not “overdetermined” and they do not enter into computation in contrast to the method proposed by Assous *et al.* [2].

It is easy by using the div–curl method as in Section 2.2 to prove that φ and χ in (3.3) are dummy variables, i.e., $\varphi \equiv 0$ and $\chi \equiv 0$ in Ω ; therefore system (3.3) is equivalent to system (3.1) (see Jiang *et al.* [26] for details). The first-order system (3.3) has eight equations, eight unknowns, and four boundary conditions on each part of the boundary and, thus, is properly determined. It is valid for static, transient, and time-harmonic cases.

In static cases, the time-derivative terms in (3.3a) and (3.3b) disappear, and $\sigma \mathbf{E}$ is included into the given current density. The system (3.3) becomes two independent div–curl systems for the electric field and the magnetic field, respectively. In Section 2.2, we have shown that each div–curl system is elliptic.

In time-harmonic cases, when the time factor $e^{j\omega t}$ is used and suppressed, the time-derivative terms become the zero-order terms, and system (3.3) becomes two coupled div–curl systems. The coupling is through the zero-order terms. The principle part, i.e., the first-order derivative terms which classify the system, still have the div–curl structure, and thus the whole system is elliptic.

In transient cases, the whole system (3.3) is hyperbolic. However, in time-domain numerical methods, the time-

derivative terms are discretized by explicit or implicit finite differences; hence the time-derivative terms become the zero-order terms in the space domain. For each time step, the time-discretized system is still elliptic.

In summary, in all cases, system (3.3) is properly determined and is elliptic in the space domain. Since system (3.1) is equivalent to system (3.3), it is indeed properly determined and also elliptic in the space domain. Therefore, the divergence equations (3.1c), (3.1d) and the boundary conditions (3.1f), (3.1h) are not “redundant,” and must always be taken into account.

3.3. The Importance of Divergence Equations

It is commonly believed that the divergence equations (3.1c) and (3.1d) are “redundant” for transient and time-harmonic problems and, thus, are neglected in computation. This misconception is the true origin of spurious or inaccurate solutions in computational electromagnetics due to the following reasons:

(1) The Maxwell equations were established by James Clerk Maxwell in 1873. The original first-order full Maxwell equations (3.1a)–(3.1c) reflect the general and independent laws of physics. These laws cannot be induced by each other. They govern all electromagnetic phenomena, no matter whether the problem is static, time-harmonic, or transient.

(2) By taking the divergence of (3.1a), one can conclude only that $\partial(\nabla \cdot (\mu\mathbf{H}))/\partial t = 0$, that is, $\nabla \cdot (\mu\mathbf{H}) = F(\mathbf{x})$ which can be any function of the space coordinates. In (3.1a) there is no information about this function, that is, the Gauss law (the magnetic flux density must be divergence free) cannot be induced by the Faraday law. Some literature asserts that, if the divergence of $\mu\mathbf{H}$ is zero at the beginning, it will be identically zero forever. The problem then is how can one set $\nabla \cdot (\mu\mathbf{H}) = 0$ initially. Let us examine the common practice: letting the initial field intensities be zero in the domain and the boundary conditions be correctly given on the boundary. In this case, the divergence-free condition is significantly violated near the boundary at the first time step of the computation and will be violated forever. If someone really can set the divergence to be zero at the beginning, it is in fact equivalent to adding a divergence-free equation into the system. The discussion for the electric field runs along the same line. For the similar reason, the boundary conditions (3.1f), (3.1h) are not “redundant.”

(3) From the mathematical point of view, the neglect of the divergence equations destroys the ellipticity of Maxwell’s equations in the space domain. In each curl system there are only three (odd) equations and three (odd) unknowns that cannot be elliptic in the ordinary sense. In general, the numerical methods based on a non-elliptic

system without special treatment cannot be proved to possess an optimal rate of convergence. A related investigation can be found in Jiang and Povinelli [23].

(4) For time-harmonic problems the curl equations alone will admit infinite number of eigenfunctions corresponding to the frequency $\omega = 0$ which is the so called infinitely degenerate eigenvalue. The inclusion of the divergence equations will exclude this completely non-physical situation and guarantee that only the trivial solution $\mathbf{E} = \mathbf{0}$ and $\mathbf{H} = \mathbf{0}$ corresponds to $\omega = 0$.

(5) The time marching method is often an effective approach to solve steady-state non-linear problems where the material properties depend on the electromagnetic fields. The curl equations alone are not adequate for this approach. Neither are the curl equations appropriate for solving the scattering of waves excited by a pulse wave.

4. THE SECOND-ORDER MAXWELL EQUATIONS

In this section we shall use the div–curl method to derive the second-order Maxwell equations and their boundary conditions and to show that the curl–curl equations cannot stand alone; the Helmholtz equations must be solved with the divergence conditions enforced on the corresponding part of boundary. We shall give the Galerkin method corresponding to the correct second-order Maxwell equations. We shall see that this Galerkin method is of the same form as the popular Galerkin/penalty method with the penalty parameter $s = 1$. We shall also give a simple least-squares look-alike method to obtain a correct variational formulation which rigorously justifies that $s = 1$ in the penalty method.

4.1. The Div–Curl Method

By virtue of the div–curl theorem, system (3.1) is equivalent to

$$\nabla \times \left\{ \nabla \times \mathbf{E} + \frac{\partial(\mu\mathbf{H})}{\partial t} + \mathbf{K}^{imp} \right\} = \mathbf{0} \quad \text{in } \Omega, \quad (4.1a)$$

$$\nabla \cdot \left\{ \nabla \times \mathbf{E} + \frac{\partial(\mu\mathbf{H})}{\partial t} + \mathbf{K}^{imp} \right\} = 0 \quad \text{in } \Omega, \quad (4.1b)$$

$$\mathbf{n} \cdot \left\{ \nabla \times \mathbf{E} + \frac{\partial(\mu\mathbf{H})}{\partial t} + \mathbf{K}^{imp} \right\} = 0 \quad \text{on } \Gamma_1, \quad (4.1c)$$

$$\mathbf{n} \times \left\{ \nabla \times \mathbf{E} + \frac{\partial(\mu\mathbf{H})}{\partial t} + \mathbf{K}^{imp} \right\} = \mathbf{0} \quad \text{on } \Gamma_2, \quad (4.1d)$$

$$\nabla \times \left\{ \nabla \times \mathbf{H} - \frac{\partial(\varepsilon\mathbf{E})}{\partial t} - \sigma\mathbf{E} - \mathbf{J}^{imp} \right\} = \mathbf{0} \quad \text{in } \Omega, \quad (4.1e)$$

$$\nabla \cdot \left\{ \nabla \times \mathbf{H} - \frac{\partial(\varepsilon\mathbf{E})}{\partial t} - \sigma\mathbf{E} - \mathbf{J}^{imp} \right\} = 0 \quad \text{in } \Omega, \quad (4.1f)$$

$$\mathbf{n} \times \left\{ \nabla \times \mathbf{H} - \frac{\partial(\varepsilon \mathbf{E})}{\partial t} - \sigma \mathbf{E} - \mathbf{J}^{imp} \right\} = \mathbf{0} \quad \text{on } \Gamma_1, \quad (4.1g)$$

$$\mathbf{n} \cdot \left\{ \nabla \times \mathbf{H} - \frac{\partial(\varepsilon \mathbf{E})}{\partial t} - \sigma \mathbf{E} - \mathbf{J}^{imp} \right\} = 0 \quad \text{on } \Gamma_2, \quad (4.1h)$$

$$\nabla \cdot (\varepsilon \mathbf{E}) = \rho^{imp} \quad \text{in } \Omega, \quad (4.1i)$$

$$\nabla \cdot (\mu \mathbf{H}) = 0 \quad \text{in } \Omega, \quad (4.1j)$$

$$\mathbf{n} \times \mathbf{E} = \mathbf{0} \quad \text{on } \Gamma_1, \quad (4.1k)$$

$$\mathbf{n} \cdot (\mu \mathbf{H}) = 0 \quad \text{on } \Gamma_1, \quad (4.1l)$$

$$\mathbf{n} \times \mathbf{H} = \mathbf{0} \quad \text{on } \Gamma_2, \quad (4.1m)$$

$$\mathbf{n} \cdot (\varepsilon \mathbf{E}) = 0 \quad \text{on } \Gamma_2. \quad (4.1n)$$

Due to the compatibility conditions (3.2), the divergence conditions (4.1i), (4.1j), and the boundary conditions (4.1k)–(4.1n), we may eliminate Eqs. (4.1b), (4.1c), (4.1f), and (4.1h) and rewrite system (4.1) as

$$\nabla \times \left\{ \nabla \times \mathbf{E} + \frac{\partial(\mu \mathbf{H})}{\partial t} \right\} = -\nabla \times \mathbf{K}^{imp} \quad \text{in } \Omega, \quad (4.2a)$$

$$\nabla \times \left\{ \nabla \times \mathbf{H} - \frac{\partial(\varepsilon \mathbf{E})}{\partial t} - \sigma \mathbf{E} \right\} = \nabla \times \mathbf{J}^{imp} \quad \text{in } \Omega, \quad (4.2b)$$

$$\nabla \cdot (\varepsilon \mathbf{E}) = \rho^{imp} \quad \text{in } \Omega, \quad (4.2c)$$

$$\nabla \cdot (\mu \mathbf{H}) = 0 \quad \text{in } \Omega, \quad (4.2d)$$

$$\mathbf{n} \times \mathbf{E} = \mathbf{0} \quad \text{on } \Gamma_1, \quad (4.2e)$$

$$\mathbf{n} \cdot (\mu \mathbf{H}) = 0 \quad \text{on } \Gamma_1, \quad (4.2f)$$

$$\mathbf{n} \times (\nabla \times \mathbf{H}) = \mathbf{n} \times \mathbf{J}^{imp} \quad \text{on } \Gamma_1, \quad (4.2g)$$

$$\mathbf{n} \times \mathbf{H} = \mathbf{0} \quad \text{on } \Gamma_2, \quad (4.2h)$$

$$\mathbf{n} \cdot (\varepsilon \mathbf{E}) = 0 \quad \text{on } \Gamma_2, \quad (4.2i)$$

$$\mathbf{n} \times (\nabla \times \mathbf{E}) = -\mathbf{n} \times \mathbf{K}^{imp} \quad \text{on } \Gamma_2. \quad (4.2j)$$

System (4.2) is completely equivalent to system (3.1), the validation of (4.2) guarantees the validation of (3.1). Therefore, we can use the curl equations in (3.1) to decouple \mathbf{E} and \mathbf{H} in (4.2) as usual; then we obtain

$$\begin{aligned} & \nabla \times \left\{ \nabla \times \mathbf{E} + \mu \frac{\partial}{\partial t} \left(\frac{\partial(\varepsilon \mathbf{E})}{\partial t} + \sigma \mathbf{E} \right) \right\} \\ &= -\nabla \times \mathbf{K}^{imp} - \mu \frac{\partial \mathbf{J}^{imp}}{\partial t} \quad \text{in } \Omega, \quad (4.3a) \end{aligned}$$

$$\nabla \cdot (\varepsilon \mathbf{E}) = \rho^{imp} \quad \text{in } \Omega, \quad (4.3b)$$

$$\mathbf{n} \times \mathbf{E} = \mathbf{0} \quad \text{on } \Gamma_1, \quad (4.3c)$$

$$\mathbf{n} \cdot (\varepsilon \mathbf{E}) = 0 \quad \text{on } \Gamma_2, \quad (4.3d)$$

$$\mathbf{n} \times (\nabla \times \mathbf{E}) = -\mathbf{n} \times \mathbf{K}^{imp} \quad \text{on } \Gamma_2; \quad (4.3e)$$

$$\begin{aligned} & \nabla \times (\nabla \times \mathbf{H}) + \left(\varepsilon \frac{\partial}{\partial t} + \sigma \right) \frac{\partial(\mu \mathbf{H})}{\partial t} \\ &= - \left(\varepsilon \frac{\partial}{\partial t} + \sigma \right) \mathbf{K}^{imp} + \nabla \times \mathbf{J}^{imp} \quad \text{in } \Omega, \quad (4.4a) \end{aligned}$$

$$\nabla \cdot (\mu \mathbf{H}) = 0 \quad \text{in } \Omega, \quad (4.4b)$$

$$\mathbf{n} \cdot (\mu \mathbf{H}) = 0 \quad \text{on } \Gamma_1, \quad (4.4c)$$

$$\mathbf{n} \times (\nabla \times \mathbf{H}) = \mathbf{n} \times \mathbf{J}^{imp} \quad \text{on } \Gamma_1, \quad (4.4d)$$

$$\mathbf{n} \times \mathbf{H} = \mathbf{0} \quad \text{on } \Gamma_2. \quad (4.4e)$$

We note that the curl–curl equations in (4.3) and (4.4) cannot stand alone; they must be supplemented by the divergence equations and the additional natural boundary conditions. In other words, the curl–curl equations admit more solutions than the first-order full system. This is the real reason that the numerical methods based on the curl–curl equations will give rise to spurious solutions.

It is difficult to solve a second-order curl–curl equation (4.3a) with the explicit constraint of the first-order divergence equation (4.3b), since the problem has more equations than unknowns and the first-order equation (4.3b) is hard to deal with numerically. We shall look for a simple way. By using Theorem 4 and the vector identity (2.12), system (4.3) can be reduced to

$$-\Delta \mathbf{E} + \mu \frac{\partial}{\partial t} \left(\frac{\partial(\varepsilon \mathbf{E})}{\partial t} + \sigma \mathbf{E} \right) = -\nabla \times \mathbf{K}^{imp} \quad (4.5a)$$

$$- \mu \frac{\partial \mathbf{J}^{imp}}{\partial t} - \left(\frac{1}{\varepsilon} \right) \nabla \rho^{imp} \quad \text{in } \Omega,$$

$$\nabla(\nabla \cdot (\varepsilon \mathbf{E}) - \rho^{imp}) = \mathbf{0} \quad \text{in } \Omega, \quad (4.5b)$$

$$\mathbf{n} \times \mathbf{E} = \mathbf{0} \quad \text{on } \Gamma_1, \quad (4.5c)$$

$$\nabla \cdot (\varepsilon \mathbf{E}) = \rho^{imp} \quad \text{on } \Gamma_1, \quad (4.5d)$$

$$\mathbf{n} \cdot (\varepsilon \mathbf{E}) = 0 \quad \text{on } \Gamma_2, \quad (4.5e)$$

$$\mathbf{n} \times (\nabla \times \mathbf{E}) = -\mathbf{n} \times \mathbf{K}^{imp} \quad \text{on } \Gamma_2. \quad (4.5f)$$

Due to the reasons pointed out in Section 2.3, Eq. (4.5b) can be eliminated. That is, the divergence equation (4.5b) is redundant and implicitly satisfied by the Helmholtz-type equations (4.5a) and the boundary conditions. Therefore, system (4.5) can be further simplified as

$$-\Delta \mathbf{E} + \mu \frac{\partial}{\partial t} \left(\frac{\partial(\varepsilon \mathbf{E})}{\partial t} + \sigma \mathbf{E} \right) = -\nabla \times \mathbf{K}^{imp} \quad (4.6a)$$

$$- \mu \frac{\partial \mathbf{J}^{imp}}{\partial t} - \left(\frac{1}{\varepsilon} \right) \nabla \rho^{imp} \quad \text{in } \Omega,$$

$$\mathbf{n} \times \mathbf{E} = \mathbf{0} \quad \text{on } \Gamma_1, \quad (4.6b)$$

$$\nabla \cdot (\varepsilon \mathbf{E}) = \rho^{imp} \quad \text{on } \Gamma_1 \quad (4.6c)$$

$$\mathbf{n} \cdot (\varepsilon \mathbf{E}) = 0 \quad \text{on } \Gamma_2, \quad (4.6d)$$

$$\mathbf{n} \times (\nabla \times \mathbf{E}) = -\mathbf{n} \times \mathbf{K}^{imp} \quad \text{on } \Gamma_2. \quad (4.6e)$$

Similarly, we can have

$$-\Delta \mathbf{H} + \left(\varepsilon \frac{\partial}{\partial t} + \sigma \right) \frac{\partial(\mu \mathbf{H})}{\partial t} = - \left(\varepsilon \frac{\partial}{\partial t} + \sigma \right) \mathbf{K}^{imp} + \nabla \times \mathbf{J}^{imp} \quad \text{in } \Omega, \quad (4.7a)$$

$$\mathbf{n} \cdot (\mu \mathbf{H}) = 0 \quad \text{on } \Gamma_1, \quad (4.7b)$$

$$\mathbf{n} \times (\nabla \times \mathbf{H}) = \mathbf{n} \times \mathbf{J}^{imp} \quad \text{on } \Gamma_1, \quad (4.7c)$$

$$\mathbf{n} \times \mathbf{H} = 0 \quad \text{on } \Gamma_2, \quad (4.7d)$$

$$\nabla \cdot (\mu \mathbf{H}) = 0 \quad \text{on } \Gamma_2. \quad (4.7e)$$

Since we are dealing with a second-order problem in the time domain, we have to add initial conditions for $\partial \mathbf{E} / \partial t$ and $\partial \mathbf{H} / \partial t$; see Assous *et al.* [2].

We note that the divergence conditions are required to be satisfied only on a part of the boundary. We will rigorously prove this in Section 4.3 by using the least-squares method. As in Section 2.3 for the div–curl system, one may enforce the divergence conditions on the whole boundary Γ in (4.6) and (4.7) and show that the divergence conditions are satisfied in the domain Ω .

The Helmholtz-type equations (4.6a) and (4.7a) can be found in all text books on electromagnetics. However, it seems that all these books claim that the Helmholtz equation must be solved with the divergence equation satisfied in the whole domain and do not mention that it needs additional boundary conditions. Our rigorous derivation using the div–curl method shows that the Helmholtz equation can stand alone and the divergence equation should be satisfied only on a part of the boundary.

The advantages of using the Helmholtz equation over the curl–curl equation are obvious: one avoids the difficulty involving the explicit satisfaction of the divergence equations; instead one solves three decoupled second-order equations with coupled boundary conditions.

4.2. The Galerkin Method

One may elect to use, for example, the finite difference method, to solve the Helmholtz-type systems (4.6) or (4.7). Usually, the finite difference method is based on rectangular structural grids. In this case, for example, the divergence condition (4.7e) can be simplified as the Neumann boundary condition:

$$\frac{\partial}{\partial n} H_n = 0 \quad \text{on } \Gamma_2.$$

For complex geometry it is not straightforward to implement the Neumann boundary condition in the finite difference method. By using the finite element method based on a variational principle, even the divergence conditions on the boundary do not appear. In the following we derive the variational formulation corresponding to (4.6).

By taking into account the vector identity (2.12), the Galerkin formulation associated with (4.6) is: find \mathbf{E} satisfying (4.6b) and (4.6d) such that

$$\begin{aligned} & (\nabla \times \{\nabla \times \mathbf{E} + \mathbf{K}^{imp}\}, \mathbf{E}^*) + \langle \nabla \times \mathbf{E} + \mathbf{K}^{imp}, \mathbf{n} \times \mathbf{E}^* \rangle_{\Gamma_2} \\ & + (-\nabla \{\nabla \cdot \mathbf{E} - \rho^{imp} / \varepsilon\}, \mathbf{E}^*) \\ & + \langle \nabla \cdot \mathbf{E} - \rho^{imp} / \varepsilon, \mathbf{n} \cdot \mathbf{E}^* \rangle_{\Gamma_1} \\ & + \left(\mu \frac{\partial}{\partial t} \left\{ \frac{\partial(\varepsilon \mathbf{E})}{\partial t} + \sigma \mathbf{E} \right\}, \mathbf{E}^* \right) \\ & + \left(\mu \frac{\partial \mathbf{J}^{imp}}{\partial t}, \mathbf{E}^* \right) = 0 \end{aligned} \quad (4.8)$$

for all \mathbf{E}^* satisfying (4.6b) and (4.6d). By virtue of Green's formula, the statement (4.8) can be simplified to a more symmetric form: find \mathbf{E} satisfying (4.6b) and (4.6d) such that

$$\begin{aligned} & (\nabla \times \mathbf{E}, \nabla \times \mathbf{E}^*) + (\nabla \cdot \mathbf{E}, \nabla \cdot \mathbf{E}^*) \\ & + \left(\mu \frac{\partial}{\partial t} \left\{ \frac{\partial(\varepsilon \mathbf{E})}{\partial t} + \sigma \mathbf{E} \right\}, \mathbf{E}^* \right) \\ & = -(\mathbf{K}^{imp}, \nabla \times \mathbf{E}^*) \\ & + (\rho^{imp} / \varepsilon, \nabla \cdot \mathbf{E}^*) - \left(\mu \frac{\partial}{\partial t} \mathbf{J}^{imp}, \mathbf{E}^* \right) \end{aligned} \quad (4.9)$$

for all \mathbf{E}^* satisfying (4.6b) and (4.6d).

For time-harmonic(eigenvalue) problems with $\sigma = 0$, the variational formulation takes the form

$$(\nabla \times \mathbf{E}, \nabla \times \mathbf{E}^*) + (\nabla \cdot \mathbf{E}, \nabla \cdot \mathbf{E}^*) - \omega^2 \mu \varepsilon (\mathbf{E}, \mathbf{E}^*) = 0, \quad (4.10)$$

where ω is the angular frequency. The formulations for the magnetic field are similar.

The variational formulations (4.9) and (4.10) are of the same structure as the most popular Galerkin/penalty formulations in the literature. However, in contrast to the commonly used penalty formulation, there is no free parameter in the Galerkin formulation (4.9) and (4.10). In

other words, the penalty parameter $s = 1$ should be chosen in the penalty method in order for the penalty method to correspond to the Helmholtz-type equations (4.6).

If the second term in (4.10), which is related to the divergence-free condition, is deleted, one obtains the commonly used incorrect variational formulation that corresponds to solving only the curl–curl equation. One can see that in this case there exists an infinitely degenerate eigenvalue $\omega = 0$. This trouble is caused by incorrect mathematical formulation. In the correct formulation (4.10), due to Theorem 3 there is only a trivial solution $\mathbf{E} = \mathbf{0}$ corresponding to $\omega = 0$. In other words, the variational formulation (4.10) will not give rise to spurious modes.

We emphasize again that the spurious solutions in the computation of waveguide, resonator, scattering wave, and eddy current problems are really caused by wrong analytical formulations. As for the polluted solutions in the MHD stability analysis we refer to Gruber and Rappaz [17] and the references therein.

4.3. The Least-Squares Look-Alike Method

In Section 4.1 the div–curl method is employed to derive the second-order (Helmholtz-type) Maxwell equations and their boundary conditions that guarantee no spurious solutions. But there we cannot make sure that the divergence conditions should be specified only on a part of the boundary. In this section we give a more powerful method to derive equivalent higher-order equations and rigorously prove the statement made in Section 4.1.

Consider the div–curl system for the electric field

$$\nabla \times \mathbf{E} = -\frac{\partial(\boldsymbol{\mu}\mathbf{H})}{\partial t} - \mathbf{K}^{imp} \quad \text{in } \Omega, \quad (4.11a)$$

$$\nabla \cdot \mathbf{E} = \rho^{imp}/\varepsilon \quad \text{in } \Omega, \quad (4.11b)$$

$$\mathbf{n} \times \mathbf{E} = \mathbf{0} \quad \text{on } \Gamma_1, \quad (4.11c)$$

$$\mathbf{n} \cdot (\varepsilon\mathbf{E}) = 0 \quad \text{on } \Gamma_2, \quad (4.11d)$$

where \mathbf{H} is assumed to be known and to satisfy Eq. (3.1b) and the boundary conditions (3.1f) and (3.1g) and the source terms satisfy the compatibility conditions (3.2a)–(3.2e). In other words, when the magnetic field and the sources are given, the solution of (4.11) will give the corresponding electric field. Obviously, system (4.11) is a typical div–curl system that has been investigated in Section 2.

Following the steps in Section 2.4, we can derive the variational formulation which corresponds to system (4.6). We define the quadratic functional

$$I(\mathbf{E}) = \|\nabla \times \mathbf{E} + \frac{\partial(\boldsymbol{\mu}\mathbf{H})}{\partial t} + \mathbf{K}^{imp}\|^2 + \|\nabla \cdot \mathbf{E} - \rho^{imp}/\varepsilon\|^2,$$

in which \mathbf{E} satisfies the boundary conditions (4.11c),

(4.11d). The minimization of I leads to the variational formulation

$$\begin{aligned} (\nabla \times \mathbf{E} + \frac{\partial(\boldsymbol{\mu}\mathbf{H})}{\partial t} + \mathbf{K}^{imp}, \nabla \times \mathbf{E}^*) \\ + (\nabla \cdot \mathbf{E} - \rho^{imp}/\varepsilon, \nabla \cdot \mathbf{E}^*) = 0, \end{aligned} \quad (4.12)$$

where $\mathbf{E}^* = \delta\mathbf{E}$ and satisfies the same boundary conditions as \mathbf{E} . Since \mathbf{H} satisfies (3.1b) and (3.1g), from (4.12) we obtain a variational formulation which is exactly the same as (4.9). By using Green’s formula, from (4.9) we can obtain the Euler–Lagrange equation (4.6a) and the natural boundary condition (4.6c) and (4.6e). That is, the correctness of (4.6) or (4.7) is completely proved.

Now we understand that the variational formulation (4.9), the Helmholtz-type equation (4.6a) and its boundary conditions, and the first-order system (4.11) are equivalent to one another. However, the finite element method based on (4.9) has superior advantages: the divergence condition (4.11b) is automatically satisfied and the test and trial functions are required to satisfy only the essential boundary conditions (4.11c), (4.11d).

We remark that the procedure in this section to obtain the formulation (4.9) is not a true least-squares approach, because (1) we have assumed that \mathbf{H} is given and satisfies (3.1b) and, hence, \mathbf{H} is not subject to the variation; (2) the true least-squares method always leads to a symmetric bilinear form; here the σ -related term is not symmetric. Even so, this procedure is mathematically justifiable. It is nothing but a rigorous method to derive the Galerkin variational formulation corresponding to the Helmholtz-type equations (4.6a) and their boundary conditions. All derivation provided in this section has rigorously proved that the penalty parameter in the Galerkin/penalty method should be equal to one.

5. THE LEAST-SQUARES METHOD FOR FIRST-ORDER MAXWELL EQUATIONS

In this section we briefly give the formulations of the LSFEM for the general first-order partial differential equations and apply LSFEM to solving the time-harmonic first-order Maxwell equations.

5.1. The General Formulation

The least-squares method for the linear operator equation $\mathbf{A}\mathbf{u} = \mathbf{f}$ formally is equivalent to the solution of the higher-order equation $\mathbf{A}^*\mathbf{A}\mathbf{u} = \mathbf{A}^*\mathbf{f}$ with $\mathbf{A}\mathbf{u} = \mathbf{f}$ serving as an additional natural boundary condition, where \mathbf{A}^* is the adjoint of \mathbf{A} in the inner product generated by the L_2 norm. When directly applied to second-order equations this approach requires the use of C^1 finite elements and leads to ill-conditioned discrete systems. In order to use

simple C^0 elements and obtain a better-conditioned algebraic system, the least-squares method discussed here is based on the first-order system. The formulation of the least-squares finite element method for general first-order steady-state boundary-value problems can be found in Jiang and Povinelli [22]. This formulation can be directly applied to the solution of the first-order steady-state and time-harmonic Maxwell equations. For time-dependent problems one always can use an appropriate finite difference method in the temporal domain, such as the backward Euler scheme or the Crank–Nicolson scheme, to discretize the time-derivative terms so that in each time-step the problems are converted into boundary-value problems, see Wu and Jiang [69] for an example. For completeness, we briefly derive the general least-squares formulation.

We consider the linear boundary-value problem

$$\mathbf{A}\mathbf{u} = \mathbf{f} \quad \text{in } \Omega, \quad (5.1a)$$

$$\mathbf{B}\mathbf{u} = \mathbf{g} \quad \text{on } \Gamma, \quad (5.1b)$$

where \mathbf{A} is a first-order partial differential operator:

$$\mathbf{A}\mathbf{u} = \sum_{i=1}^{n_d} \mathbf{A}_i \frac{\partial \mathbf{u}}{\partial x_i} + \mathbf{A}_0 \mathbf{u}, \quad (5.2)$$

in which $\Omega \in \mathbb{R}^{n_d}$ is a bounded domain with a piecewise smooth boundary Γ , $n_d = 2$ or 3 represents the number of space dimensions, $\mathbf{u}^T = (u_1, u_2, \dots, u_m)$ is a vector of m unknown functions of $\mathbf{x} = (x_1, \dots, x_{n_d})$, \mathbf{A}_i and \mathbf{A}_0 are $n \times m$ matrices which depend on \mathbf{x} , \mathbf{f} is a given vector-valued function, \mathbf{B} is a boundary algebraic operator, and \mathbf{g} is a given vector-valued function on the boundary. Without loss of generality we assume that the vector \mathbf{g} is null. We should mention that the number of equations n in the system (5.1a) must be greater than or equal to the number of unknowns m .

Considering the boundary condition of the boundary-value problem, we also define the function space

$$\mathbf{V} = \{\mathbf{v} \in H^1(\Omega)^m \mid \mathbf{B}\mathbf{v} = \mathbf{0} \text{ on } \Gamma\}. \quad (5.3)$$

Let us suppose that $\mathbf{f} \in \mathbf{L}_2(\Omega)$ and $\mathbf{A} : \mathbf{V} \rightarrow \mathbf{L}_2(\Omega)$. For an arbitrary trial function $\mathbf{v} \in \mathbf{V}$, we define the residual function:

$$\mathbf{R} = \mathbf{A}\mathbf{v} - \mathbf{f} \quad \text{in } \Omega. \quad (5.4)$$

In general the residual \mathbf{R} is not equal to zero, except \mathbf{v} is equal to the exact solution \mathbf{u} . The squared distance between $\mathbf{A}\mathbf{v}$ and \mathbf{f} will be nonnegative:

$$\|\mathbf{R}\|_0^2 = \int_{\Omega} (\mathbf{A}\mathbf{v} - \mathbf{f})^2 d\Omega \geq 0. \quad (5.5)$$

A solution \mathbf{u} to the problem (5.1) can thus be interpreted as a member of \mathbf{V} that minimizes the squared distance between $\mathbf{A}\mathbf{v}$ and \mathbf{f} :

$$0 = \|\mathbf{R}(\mathbf{u})\|_0^2 \leq \|\mathbf{R}(\mathbf{v})\|_0^2 \quad \forall \mathbf{v} \in \mathbf{V}.$$

The least-squares method consists of seeking a minimizer of the squared distance $\|\mathbf{A}\mathbf{v} - \mathbf{f}\|_0^2$ in \mathbf{V} . We write the quadratic functional in (5.5) as

$$I(\mathbf{v}) = \|\mathbf{A}\mathbf{v} - \mathbf{f}\|_0^2 = (\mathbf{A}\mathbf{v} - \mathbf{f}, \mathbf{A}\mathbf{v} - \mathbf{f}). \quad (5.6)$$

A necessary condition that $\mathbf{u} \in \mathbf{V}$ be a minimizer of the functional I in (5.6) is that its first variation vanish at \mathbf{u} for all admissible \mathbf{v} . That is,

$$\lim_{\tau \rightarrow 0} \frac{d}{d\tau} I(\mathbf{u} + \tau \mathbf{v}) \equiv 2 \int_{\Omega} (\mathbf{A}\mathbf{v})^T (\mathbf{A}\mathbf{u} - \mathbf{f}) d\Omega = \mathbf{0} \quad \forall \mathbf{v} \in \mathbf{V}.$$

Thus, the least-squares method leads us to the variational boundary-value problem: Find $\mathbf{u} \in \mathbf{V}$ such that

$$B(\mathbf{u}, \mathbf{v}) = F(\mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{V}, \quad (5.7a)$$

where

$$B(\mathbf{u}, \mathbf{v}) \equiv (\mathbf{A}\mathbf{u}, \mathbf{A}\mathbf{v}), \quad (5.7b)$$

$$F(\mathbf{v}) \equiv (\mathbf{f}, \mathbf{A}\mathbf{v}). \quad (5.7c)$$

In the finite element analysis, we first subdivide the domain as a union of finite elements and then introduce an appropriate finite element basis. Let N_n denote the number of nodes for one element and ψ_j denote the element shape functions. If equal-order interpolations are employed, that is, for all unknown variables the same finite element is used, we can write the expansion in each element

$$\mathbf{u}_h^e(\mathbf{x}) = \sum_{j=1}^{N_n} \psi_j(\mathbf{x}) \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_m \end{pmatrix}_j, \quad (5.8)$$

where $(u_1, u_2, \dots, u_m)_j$ are the nodal values at the j th node, and h denotes the mesh parameter.

Introducing the finite element approximation defined in (5.8) into the variational statement (5.7), we have the linear algebraic equations

$$\mathbf{K}\mathbf{U} = \mathbf{F}, \quad (5.9)$$

where \mathbf{U} is the global vector of nodal values. The global matrix \mathbf{K} is assembled from the element matrices

$$\mathbf{K}_e = \int_{\Omega_e} (\mathbf{A}\psi_1, \mathbf{A}\psi_2, \dots, \mathbf{A}\psi_{N_n})^T (\mathbf{A}\psi_1, \mathbf{A}\psi_2, \dots, \mathbf{A}\psi_{N_n}) d\Omega, \quad (5.10)$$

in which $\Omega_e \subset \Omega$ is the domain of the e th element, \mathbf{T} denotes the transpose, and the vector \mathbf{F} is assembled from the element vectors,

$$\mathbf{F}_e = \int_{\Omega_e} (\mathbf{A}\psi_1, \mathbf{A}\psi_2, \dots, \mathbf{A}\psi_{N_n})^T \mathbf{f} d\Omega, \quad (5.11)$$

in (5.10) and (5.11):

$$\mathbf{A}\psi_j = \sum_{i=1}^{n_d} \frac{\partial \psi_j}{\partial x_i} \mathbf{A}_i + \psi_j \mathbf{A}_0. \quad (5.12)$$

From the above derivation we can immediately find out or further prove that:

(1) the least-squares method is universal for all types of first-order partial differential equations, no matter whether they are elliptic, hyperbolic, parabolic, or mixed; the only requirement is that they have a unique solution (see Mikhlin [39] and Marchuk [38]);

(2) the LSFEM leads to a symmetric positive definite algebraic system which can be solved efficiently by matrix-free iterative methods, such as the element-by-element preconditioned conjugate gradient method, and thus the parallelization and large-scale 3D computation is made easy;

(3) the LSFEM formulation and its coding are general; therefore for a new problem one needs only to supply the coefficients of the system of equations, the load vector, and the boundary conditions;

(4) the LSFEM is robust, no special treatments, such as upwinding, staggered grids, operator splitting, etc. are needed; the LSFEM leads to a minimization problem rather than a saddle-point problem; thus simple equal-order interpolations can be employed;

(5) the LSFEM can often be proved to have optimal numerical properties including an optimal rate of convergence;

(6) the LSFEM satisfies easily the divergence conditions in electromagnetics.

5.2. Time-Harmonic Fields

For three-dimensional time-harmonic fields, the first-order full Maxwell equations can be written as

$$\nabla \times \mathbf{E} + j\omega\mu\mathbf{H} = -\mathbf{K}^{imp} \quad \text{in } \Omega, \quad (5.13a)$$

$$\nabla \times \mathbf{H} - j\omega\varepsilon\mathbf{E} = \mathbf{J}^{imp} \quad \text{in } \Omega, \quad (5.13b)$$

$$\nabla \cdot \mathbf{E} = 0 \quad \text{in } \Omega, \quad (5.13c)$$

$$\nabla \cdot \mathbf{H} = 0 \quad \text{in } \Omega, \quad (5.13d)$$

where the time factor $e^{j\omega t}$ is used and suppressed, ω is the given angular frequency and not equal to the resonant frequencies of this problem, \mathbf{E} and \mathbf{H} are the complex electric and magnetic field intensities, respectively, \mathbf{J}^{imp} and \mathbf{K}^{imp} are imposed harmonic sources of electric and magnetic current density, respectively. For simplicity, ε and μ are constant scalars for homogeneous isotropic media. The field equations are supplemented by the same homogeneous boundary conditions as (3.1e)–(3.1h). The source terms satisfy the compatibility conditions similar to (3.2).

Separating the real and imaginary parts in (5.13) leads to

$$\nabla \times \mathbf{E}_r - \omega\mu\mathbf{H}_i = -\mathbf{K}_r^{imp} \quad \text{in } \Omega, \quad (5.14a)$$

$$\nabla \times \mathbf{E}_i + \omega\mu\mathbf{H}_r = -\mathbf{K}_i^{imp} \quad \text{in } \Omega, \quad (5.14b)$$

$$\nabla \times \mathbf{H}_r + \omega\varepsilon\mathbf{E}_i = \mathbf{J}_r^{imp} \quad \text{in } \Omega, \quad (5.14c)$$

$$\nabla \times \mathbf{H}_i - \omega\varepsilon\mathbf{E}_r = \mathbf{J}_i^{imp} \quad \text{in } \Omega, \quad (5.14d)$$

$$\nabla \cdot \mathbf{E}_r = 0 \quad \text{in } \Omega, \quad (5.14e)$$

$$\nabla \cdot \mathbf{E}_i = 0 \quad \text{in } \Omega, \quad (5.14f)$$

$$\nabla \cdot \mathbf{H}_r = 0 \quad \text{in } \Omega, \quad (5.14g)$$

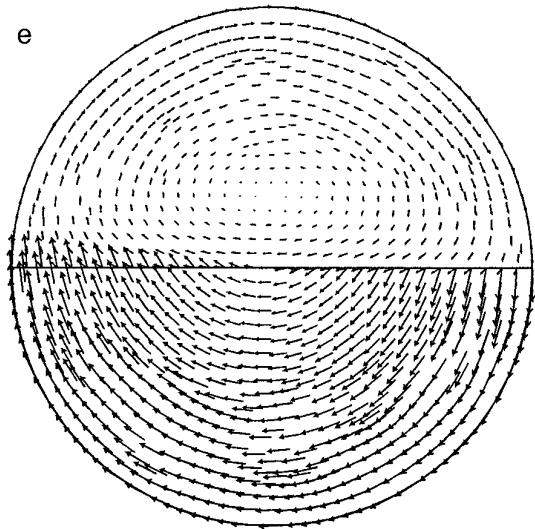
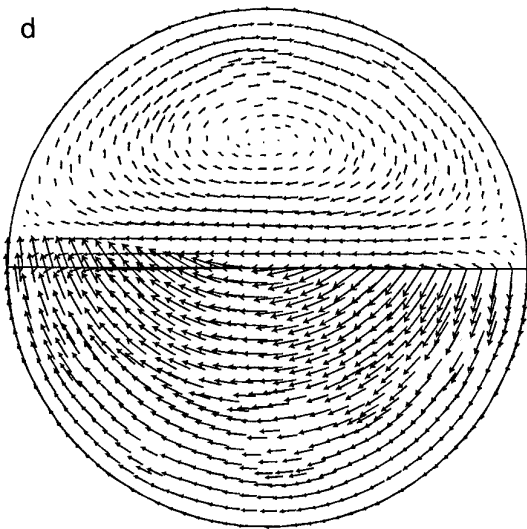
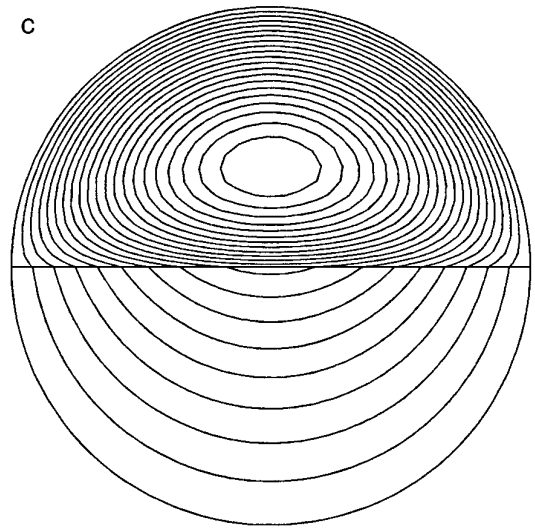
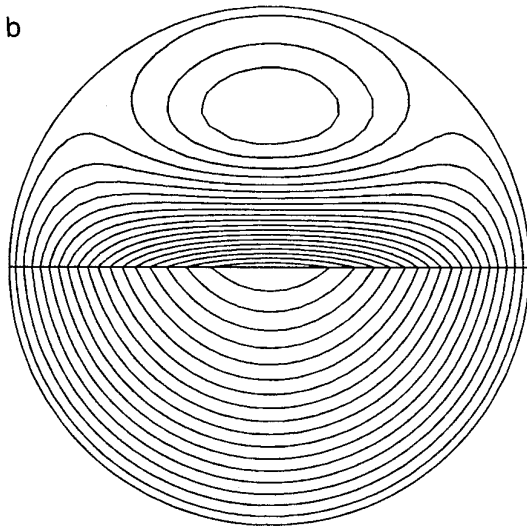
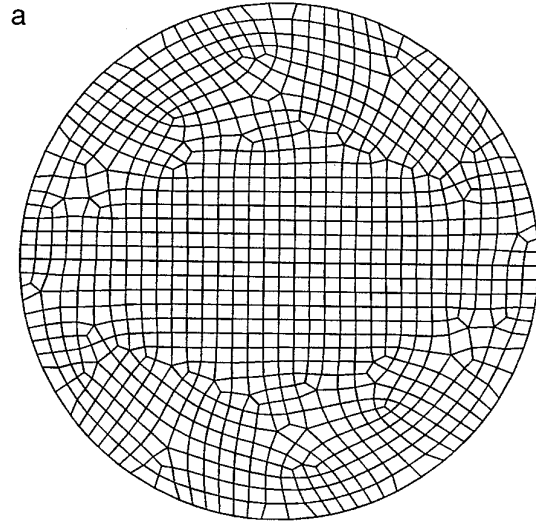
$$\nabla \cdot \mathbf{H}_i = 0 \quad \text{in } \Omega. \quad (5.14h)$$

Obviously, system (5.14) is elliptic, since its principle part consists of four div–curl systems. For the solution of (5.14) the least-squares variational formulation is: find $\mathbf{u} = (\mathbf{E}_r, \mathbf{E}_i, \mathbf{H}_r, \mathbf{H}_i) \in \mathcal{H}$ such that

$$B(\mathbf{u}, \mathbf{v}) = L(\mathbf{v}) \quad \forall \mathbf{v} = (\mathbf{E}_r^*, \mathbf{E}_i^*, \mathbf{H}_r^*, \mathbf{H}_i^*) \in \mathcal{H}, \quad (5.15)$$

where $\mathcal{H} = \{\mathbf{u} \in H^1(\Omega)^3 \times H^1(\Omega)^3 \times H^1(\Omega)^3 \times H^1(\Omega)^3 \mid \mathbf{n} \times \mathbf{E} = \mathbf{0} \text{ on } \Gamma_1, \mathbf{n} \cdot \mathbf{H} = 0 \text{ on } \Gamma_1, \mathbf{n} \times \mathbf{H} = \mathbf{0} \text{ on } \Gamma_2, \mathbf{n} \cdot \mathbf{E} = 0 \text{ on } \Gamma_2\}$, and $B(\cdot, \cdot)$ is the bilinear form

$$\begin{aligned} B(\mathbf{u}, \mathbf{v}) = & (\nabla \times \mathbf{E}_r - \omega\mu\mathbf{H}_i, \nabla \times \mathbf{E}_r^* - \omega\mu\mathbf{H}_i^*) \\ & + (\nabla \times \mathbf{E}_i + \omega\mu\mathbf{H}_r, \nabla \times \mathbf{E}_i^* + \omega\mu\mathbf{H}_r^*) \\ & + (\nabla \times \mathbf{H}_r + \omega\varepsilon\mathbf{E}_i, \nabla \times \mathbf{H}_r^* + \omega\varepsilon\mathbf{E}_i^*) \\ & + (\nabla \times \mathbf{H}_i - \omega\varepsilon\mathbf{E}_r, \nabla \times \mathbf{H}_i^* - \omega\varepsilon\mathbf{E}_r^*) \\ & + (\nabla \cdot \mathbf{E}_r, \nabla \cdot \mathbf{E}_r^*) + (\nabla \cdot \mathbf{E}_i, \nabla \cdot \mathbf{E}_i^*) \\ & + (\nabla \cdot \mathbf{H}_r, \nabla \cdot \mathbf{H}_r^*) + (\nabla \cdot \mathbf{H}_i, \nabla \cdot \mathbf{H}_i^*), \end{aligned} \quad (5.16a)$$



and $L(\cdot)$ is the linear form

$$\begin{aligned} L(\mathbf{v}) = & (-K_i^{imp}, \nabla \times \mathbf{E}_r^* - \omega \mu \mathbf{H}_i^*) \\ & + (-K_i^{imp}, \nabla \times \mathbf{E}_i^* + \omega \mu \mathbf{H}_r^*) \\ & + (J_r^{imp}, \nabla \times \mathbf{H}_r^* + \omega \varepsilon \mathbf{E}_i^*) \\ & + (J_i^{imp}, \nabla \times \mathbf{H}_i^* - \omega \varepsilon \mathbf{E}_r^*). \end{aligned} \quad (5.16b)$$

Obviously, the bilinear form $B(\mathbf{u}, \mathbf{v})$ in (5.16a) is symmetric and continuous, and the linear form $L(\mathbf{v})$ in (5.16b) is continuous. One may prove that if the frequency of the exciting source is not equal to the resonant frequencies of this electromagnetic system, then the bilinear form $B(\mathbf{u}, \mathbf{u})$ is coercive. By virtue of the Lax–Milgram theorem, the least-squares solution uniquely exists and the corresponding finite element solution is of an optimal rate of convergence. In fact, the following statement is the consequence of the coerciveness of the bilinear form $B(\mathbf{u}, \mathbf{u})$. We will prove it in our future reports.

The LSFEM based on (5.15) has an optimal rate of convergence and an optimal satisfaction of divergence-free conditions:

$$\|\mathbf{E}_r - \mathbf{E}_{rh}\|_0 \leq Ch^{k+1}\|\mathbf{u}\|_{k+1}, \quad \|\nabla \cdot \mathbf{E}_{rh}\|_0 \leq Ch^k\|\mathbf{u}\|_{k+1}, \quad (5.17a)$$

$$\|\mathbf{E}_i - \mathbf{E}_{ih}\|_0 \leq Ch^{k+1}\|\mathbf{u}\|_{k+1}, \quad \|\nabla \cdot \mathbf{E}_{ih}\|_0 \leq Ch^k\|\mathbf{u}\|_{k+1}, \quad (5.17b)$$

$$\|\mathbf{H}_r - \mathbf{H}_{rh}\|_0 \leq Ch^{k+1}\|\mathbf{u}\|_{k+1}, \quad \|\nabla \cdot \mathbf{H}_{rh}\|_0 \leq Ch^k\|\mathbf{u}\|_{k+1}, \quad (5.17c)$$

$$\|\mathbf{H}_i - \mathbf{H}_{ih}\|_0 \leq Ch^{k+1}\|\mathbf{u}\|_{k+1}, \quad \|\nabla \cdot \mathbf{H}_{ih}\|_0 \leq Ch^k\|\mathbf{u}\|_{k+1}, \quad (5.17d)$$

where \mathbf{E}_{rh} , \mathbf{E}_{ih} , \mathbf{H}_{rh} , \mathbf{H}_{ih} are the finite element solutions and k is the order of complete polynomials in the equal-order finite element interpolation.

5.3. Time-Harmonic TE Waves

For time-harmonic TE waves the first-order Maxwell equations are

$$j\omega \mu H_z + \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = 0 \quad \text{in } \Omega, \quad (5.18a)$$

$$j\omega \varepsilon^* E_x - \frac{\partial H_z}{\partial y} = 0 \quad \text{in } \Omega, \quad (5.18b)$$

$$j\omega \varepsilon^* E_y + \frac{\partial H_z}{\partial x} = 0 \quad \text{in } \Omega, \quad (5.18c)$$

$$\frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} = 0 \quad \text{in } \Omega, \quad (5.18d)$$

in which $\varepsilon^* = \varepsilon_r + j\varepsilon_i = \varepsilon - j\sigma/\omega$ is the complex permittivity. For a complete description of TE wave problems appropriate boundary conditions should be included. One may consider, for example,

$$H_z = \text{const} \quad \text{on } \Gamma, \quad (5.18e)$$

$$E_x n_x + E_y n_y = 0 \quad \text{on } \Gamma. \quad (5.18f)$$

The condition (5.18e) is an inhomogeneous version corresponding to (3.1g), and (5.18f) is a 2D version of (3.1h). We also note that the boundary conditions (5.18e), (5.18f) satisfy the boundary compatibility condition

$$j\omega \varepsilon^* (E_x n_x + E_y n_y) = \frac{\partial H_z}{\partial y} n_x - \frac{\partial H_z}{\partial x} n_y \quad \text{on } \Gamma, \quad (5.19)$$

which is obtained by taking the operation $\mathbf{n} \cdot$ to Eqs. (5.18b) and (5.18c).

In system (5.18) there are three unknowns and four equations, and thus the divergence-free equation (5.18d) seems ‘‘redundant.’’ By introducing a dummy variable into system (5.18) as in Section 3.2 (see Jiang *et al.* [26] for details), we can prove that System (5.18) is not ‘‘overdetermined,’’ but is indeed properly determined and elliptic.

For numerical calculation separating the real and imaginary parts in (5.18a)–(5.18d) leads to

$$-\omega \mu H_{zi} + \frac{\partial E_{yr}}{\partial x} - \frac{\partial E_{xr}}{\partial y} = 0 \quad \text{in } \Omega, \quad (5.20a)$$

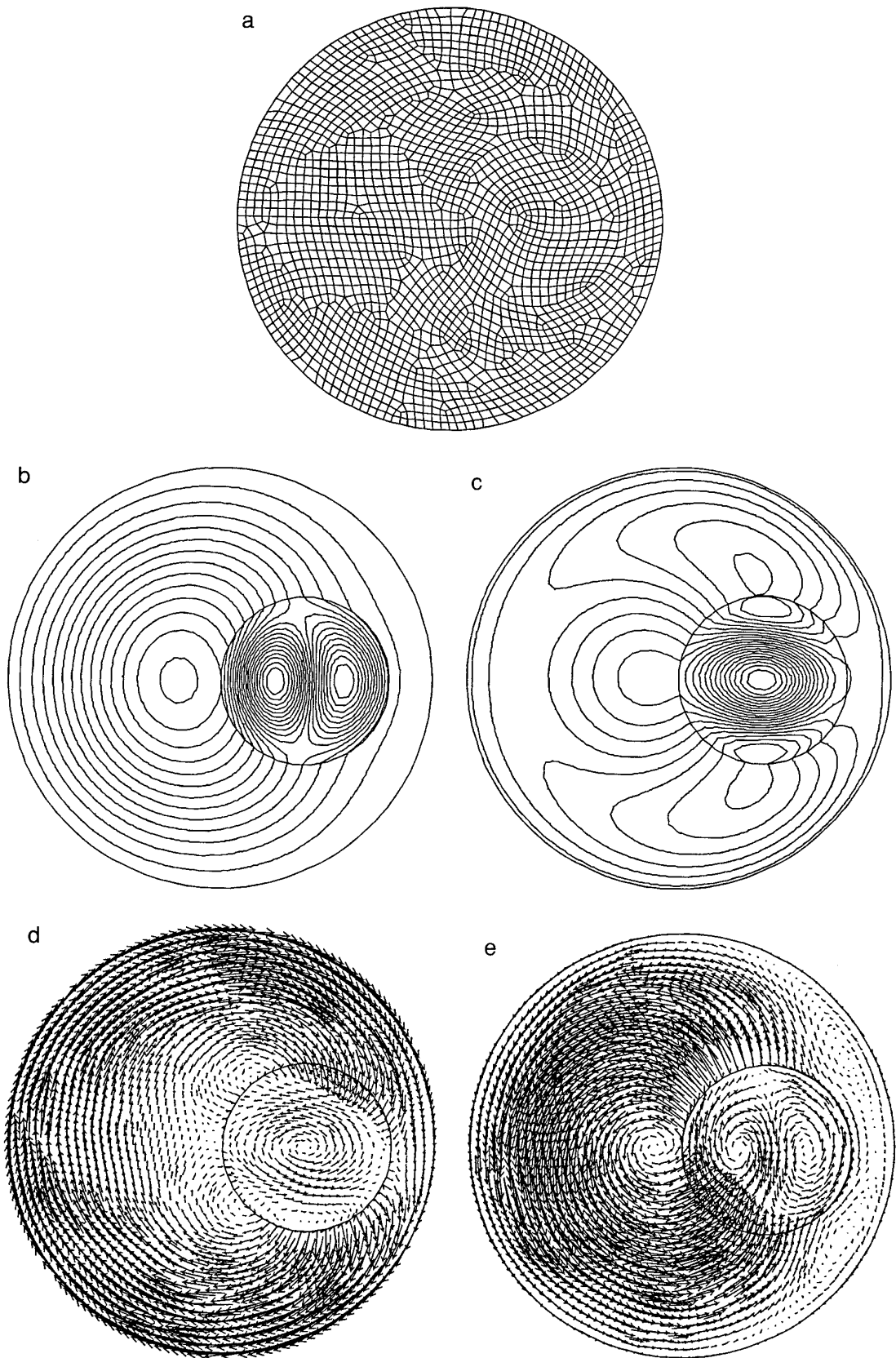
$$-\omega (\varepsilon_r E_{xi} + \varepsilon_i E_{xr}) - \frac{\partial H_{zr}}{\partial y} = 0 \quad \text{in } \Omega, \quad (5.20b)$$

$$-\omega (\varepsilon_r E_{yi} + \varepsilon_i E_{yr}) + \frac{\partial H_{zr}}{\partial x} = 0 \quad \text{in } \Omega \quad (5.20c)$$

$$\frac{\partial E_{xr}}{\partial x} + \frac{\partial E_{yr}}{\partial y} = 0 \quad \text{in } \Omega, \quad (5.20d)$$

$$\omega \mu H_{zr} + \frac{\partial E_{yi}}{\partial x} - \frac{\partial E_{xi}}{\partial y} = 0 \quad \text{in } \Omega, \quad (5.20e)$$

FIG. 1. (a) The split cylinder and the mesh. (b) Contours of constant magnetic field intensity H_r . (c) Contours of constant magnetic field intensity H_i . (d) Vectors of the computed electric field intensity \mathbf{E}_r . (e) Vectors of the computed electric field intensity \mathbf{E}_i .



$$\omega(\varepsilon_r E_{xr} - \varepsilon_i E_{xi}) - \frac{\partial H_{zi}}{\partial y} = 0 \quad \text{in } \Omega, \quad (5.20f)$$

$$\omega(\varepsilon_r E_{yr} - \varepsilon_i E_{yi}) + \frac{\partial H_{zi}}{\partial x} = 0 \quad \text{in } \Omega, \quad (5.20g)$$

$$\frac{\partial E_{xi}}{\partial x} + \frac{\partial E_{yi}}{\partial y} = 0 \quad \text{in } \Omega. \quad (5.20h)$$

Of course, in (5.20) the medium properties are different for different medium regions.

At the interface Γ_{int} between two contiguous media (+) and (−) the following general conditions should be satisfied:

$$\mathbf{n} \times \mathbf{E}^+ = \mathbf{n} \times \mathbf{E}^- \quad \text{on } \Gamma_{\text{int}}, \quad (5.21a)$$

$$\mathbf{n} \times \mathbf{H}^+ = \mathbf{n} \times \mathbf{H}^- \quad \text{on } \Gamma_{\text{int}}, \quad (5.21b)$$

$$\mathbf{n} \cdot (\varepsilon^{*+} \mathbf{E}^+) = \mathbf{n} \cdot (\varepsilon^{*-} \mathbf{E}^-) \quad \text{on } \Gamma_{\text{int}}, \quad (5.21c)$$

$$\mathbf{n} \cdot (\mu^+ \mathbf{H}^+) = \mathbf{n} \cdot (\mu^- \mathbf{H}^-) \quad \text{on } \Gamma_{\text{int}}. \quad (5.21d)$$

For two-dimensional TE waves the interface condition (5.21d) is automatically satisfied and (5.21b) becomes

$$H_z^+ = H_z^-.$$

In the LSFEM the treatment of the interface conditions is not difficult. As in other node-based finite element methods, the nodes on the interface should be double-numbered. If a direct solver is employed for solving the discretized system, two approaches are available: a simple way is to include the interface conditions into the least-squares functional; a better way is to use the conditions (5.21a)–(5.21d) to modify the global stiffness matrix in the discretized system. If the conjugate gradient method is used, one just simply chooses the unknowns related to the medium (+) (or (−)) as the true unknowns and keeps the conditions (5.21a)–(5.21d) satisfied for each solution vector.

Since the general formulation of the LSFEM has been given in Section 5.1, it is not necessary to write down the special one for the problem discussed in this section. One only needs to substitute the coefficients of (5.20) and the boundary conditions into a general-purpose LSFEM code.

We consider two test problems that are taken from Paulsen and Lynch [48]; see also Jin [27, p. 167], in which the spurious solutions given by the curl–curl formulation as well as the correct solutions are illustrated.

The first example is a cylinder ($R = 25$) which is split into two regions having different complex permittivity. For the top region, $\varepsilon_r^+ = 3.0$, $\varepsilon_i^+ = -5.0$, and $\mu^+ = 1.0$; for the bottom region, $\varepsilon_r^- = 1.0$, $\varepsilon_i^- = 0.0$, and $\mu^- = 1.0$. This cylinder is excited by a uniform $H_z|_{\Gamma} = (1, 0)$ (with $\omega = 0.05$) imposed on the outer boundary. All variables in this problem are discretized by 932 bilinear elements with 1016 nodes shown in Fig. 1(a). The one-point Gaussian quadrature is used for evaluating the element matrices. The contours of the computed real and imaginary magnetic field intensity are shown in Figs. 1(b) and (c), respectively. The vector plots of the real and imaginary electric field intensity are illustrated in Figs. 1(d) and (e), respectively.

In the second example, a smaller off-center cylinder ($R = 0.1$) is embedded in a larger cylinder ($R = 0.25$). The material properties for the outer region are $\varepsilon_r^+ = 0.0981$, $\varepsilon_i^+ = -0.0196$, and $\mu^+ = 1.0$; for the inner region $\varepsilon_r^- = 1.0$, $\varepsilon_i^- = 0.0$, and $\mu^- = 1.0$. A uniform $H_z|_{\Gamma} = (1, -0.15)$ (with $\omega = 44.7$) is imposed on the outer boundary. Figure 2(a) shows the mesh with 2027 bilinear elements and 2165 nodes. The contours of the computed real and imaginary magnetic field intensity are shown in Fig. 2(b, c), respectively. The vector plots of the real and imaginary electric field intensity are illustrated in Fig. 2(d, e), respectively.

As expected all computed results by the LSFEM are free of spurious modes.

6. CONCLUSIONS

(1) The system of the first-order full Maxwell equations seems “overdetermined,” because it has more equations than unknowns. By taking into account of its div–curl structure and introducing the dummy variables it proves to be properly determined and elliptic in the space domain. The information provided by the divergence equations is not completely contained in the curl equations. Therefore, the divergence equations must be explicitly included in the first-order system to assure the uniqueness of the solution in steady-state cases, to exclude the infinite degenerate eigenvalue in time-harmonic cases and to guarantee the accuracy of the numerical solution for time-varying cases.

(2) The least-squares method and the div–curl method are mathematically rigorous and useful tools for the derivation of correct second-order Maxwell’s equations and their boundary conditions. The curl–curl equations cannot stand alone, they must be supplemented by the divergence equations and additional natural boundary conditions to eliminate the spurious solutions.

FIG. 2. (a) The off-center cylinder. (b) Contours of constant magnetic field intensity H_r . (c) Contours of constant magnetic field intensity H_i . (d) Vectors of the computed electric field intensity \mathbf{E}_r . (e) Vectors of the computed electric field intensity \mathbf{E}_i .

(3) The Helmholtz-type equations with appropriate natural boundary conditions, derived by the div-curl method or the least-squares method, can guarantee the implicit satisfaction of the divergence equations. For the solution of the Helmholtz-type equations the divergence conditions of the electric field and the magnetic field need to be enforced only on the electric wall and the magnetic symmetry wall, respectively.

(4) The variational formulation corresponding to the Helmholtz-type equations can be derived by using the least-squares look-alike method. This formulation theoretically justifies that the penalty parameter in the Galerkin/penalty method should be taken as one. The advantage of this formulation is that the trial and test functions need only to satisfy the conditions related to the essential boundary conditions.

(5) The node-based least-squares finite element method (LSFEM) can be used to solve both static and time-varying first-order Maxwell equations directly and efficiently with the divergence equations satisfied easily. The introduction of vector potentials and the gauging method, the edge element method, the staggered grid, up-winding, and non-equal-order elements, etc. all turn out to be unnecessary.

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