Second-Order Procedure for Modeling Dielectric Material Interfaces in Structured Nonorthogonal Finite-Difference Discretizations of Maxwell’s Equations

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Abstract—Structured nonorthogonal finite-difference discretizations of Maxwell’s equations are often employed to incorporate curved dielectric material interfaces. As part of this process, it is necessary to employ an adequate procedure to enforce the tangential field continuity conditions at the locations of the interfaces where the components of the permittivity tensor are discontinuous. This contribution proposes a second-order domain-splitting procedure that can accomplish this task without assuming that the permittivity tensor components are piecewise constant or diagonal. As explained, this feature is needed to exploit the full geometrical flexibility of structured grid generation. The proposed procedure consistently yields a global error that is second-order accurate even in extreme cases where the components of the permittivity tensor have a change of sign or a sharp jump.

Index Terms—finite difference methods, Maxwell’s equations, interface phenomena, eigenvalues and eigenfunctions.

I. INTRODUCTION

Due to the fact that finite-difference discretizations of Maxwell’s equations are usually derived using the Cartesian coordinate system, they are sometimes viewed as poorly suited to model structures with curved material interfaces. In any given coordinate system, the easiest way to specify the surfaces that represent material interfaces is by employing coordinate surfaces. In other words, by employing surfaces specified by equations of the form

\[ u^q = \text{constant} \quad \text{for} \quad q = 1, 2, 3 \]  

where \( u^q \) stands for the spatial coordinates of a general curvilinear coordinate system in 3-D. Since the coordinate surfaces of the Cartesian coordinate system are flat sheets that intersect at right angles, the Cartesian coordinate system is well suited to model structures with rectangular material interfaces and poorly suited to model structures with curved material interfaces. To facilitate the introduction of curved material interfaces, it is thus wise to derive any given discretization of Maxwell’s equations using a general curvilinear coordinate system. This observation was first made by Holland who established the basic template for carrying out a finite-difference discretization of a coordinate invariant representation of Maxwell’s equations in differential form [1]. Over the years, many enhancements have been made to Holland’s initial template [2]–[11]. In the beginning, it was common to resort to crude polyhedral representations of all the material interfaces of a given structure in order to construct the needed covariant and contravariant vector bases [1]–[7]. Subsequently, it was realized that the accuracy with which the covariant and contravariant vector bases are constructed does not have to be tied to the grid cell size used to discretize Maxwell’s equations [8]–[11]. This point was first made by Ward and Pendry [8] who explained that all the material interfaces of a structure can be described through a coordinate transformation

\[ x^p = x^p(u^q) \quad \text{for} \quad p, q = 1, 2, 3 \]  

where \( x^p \) stands for the three Cartesian coordinates. The coordinate transformation can be defined either analytically or numerically, and it is constructed so that all the material interfaces of the problem are specified by coordinate surfaces in the \( u^q \) coordinate system. By constructing a coordinate transformation in this manner, a uniform discretization in the \( u^q \) coordinate system automatically maps onto a structured nonorthogonal discretization in the Cartesian coordinate system where the grid cells conform to the geometry of the material interfaces and boundaries of the problem. When the mapping in (2) is defined analytically, the representation of the material interfaces is exact and the needed covariant and contravariant basis vectors can be constructed exactly. When the mapping in (2) is defined numerically, the set of grid points used to define the mapping must be much denser than the set of field samples used to discretize the partial derivatives in Maxwell’s equations. In this way, the global error will be dominated by the finite-difference approximations rather than by the crudeness of the geometrical representation of the material interfaces. While the explicit introduction of a coordinate transformation was certainly a step forward, nobody has previously discussed what procedure must be employed to enforce the tangential field continuity conditions at the locations of material interfaces. Developing such a procedure is not a trivial matter even for structures that contain only isotropic materials with piecewise constant \( \varepsilon \) and \( \mu \) functions. To explain why, let us consider for a moment structures that contain only such materials. When the permittivity and permeability tensors of a problem with simple materials are projected into components using the Cartesian vector basis, the resulting components have the form

\[ \varepsilon_{mn} = \varepsilon \delta_{mn} \quad \text{and} \quad \mu_{mn} = \mu \delta_{mn} \quad \text{for} \quad m, n = 1, 2, 3 \]  

where \( \delta_{mn} \) is the Kronecker delta. On the other hand, when the permittivity and permeability tensors are projected into components using the contravariant basis vectors associated with the computational coordinate system \( u^q \), the resulting components, \( \varepsilon^{pq} \) and \( \mu^{pq} \), are related to their Cartesian counterparts as follows:

\[ \varepsilon^{pq} = \sum_{m=1}^{3} \sum_{n=1}^{3} \frac{\partial u^p}{\partial x^m} \frac{\partial u^q}{\partial x^n} \varepsilon_{mn} \]  

\[ \mu^{pq} = \sum_{m=1}^{3} \sum_{n=1}^{3} \frac{\partial u^p}{\partial x^m} \frac{\partial u^q}{\partial x^n} \mu_{mn}. \]  

These relations show that, even if \( \varepsilon \) and \( \mu \) are piecewise constant, \( \varepsilon^{pq} \) and \( \mu^{pq} \) are not necessarily piecewise constant or diagonal (i.e. zero for \( p \neq q \)). Consequently, when Maxwell’s equations are discretized and solved in the computational coordinate system, it is necessary to know how to enforce the tangential field continuity conditions at the locations of the discontinuities in \( \varepsilon \) and \( \mu \) without assuming that \( \varepsilon^{pq} \) and \( \mu^{pq} \) are piecewise constant or diagonal. With the exception of the averaging method [12], previously proposed methods to enforce the tangential field continuity conditions have been formulated in Cartesian coordinates under one of the following assumptions: that \( \varepsilon^{mn} \) and \( \mu^{mn} \) have the form given in (3) with piecewise constant \( \varepsilon \) and \( \mu \) functions [13]–[17]; that \( \varepsilon^{mn} \) and \( \mu^{mn} \) are full tensors with piecewise constant components [18]; or that, in order to enforce the tangential field continuity conditions through effective material parameters, a local coordinate transformation is employed where the partial derivatives in (4) and (5) are constant [19]–[21]. As a result, none of the methods in [13]–[21] can be directly applied in the computational coordinate system without severely constraining the properties of \( \varepsilon^{pq} \) and \( \mu^{pq} \). Furthermore, while the averaging method [12] is very easy to apply, its convergence properties can deteriorate significantly whenever there is a change of sign or a sharp jump in \( \varepsilon \) or \( \mu \). Because many structures are modeled using frequency dependent \( \varepsilon \) functions that exhibit sign changes and a broad range of values, it is important to understand the limitations.
of the averaging method and to develop alternatives that perform well under such scenario. This contribution describes a second-order domain-splitting procedure to enforce the tangential field continuity conditions over a material interface where \( \varepsilon^{pq} \) is a full second-rank inhomogeneous tensor with jump discontinuities. With this objective in mind, this manuscript is organized as follows. In Section II, the general procedure to generate a finite-difference discretization of a coordinate invariant representation of Maxwell’s equations in the absence of material interfaces is briefly summarized. Subsequently, in Section III, the proposed domain-splitting procedure to enforce the tangential field continuity conditions on the grid cells adjacent to a dielectric material interface is presented. Finally, in Section IV, the performance of the proposed procedure is evaluated using a simple eigenvalue problem. Since the enforcement of the continuity conditions at a material interface is an issue involving only the spatial derivatives, everything is done in the frequency domain where only the spatial derivatives are present. For conciseness, the frequency and spatial dependence of all quantities is omitted.

II. COORDINATE INVARIANT FINITE-DIFFERENCE DISCRETIZATION OF MAXWELL’S EQUATIONS

To generate a coordinate invariant projection of the differential form of Maxwell’s equations using the covariant \((g_{ij})\) and contravariant \((g^{ij})\) basis vectors associated with the \(u^i\) coordinate system, the procedure outlined in [22] must be followed. For the curl equations, the procedure leads to

\[
\begin{align*}
\frac{1}{\sqrt{g}} \left( \frac{\partial e_s}{\partial u^i} - \frac{\partial e_i}{\partial u^s} \right) &= -j\omega b^p, \\
\frac{1}{\sqrt{g}} \left( \frac{\partial h_i}{\partial u^s} - \frac{\partial h_s}{\partial u^i} \right) &= j\omega d^p
\end{align*}
\]

(6)

(7)

where \( g = \det(g_{ij}) \) and \( g_{ij} \) represents the covariant metric tensor components. The set of free indices \( \{p, q, s\} \) must be equated to the three sets \( \{1, 2, 3\}, \{3, 1, 2\} \) and \( \{2, 3, 1\} \) in order to obtain the three components of the two curl equations. For the constitutive relations, the procedure results in

\[
b_p = \sum_{q=1}^{3} \mu^{pq} h_q \quad \text{and} \quad d_p = \sum_{q=1}^{3} \varepsilon^{pq} e_q.
\]

(8)

The constitutive relations are assumed to be linear, but the materials of the structure can still be lossy, dispersive, inhomogenous and anisotropic. Nevertheless, to avoid ending up with results that are difficult to verify from a physical standpoint, homogeneous isotropic materials are henceforth employed. The permeability and permittivity tensor components that correspond to such properties were already given in (3)-(5). While this simplification facilitates the testing of the proposed domain-splitting procedure, anisotropic and inhomogeneous materials can be introduced simply by inserting the appropriate \( \varepsilon^{mn} \) and \( M^{mn} \) tensors into (4) and (5). When the expressions for \( \varepsilon^{mn} \) and \( M^{mn} \) given in (3) are substituted into (4) and (5), a useful simplification is obtained:

\[
\varepsilon^{pq} = \varepsilon g^{pq} \quad \text{and} \quad \mu^{pq} = \mu g^{pq}
\]

(9)

where \( g^{pq} \) stands for the contravariant metric tensor components. In an effort to balance completeness and conciseness, the proposed domain-splitting procedure is presented in 2-D rather than 3-D. Working in 2-D does not limit the applicability of the proposed methodology to 2-D structures because the 3-D version can be constructed by applying the 2-D version to all the 3-D grid planes that are perpendicular to any given material interface. To introduce a 2-D reduction of (6)-(8), two assumptions are made: that \( x^3 = u^3 \), and that nothing varies along the \( x^3 \)-axis. Under these assumptions, equations (6)-(8) split into two independent sets: the TE\(^3\) and the TM\(^3\). Since both sets are duals of each other, only the TE\(^3\) set is employed hereafter. After eliminating \( d^1, d^2 \) and \( b^1 \), the TE\(^3\) set reduces to the following three equations:

\[
\begin{align*}
\frac{\partial e_2}{\partial u^1} - \frac{\partial e_1}{\partial u^2} &= -j\omega \mu^{33} h_3, \\
\frac{\partial h_3}{\partial u^2} &= j\omega e^{31} e_1 + j\omega e^{32} e_2, \\
\frac{\partial h_3}{\partial u^1} &= -j\omega e^{21} e_1 - j\omega e^{22} e_2
\end{align*}
\]

(10)

(11)

(12)

where \( \mu^{33} = \sqrt{g} \mu^{33} \) and \( \varepsilon^{pq} = \sqrt{g} \varepsilon^{pq} \) for \( p, q = 1, 2 \).

(13)

As long as \( \mu^{33} \) and \( \varepsilon^{pq} \) are smooth, it is straightforward to discretize (10)-(12) using second-order staggered finite-difference approximations; the staggered grid cell structure described in Fig. 1. Since a cavity with perfect electric conductor (PEC) boundaries is used in Section IV to test the proposed domain-splitting procedure, the boundary conditions are understood to be:

\[
e_1 = 0 \quad \text{for} \quad u^2 = 0 \quad \text{and} \quad u^2 = \ell_2; \tag{14}
\]

\[
e_2 = 0 \quad \text{for} \quad u^1 = 0 \quad \text{and} \quad u^1 = \ell_1.
\]

(15)

In the absence of material interfaces, the discretization of (10)-(12) subject to (14) and (15) generates a complete linear system of equations that can be casted into an eigenvalue problem of the form

\[
Mv = \omega Nv
\]

(16)
As implied by (9), a jump in resulting eigenvalues are referred to as the characteristic frequencies.\(\varepsilon\) of this form can be solved using the QZ algorithm [23], and the column vector \(v\) where matrices \(M\) and \(N\) are square, sparse and real, and the column vector \(v\) collects all the field samples. An eigenvalue problem of this form can be solved using the QZ algorithm [23], and the resulting eigenvalues are referred to as the characteristic frequencies. As implied by (9), a jump in \(\varepsilon\) will introduce a jump in \(\varepsilon^{pq}\) for all \(p, q = 1, 2\). Such a discontinuity is needed to model the presence of a dielectric material interface, and it can be incorporated into the discretization process as described in the next section.

III. PROPOSED DOMAIN-SPLITTING PROCEDURE

As pointed out in the Introduction, the coordinate transformation must be constructed so that any discontinuity in the components of \(\varepsilon^{pq}\) occurs over a surface—or, in the 2-D case, a line—described by an equation of the form given earlier in (1). For conciseness, the structure under analysis is assumed to contain a single dielectric material interface along a line described by \(u^1 = \text{constant}\). If the coordinate transformation is constructed carefully, the material interface can always be made to coincide with one of the grid cell boundaries defined by

\[
u^1 = M \Delta u^1 \quad (17)
\]

where \(M\) is an integer in the range \(0 < M < N_1\). By placing this small constraint on the way the coordinate transformation is constructed, the discontinuity in \(\varepsilon^{pq}\) for \(p, q = 1, 2\) always coincides with the grid cell boundary where the \(\varepsilon_{21} |_{M+1/2} j+1/2\) samples are located. Requiring the material interface to line up with the grid cell boundaries facilitates the development of the proposed domain-splitting procedure by preserving the validity of the discrete equations that derive from (10) and (11). Only the discretization that derives from (12) must be modified because

\[
\frac{\partial h_3}{\partial u^1}\bigg|_{u^1 = M \Delta u^1} = \hat{g}.
\]

This follows from the fact that

\[
\lim_{u^1 \to M \Delta u^1} \varepsilon^{2q} \neq \lim_{u^1 \to M \Delta u^1} \varepsilon^{2q} \quad (19)
\]

and that \(\varepsilon^2\) must be continuous across the dielectric material interface. To remedy the fact that \(h_3\) is not differentiable at the interface, the computational domain is partitioned into two separate regions as described in Fig. 2. The cut is made along the line described by (17) so that the ambiguity in the values of the material tensors is removed by assigning the left limit values to the first region and the right limit values to the second region. This strategy is similar to that employed in [13], [17] under a Cartesian coordinate system. In order to create a second-order accurate discretization of (12), one extra column of grid cells is added to the right of the first region and a second extra column of grid cells is added to the left of the second region as illustrated in Fig. 2. The field samples in the newly introduced columns of grid cells are referred to as ghost samples, and they are labeled with tildes in Fig. 2 to distinguish them from the field samples in the original grid. The ghost samples are simply smooth extensions of the electric and magnetic fields profiles that are needed to make \(h_3\) differentiable at the interface. Their role is to act as placeholders for the two different values of the field derivatives that arise from using either the left or the right limits in (19). By making use of the ghost field samples, it is possible to discretize (12) at the material interface knowing that, because the \(h_3\) profile will be smooth in either of the two regions, the resulting finite-difference
Discretizing (22) with (21) substituted into both sides using the field samples from the first region results in
\[
\frac{\hat{h}_3}{M+\frac{1}{2},j+\frac{1}{2}} - \hat{h}_3|_{M-\frac{1}{2},j+\frac{1}{2}} = j\omega \varepsilon_{22} |_{M+j+\frac{1}{2}} + \varepsilon_1 |_{M+j+\frac{1}{2}} + \frac{1}{4} \varepsilon_{11} |_{M+j+\frac{1}{2}} + \frac{1}{4} \varepsilon_{11} |_{M-j-\frac{1}{2}}.
\]
\[
+ j\omega \varepsilon_{21} |_{M,j+\frac{1}{2}} \varepsilon_{12} |_{M,j+\frac{1}{2}} = 0 \quad \text{for} \quad j = 0, 1, \ldots, N_2 - 2.
\]
(20)

A similar discretization can be carried out using the field samples from the second region. Of course, to completely specify the expanded system of equations, the values of the ghost samples in both regions must be linked by the continuity of \( \hat{h}_3 \) and \( \varepsilon_2 \) at the material interface. As shown in Fig. 2, there are three \( \hat{e}_2 \)-samples, two \( \hat{h}_3 \)-samples and two \( \hat{e}_1 \)-samples on each row of grid cells. Consequently, a total of seven independent linking equations are needed to completely specify the expanded system of equations. For conciseness, only one of the linking equations is derived here; the remaining derivations can be found in [22]. To derive the chosen linking equation, both sides of (10) must be first differentiated with respect to \( u^1 \). Substituting (12) into the right hand side of the result and solving for \(-\omega^2 \varepsilon_2\) yields the following expression:

\[
-\omega^2 \varepsilon_2 = \frac{1}{\mu^{33} \varepsilon_{22}} \left( \frac{\partial^2 \varepsilon_{22}}{\partial u^1} - \frac{\partial^2 \varepsilon_{11}}{\partial u^1} \frac{\partial^2 \varepsilon_{22}}{\partial u^2} + \omega^2 \mu^{33} \varepsilon_{22} \varepsilon_{11} + j\omega \mu^{33} \hat{h}_3 \right)
\]
(21)

The continuity of \( \varepsilon_2 \) demands that
\[
\lim_{u^1 \to M \Delta u^{1-}} (-\omega^2 \varepsilon_2) = \lim_{u^1 \to M \Delta u^{1+}} (-\omega^2 \varepsilon_2)
\]
(22)

Discretizing (22) with (21) substituted into both sides using the field samples in the first region to discretize the partial derivatives associated with the left limit and the field samples in the second region to discretize the partial derivatives associated with the right limit at the point \((M \Delta u^{1}, j + 1/2)\) using second-order finite-difference approximations leads to an equation linking the ghost field samples in both regions. As mentioned earlier, the averaging procedure is the only previously proposed procedure to enforce the tangential field continuity conditions at the location of a material interface that can be applied to a coordinate invariant projection of Maxwell’s equations. The averaging procedure does have the advantage of being easy to implement; however, the averaging procedure discretizes (12) directly using averaged \( \hat{e}_{11}^{33} \) and \( \varepsilon_{12}^{32} \) values without acknowledging that, because of the lack of differentiability of \( h_3 \) with respect to \( u^1 \) at the interface, the local truncation error of the resulting finite-difference expression is undefined. As a result, the convergence properties of the averaging procedure are unpredictable. In fact, whenever \( e \) changes sign or has a sharp jump across a dielectric material interface, the global error performance can deteriorate significantly. To demonstrate this, the performance of the averaging procedure is compared with that of the proposed domain-splitting procedure in the next section using the partially filled PEC cavity described in Fig. 3.

To document the effect of introducing a sign change or a sharp jump in \( e \), the dielectric material that fills the second half of the cavity was given the six different \( \varepsilon_r \) values shown in Fig. 3. The vacuum-dielectric interface can be analyzed as described in Section III by employing the following 2-D coordinate transformation:

\[
x^1 = u^1 \left( 1 + \frac{1}{12} \sin \left( \frac{\pi}{\ell_1} u^1 \right)^3 \cos \left( \frac{\pi}{\ell_2} u^2 \right) \right)
\]
(23)

\[
x^2 = u^2 \left( 1 + \frac{1}{6} \cos \left( \frac{\pi}{\ell_1} u^1 \right) \sin \left( \frac{\pi}{\ell_2} u^2 \right)^3 \right)
\]
(24)

where \(0 \leq u^1 \leq \ell_1\) and \(0 \leq u^2 \leq \ell_2\). To visualize the geometric properties of this coordinate transformation, coordinate line plots are provided in Fig. 4. Because the line \( u^1 = \ell_1/2 \) describes the vacuum-dielectric interface, the material tensor components are simply

\[
\varepsilon_{pq} = \begin{cases} e_0 g_{pq}^0, & u^1 < \ell_1/2 \\ e_0 e_r g_{pq}^r, & u^1 > \ell_1/2 \end{cases} \quad \text{for} \quad p, q = 1, 2
\]
(25)

and \(\mu^{23} = \mu_0\). For all six \( e_r \) cases, the eigenvalue problem was solved for the smallest \( \omega \) for which \( e_1, e_2 \) and \( h_3 \) are all nonzero. To keep a balanced grid aspect ratio, the number of grid points were constrained so that \( N_1 = 2N + 1 \) and \( N_2 = N + 1 \) where \( N \) is an even positive integer. By making \( N \) even, the discontinuity in the material tensors always lies along the grid cell boundary defined by \( u^1 = N \Delta u^1 = \ell_1/2 \). To evaluate convergence rates, coarse \((N = 16, 20, 24)\), medium \((N = 32, 40, 48)\), dense \((N = 64, 80, 96)\) as well as very dense \((N = 128)\) grids were employed. To measure the
global error, normalized energy norms of \( \epsilon_1, \epsilon_2 \) and \( h_3 \) are employed. More specifically,

\[
\| \hat{h}_3 \|_2 = \sqrt{\int_0^{\xi_1} \int_0^{\xi_2} |h_3 - \hat{h}_3|^2 \, du^1 \, du^2}
\]

(26)

where \( h_3 \) is a very accurate reference value and \( \hat{h}_3 \) the numerical estimate obtained by solving the eigenvalue problem in (16) for a given \( N \). When Maxwell’s equations are discretized using finite-difference approximations with a second-order local truncation error, the hope is that

\[
\| \hat{\epsilon}_1 \|_2, \| \hat{\epsilon}_2 \|_2 \quad \text{and} \quad \| \hat{h}_3 \|_2 \propto \frac{1}{N^2} \quad \text{where} \quad R \approx 2.
\]

(27)

To obtain an estimate of \( R \)—which is also known as the order of accuracy—it is useful to plot the aforementioned energy norms as a function of \( N \) using a logarithmic scale. Such plots are given in Fig. 5 for the proposed domain-splitting method and in Fig. 6 for the averaging method. An estimate of \( R \) can then be obtained from a linear least-squares fit to

\[
\begin{align*}
R_1 &= - \log_{10} \left( \frac{\| \hat{\epsilon}_1 \|_2}{\log_{10}(N)} \right) \\
R_2 &= - \log_{10} \left( \frac{\| \hat{\epsilon}_2 \|_2}{\log_{10}(N)} \right) \\
R_3 &= - \log_{10} \left( \frac{\| \hat{h}_3 \|_2}{\log_{10}(N)} \right)
\end{align*}
\]

(28)-(30)

by choosing

\[
R = \min\{R_1, R_2, R_3\}.
\]

(31)

Fits for (28)-(30) are given in Figs. 5 and 6 for each of the six \( \epsilon_r \) cases under consideration. From these fits, it is easy to see that the proposed procedure produces a much more consistent convergence performance than the averaging procedure, and, with the exception of the case \( \epsilon_r = -1 \), the proposed procedure always leads to second-order convergence \( (R \approx 2) \). For the particular case \( \epsilon_r = -1 \), the cavity is difficult to analyze with coarse discretizations due to the sharp features present in the solution, which is shown in Fig. 7. Nonetheless, for dense discretizations \( (N \geq 64) \), the proposed domain-splitting procedure does exhibit a second-order convergence behavior.

V. CONCLUSION

In summary, a domain-splitting procedure to enforce the tangential field continuity conditions at the location of a dielectric material interface has been presented. Unlike previously proposed alternatives, the proposed procedure was formulated assuming that the permittivity tensor is a full second-rank inhomogeneous tensor with jump discontinuities at the location of the interface. Such feature is needed in order to exploit the full geometrical flexibility of structured grids. The proposed procedure consistently leads to second-order convergence even in extreme cases where the \( \epsilon^{\text{pp}} \) components have a change of sign or a sharp jump. As demonstrated, the proposed domain-splitting procedure consistently outperforms a simple averaging procedure, which is the most commonly employed alternative.

REFERENCES


