Interfacial Numerical Dispersion and New Conformal FDTD Method

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Abstract

This article shows the interfacial relation in electrodynamics shall be corrected in discrete grid form which can be seen as certain numerical dispersion beyond the usual bulk type. Furthermore we construct a lossy conductor model to illustrate how to simulate more general materials other than traditional PEC or simple dielectrics, by a new conformal FDTD method which main considers the effects of penetrative depth and the distribution of free bulk electric charge and current.

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1 Introduction

Bulk dynamics and boundary conditions are two essential ingredients for solving a concrete physical problem. In computational electromagnetic, it is well known finite difference form of wave equation in bulk leads to numerical dispersion which is measured by the factor $\frac{\sin x}{x}$, where $x$ is proportional to the grid size. If the grid length is smaller than $\frac{\lambda}{12}$, then the dispersive factor approximates to 1 which means the error due to this numerical dispersion can always be ignored in problem. However, beyond this traditional bulk numerical dispersion (BND), we find discrete process in simulation as in Finite-Difference Time-Domain (FDTD) approach also generates certain unphysical anti-dispersion effects on the boundary which can be defined as the interfacial numerical dispersion (IND). If we ignore this effect, we shall get the staircase approximation grid representation of the curved boundary, which is just one of the shortcomings of traditional FDTD method. Instead, we find interfacial relation in usual electrodynamics must be corrected in grid variable form due to IND, and some treatments in conformal FDTD method before as in perfect electric conductor (PEC) or dielectric materials can be seen as special cases of the new relation.

Traditional conformal FDTD (CFDTD) often deal with PEC [1-10] and simple dielectrics [11-15]. In former case, the electric field in material can be ignored due to the penetrative depth is far less than one grid length due to the lossy parameter $p = \sigma \varepsilon \omega \gg 1$ and in later case simple denote near lossless, i.e. $p = \sigma \varepsilon \omega \ll 1$.

For general dispersive and lossy media like Lorentz model, the related Conformal FDTD approach is difficult due to the permittivities in the interfacial relation involve complex dependence of the frequency and in corresponding time-domain algorithm this shall turns to be involve with high order time derivatives.

However, for a large class of lossy dielectrics, whose penetrative depth $\delta$ is between PEC and perfect electric insulator (PEI), more exactly in which the lossy parameter $p = \sigma \varepsilon \omega \sim 1$ or the $\delta$ is about several grids' length, if we can ignore the influence of the resonance frequency in the problem or the involved electromagnetical frequency is far away from the material resonance frequencies, we can use certain conductivity model as the dispersive model and get a (theoretical) more effective CFDTD method called lossy conductor CFDTD (LCCFDTD), which consider the effects of IND, surface/volume free electric current/charge, penetrative depth and conformal angle (defined as the angle between the cross-section of interface and the grid line) in more physical way. Especially our method is more suitable for the FDTD simulation of the problems like the design of microwave dark chamber with strong absorber materials.
2 Grid representation of interfacial relation

Consider the 2-dimensional TE case below without loss of generality. First we define the angle $\theta$ between the tangent line at the interfacial point and the grid line as the conformal angle. The grid line at the boundary is divided into two parts on which two electric fields is uniform distributed as $E$ in air and $E'$ in materia. General case of arbitrary two medias is similar.

For PEC model, the inside field can be assumed to be vanished. But for general materials or even as in nondispersive, lossless dielectrics, to obtain a conformal algorithm instead of naive staircase approximation, we have to discuss the interfacial relation between $E$ and $E'$. In continuous electrodynamics theory we have following boundary relations:

\begin{align}
E_n &= E'_n \\
H_n &= H'_n + \alpha \\
D_\perp &= D'_\perp + \rho \\
B_\perp &= B'_\perp
\end{align}

where $\alpha$ is line density of free surface electrical current and $\rho$ is surface density of free electrical charge. Here we only consider the simplest case in which $\alpha, \rho$ vanish and permittivity is a real const. In next section we may show how to deal with nonzero $\alpha, \rho$ and complex permittivity for a more general model of materials.

As we know, for certain frequency only two of above interfacial relations are independent and here we use (1) (3), i.e.

\begin{align*}
E_n &= E'_n, \quad E_\perp = \varepsilon_r E'_\perp, \quad \varepsilon_r = \varepsilon/\varepsilon_0.
\end{align*}

This interfacial relation indicate $E, E'$ can’t be along same direction through the interface, i.e. the refraction phenomena exist or for general case if the permittivity as function of the frequency, electromagntical waves of different frequency shall refract to different directions, i.e. dispersive phenomena appears. However, in discrete grid simulation, $E, E'$ have to be along same grid line and this in fact introduces extra error. Like the discrete treatment for wave equation in bulk will produces numerical dispersion, the effect of this elimination of physical refraction or dispersion on interface due ro simulation method as FDTD can be seen as certain interfacial numerical dispersion (IND). Hence we should take one of two fields on the same boundary grid line as projection of the refraction field along the grid line, take $E$ for instance and the relation between $E, E'$ give the grid representation of physical interfacial relation (1), (3).
By a simple geometrical analysis indicated by figure 1 above, we find this grid interfacial relation,

\[ E = (\cos^2 \theta + \varepsilon_r \sin^2 \theta)E' = \varepsilon_r(\theta)E'. \]  

(5)

It’s direct to see several special correct results. First take \( \varepsilon_r = 1 \) i.e. for grid in same materia, \( E = E' \) as our basic assumption in simulation. Second, consider \( \theta = 0 \), i.e. the coincident case of grid choice, \( E = E' \), as same as traditional FDTD. Third, if \( \theta = \frac{\pi}{2} \), as the translation case for coincident grid choice, we get \( E = \varepsilon_rE' \) or equivalently as \( E_{\|} = E'_{\|} = 0, \ D_{\perp} = D'_{\perp} \).

3 Lossy conductor model and conformal FDTD

To deal with more general materials as needed in most applications, we construct a lossy conductor model and for simplicity, we assume the boundary of materia is flat, i.e the tangent line at the interfacial point is coincident with the boundary. New model main considers a reasonable generalization of the surface distribution of free electric charge and current in well conductor model (WEC) via a special discrete treatment.

First we introduce a kind of lossy conductor conformal grid (LCCG), and take a 2-dimensional cross-section of a rotated planar interface for example as figure 2 shows. Except usual field nodes, this grid have four material points \( a, b, c, d \) and a new grid parameter \( B \) called grid penetrative number. For the grid outside of the material \( B = 0 \) and on the geometrical boundary of media \( B = 1 \). For the grids in the material, \( B = \min([D_i/ds])+1 \), where \( D_i \) is the distance between the grid’s center node and the tangent line of interface, \([x]\) is the maximal integer less than \( x \), \( ds \) denote the size of grid. In fact we can take its relative coordinate of the nearest interfacial grid as its \( B \) value.

Only two material points in a grid are independent which are determined by the dividing character of the boundary grids, while other two points if needed can be obtained via translation of the line which connects the two independent points as figure 2 shows. In fact like
The traditional subgrid method which introduces four field nodes in a grid to construct the relative small grids, our new conformal method also consider new sub nodes which describe the geometry of material boundary and this process don’t introduces new field nodes to increase the complexity of computation.

The start point of conformal method is the integrated form of Maxwell equation below:
\[
\frac{\partial}{\partial t}\int_S \mu H \cdot dS = -\oint_{\partial S} E \cdot dl.
\] (6)

For the case of figure 2, by discretion of above equation we have iterated equation for magnetic field \(H\),
\[
H^{n+\frac{1}{2}}(i,j) = H^{n-\frac{1}{2}}(i,j) + \frac{\Delta t}{\mu S(i,j)} \left\{ E_x^n(i,j + \frac{1}{2})l_x(i,j) + E_y^n(i,j + \frac{1}{2})l_y'(i,j) \right. \\
- E_x^n(i,j - \frac{1}{2})l_x(i, j - 1) - E_y^n(i,j - \frac{1}{2})l_y'(i, j - 1) \\
+ E_y^n(i - \frac{1}{2},j)l_y(i - 1, j) + E_x^n(i - \frac{1}{2},j)l_x'(i - 1, j) \\
- E_y^n(i + \frac{1}{2},j)l_y(i,j) - E_x^n(i + \frac{1}{2},j)l_x'(i,j) \right\}
\]

Note we can just take some terms in above formula to be zero for other cases of division. In the situation of figure 2, we also have some constraints on the length variables due to two independent material points in a grid,
\[
l'_y(i,j) = l'_y(i - 1, j), \quad l'_y(i,j - 1) = l_x(i,j) \cdot \frac{l_y'(i,j)}{l_y(i - 1, j)}, \\
l_x + l'_x = \Delta x, \quad l_y + l'_y = \Delta y; \quad \frac{l_T(i,j)}{l_T(i,j)} = \frac{l_y(i,j)}{l_y'(i,j)}.
\]

It’s easy to see that the usual PEC conformal algorithm is just as the special case for which \(S(i,j)\) denote the area of the outside cell and
\[
E_x(i,j + \frac{1}{2}) = E'_x(i,j + \frac{1}{2}), \quad E_y(i - \frac{1}{2},j) = E'_y(i - \frac{1}{2},j); \\
E_x(i,j - \frac{1}{2}) = 0, \quad E'_y(i + \frac{1}{2},j) = 0.
\]

By the symmetry of electric grids and magnetic grids in FDTD method, it’s not necessary to do conformal treatment for electric grids, i.e. the iteration of electrical field is same as in traditional FDTD which is just by discretion of another Maxwell integrated equation:
\[
\oint_{\partial S} H \cdot dl = \frac{\partial}{\partial t}\int_S D \cdot ds + \int_S J \cdot ds.
\]

Note in our lossy conductor model, the conductivity \(\sigma\) is not zero which require the term of free electric current.

To deal with the effects of the free electric charge and penetrative depth, we take a special discrete treatment for the distribution of free
bulk electric current in our grid system, which assumes the free electric charge only distribute uniformly on the transverse grid line \( l_T \) and the electric current just conduct along the perpendicular direction of the grid plane. Thus no electric charge and current on the grid line in our model and especially the transverse line \( l_T \) in one grid just denote the unit transverse line which appears in the definition of free surface electric current \( \alpha \) in (2).

By a simple deduction like for the lossless model, we can get the generalization of formula (5) in lossy conductor model,

\[
E = (\cos^2 \theta + \left( \varepsilon_r - \frac{\sigma_r}{j\omega} + \frac{|\alpha|}{\varepsilon_0 v E'_\perp} \right) \sin^2 \theta) E' \\
= (\cos^2 \theta + \varepsilon_r \sin^2 \theta) E' - \varepsilon_r(\theta) E'.
\]

where \( |\alpha| = \sigma E' l_T \) as the electric current through the unit transverse line \( l_T \) and \( v \) is the velocity of the electromagnetical wave in the material and clearly \( v = \frac{c}{\sqrt{\varepsilon_r \mu_r}} \), where the refraction lossy parameter

\[
L = \sqrt{\frac{1 + \sqrt{1 + p^2}}{2}}, \quad p = \frac{\sigma_r}{\varepsilon_r \omega}, \quad \sigma_r = \sigma / \varepsilon_0.
\]

Finally we obtain the grid interfacial relation of lossy conductor model:

\[
E = (\cos^2 \theta + \left( \varepsilon_r - \frac{\sigma_r}{j\omega} + \frac{l_T \sigma_r \sqrt{\varepsilon_r \mu_r} L \sin \theta}{c \sin \theta} \right) \sin^2 \theta) E' \quad (7)
\]

To apply above formula in conformal FDTD scheme, we have to make some approximations and furthermore turn it to the iteration relation in time domain.

- **Half order and IND corrected approximation (HIND):** \( l_T = 0 \) (ignore the distribution of free electrical current)

\[
E = (\cos^2 \theta + \left( \varepsilon_r - \frac{\sigma_r}{j\omega} \right) \sin^2 \theta) E' \quad (8)
\]

\[
\frac{\partial E}{\partial t} = (\cos^2 \theta + \varepsilon_r \sin^2 \theta) \frac{\partial E'}{\partial t} - \sigma_r \sin^2 \theta \cdot E'. \quad (9)
\]

- **First order and IND corrected approximation (FIND):** \( l_T \neq 0, \quad L \approx 1 \)

\[
E = (\cos^2 \theta + \left( \varepsilon_r - \frac{\sigma_r}{j\omega} + \frac{l_T \sigma_r \sqrt{\varepsilon_r \mu_r}}{c \sin \theta} \right) \sin^2 \theta) E' \quad (10)
\]

\[
\frac{\partial E}{\partial t} = (\cos^2 \theta + \left( \varepsilon_r + \frac{l_T \sigma_r \sqrt{\varepsilon_r \mu_r}}{c \sin \theta} \right) \sin^2 \theta) \frac{\partial E'}{\partial t} - \sigma_r \sin^2 \theta \cdot E'. \quad (11)
\]

- **Second order and IND corrected approximation (SIND):** \( l_T \neq 0, \quad L \approx 1 + \frac{p^2}{8} \)

\[
E = (\cos^2 \theta + \left( \varepsilon_r - \frac{\sigma_r}{j\omega} + \frac{l_T \sigma_r \sqrt{\varepsilon_r \mu_r}}{c \sin \theta} \right) \sin^2 \theta) E' \quad (12)
\]

\[
\frac{\partial^2 E}{\partial t^2} = (\cos^2 \theta + \left( \varepsilon_r + \frac{l_T \sigma_r \sqrt{\varepsilon_r \mu_r}}{c \sin \theta} \right) \sin^2 \theta) \frac{\partial^2 E'}{\partial t^2} - \sigma_r \sin^2 \theta \cdot \frac{\partial E'}{\partial t} - \frac{l_T \sigma_r \sqrt{\varepsilon_r \mu_r}}{8c^2 \sin^2 \theta} \sin \theta E'. \quad (13)
\]
• Geometric boundary conformal FDTD:

Only consider above conformal treatment for the geometrical boundary grid in which $B = 1$. Thus in the iteration equation of magnetic field we have

$$E_x(i, j - \frac{1}{2}) = E'_x(i, j - \frac{1}{2}), \quad E_y(i + \frac{1}{2}, j) = E'_y(i + \frac{1}{2}, j)$$

and $E_x(i, j + \frac{1}{2}), \quad E_y(i - \frac{1}{2}, j)$ can be determined by $E'_x(i, j + \frac{1}{2}), \quad E'_y(i - \frac{1}{2}, j)$ via the discrete form of the equation (9), (11) and (13). For $B > 1$, we set $E = E'$ which means we have ignored the effect of penetrative depth in this scheme.

• Penetrative boundary conformal FDTD:

Consider above conformal treatment for the penetrative boundary grid in which $1 \leq B \leq \lfloor \frac{\delta}{\Delta l} \rfloor, \quad \Delta l = \min(\Delta x, \Delta y)$. For such grids we get all $E$ from $E'$ via discrete form of (9), (11) and (13). The grid with $B = \lfloor \frac{\delta}{\Delta l} \rfloor + 1$ will be treated as geometric boundary grid while for $B > \lfloor \frac{\delta}{\Delta l} \rfloor + 1$ we just set $E = E'$. Especially for PEC case, $\lfloor \frac{\delta}{\Delta l} \rfloor = 0$ and $E' = 0$ as in traditional way.

Although the penetrative depth $\delta$ is an important physical quantity which can be determined by the electromagnetic parameters of the material exactly, we can take it as an adjustable parameter called lossy depth $\delta_l$ for practical use. It can be set by the precision and cost of computation in a problem and penetrative depth $\delta$ could just be its default value.

4 Discussion

We know electrodynamics manifest Lorentz symmetry or Maxwell equations in continuous spacetime is covariant under the translation and rotation, while in discrete grid spacetime such Poincare symmetry is broken. For flat boundary material, we find formula (5) considers the exact effect of conformal angle in the interfacial relation such that the simulation physical result is independent of grid system in the sense of global translation and rotation, or in other words for flat boundary case the shape of material in simulation is invariant of grid translation and rotation which is more physical unlike in traditional FDTD. In this manner we could say our IND corrected conformal FDTD have restored certain 3-dimensional space symmetry and especially it manifests the consistence between the conformal and nonconformal algorithm.

There are several directions to generalize above section’s result.

First, if the boundary is curved, the tangent line at the interfacing point shall not be along $l_T$. One simple way to deal with this case is to define the angle between the tangent line and transversal line $l_T$ as relative conformal angle $\theta_r$ and the conformal angle still to be the one between $l_T$ and the grid line. If $\theta_r \leq \frac{\pi}{2}$, such boundary’s treatment can be approximated by transversal line boundary as done in previous, while $\theta_r > \frac{\pi}{2}$, we’d better approximate the boundary in this direction by the complete grid line, i.e. $E = E'$. 7
Second, our LCCFDTD method only considers the electrical loss, it seems the magnetic loss and some special anisotropy or nonlinear or dispersive medias also can be treated in similar way [16]. It may also have applications in other numerical computational areas.

Finally, we may consider the stability problem as in traditional conformal FDTD method [17-18] and an improved absorb boundary may be obtained by the combination of a large lossy conductor material and the ideas of PML. Of course all above discussions are main in theoretical manner and it can be verified by some numerical experiments. The results may be similar with [14], i.e. the simulation of rotated problem should has good agreement with the coincidence problem as reference solution.

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