Demonstration and Suppression of Numerical Divergence Errors in FDTD Analysis of Practical Microwave Problems

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ABSTRACT – Field divergence emulation in FDTD is revisited, and new theoretical aspects as well as problems of practical importance are revealed and resolved. Various choices of divergence definition are discussed in terms of their predictive power. It is shown that total FDTD solutions inevitably violate Gauss law in dipole radiation or eigenvalue analysis. The theory of S- and P-eigenmodes is applied to understand these problems and to restore their physical solutions. Recipes for extracting correct radiation efficiency, radiation resistance, Q-factors and modal field patterns in the presence of P-modes are proposed.

I. Introduction

Over the last two decades, the FDTD method has attracted an impressive research effort, resulting in a plethora of FDTD software packages used in microwave research and engineering practice. An important rationale behind the FDTD success, and its important asset with respect to the more classical FEM, reside in the remarkable immunity to spurious modes. This can be traced back to the divergence conservation on the FDTD meshes. Thus, studies of FDTD dispersion relations (e.g.[1]..[3]) and divergence properties [4][5] are of practical importance.

The present paper contains a critical review of earlier works on the subject, reveals previously unknown divergence-violation phenomena in FDTD applications involving punctual sources, explains earlier noticed but unexplained FDTD errors, and proposes simple recipes for restoring the physical results.

II. Divergence Definitions in FDTD

While dispersion properties of FDTD eigensolutions have been investigated by many authors, e.g.[1]..[3], the properties of the resulting FDTD eigenmodes, and their divergence properties in particular, have attracted less attention [1][4][5]. With reference to Fig.1, it has been shown that the flux of *E*-fields (marked by thick arrows) through any dual cell surface (as that dashed) remains constant in time. The reasoning behind is, that if a certain *H*-field component enters an FDTD update equation of one *E*-field on one of the dual cell walls, then it also enters the update equation of another *E*-field on another wall, with an opposite sign. For example, H_z at (1.5,0.5,1) in Fig.1 will influence both E_x at (1.5,1,1) and E_y at (1,0.5,1). Based on this observation, FDTD has been claimed to conserve the numerical divergence, and hence to emulate non-divergent physical modes.

Herein we will show that both conclusions become incorrect in certain cases because they have been based on insufficient premises:

Firstly, a hypothetical FDTD system without any excitation has been considered, while in all practical problems we need to include sources. Let us imagine applying a point source to E_x at (1.5,1,1); this field will now be increased without a corresponding change in E_y at (1,0.5,1). Hence, numerical divergence will be violated.

Secondly, only the *total* divergence has been investigated so far. It is known from earlier work on FEM [6] that a *total* non-divergent solution may comprise a *physical* mode erroneously emulated with non-zero divergence, and a compensating *spurious* mode. Hence, individual treatment of FDTD eigenmodes is needed to ensure that the propagating modes will not be corrupted with non-zero divergence, if imposed e.g. by a punctual source.

We have started a systematic study of FDTD eigenmodes in [7]. A complete dispersion relation has been derived in the following factorised form:

$$P(\omega\Delta t)\ S(\omega\Delta t, \beta_x a, \beta_y a, \beta_z a) = 0 \qquad (1)$$

where:

$$P(\omega\Delta t) = \sin^2(0.5\omega\Delta t) \qquad (2)$$

$$S(\omega\Delta t, \beta_x a, \beta_y a, \beta_z a) = [-r^2 \sin^2(0.5\omega\Delta t) + \sin^2(0.5\beta_x a) + \sin^2(0.5\beta_y a) + \sin^2(0.5\beta_z a)]^2 \qquad (3)$$

Please note that eq.(1) differs from the classically presented FDTD dispersion relations [1]..[3] by revealing the P-term, responsible for the static potential mode.

The properties of P- and S-modes can now be studied independently of each other, by enforcing their respective modal dispersion relations (2) and (3) into the matrix representation of FDTD, given by eq.(8) in [7]. In particular, it can be proven that:

- S-modes are always emulated with zero divergence,
- P-modes are emulated with zero curl, but may have non-zero divergence.

Such separate evaluation of *modal* divergence allows us to predict the nature of field disturbances caused by punctual sources. We claim that any such disturbances will take the form of non-propagating P-modes. In Sections III and IV we shall further study the P-modes in radiation and eigenvalue problems.

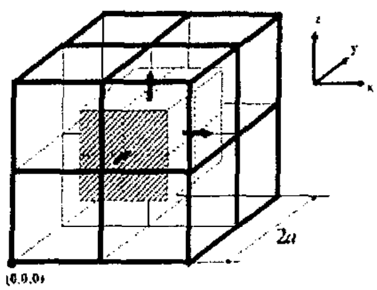

Fig.1. A cluster of eight FDTD cells with one centred dual cell for E-field divergence definition.

However, before we proceed to practical applications, let us clarify one more theoretical issue related to the FDTD divergence and previously untackled in the literature. Please note that the definition of divergence in Fig.1 is inherently *integral* and concerns the flux through the finite FDTD cell surface. In principle, we can also consider a *differential* definition denoted by $\underline{\nabla}\bullet$:

$$\underline{\nabla}\bullet E = E_{x0}\,\beta_x + E_{x0}\,\beta_x + E_{x0}\,\beta_x \qquad (4)$$

Since all modal amplitudes and propagation constants can be extracted from the FDTD simulations, we can calculate the *differential* divergence. The *integral* and *differential* definitions will always agree to the second order in small quantities. While the choice of *integral* definitions is earlier papers may seem somewhat arbitrary, we shall now provide its justification. Namely, the *integral* definition is bound to the way in which boundary and initial conditions are set up in the FDTD system. Any subtle but systematic discrepancy between zero *integral* divergence of S-modes and non-zero divergence of sources or erroneously defined boundaries will invoke compensating P-modes.

III. Dipole Radiation Problems

Consider a Hertzian dipole radiating in free space. In the literature, two models of applying excitation to the dipole have been considered (see eg.[8]):

- hard (or imposed) source – when the field calculated at the excited node by FDTD equations is replaced by the source value,
- soft (or added) source – when the source value is added to the value calculated by FDTD.

In [8] it has been found that the near-fields excited by a soft source differ by over 20% with respect to the analytical solution. Despite such a large discrepancy, and despite the fact that its satisfactory explanation has not been given in [8] - the effect has not attracted further attention. We will now attribute it to the P-mode.

Let us assume that the excited field is E_z at (1,1,1.5) in Fig.1 (vertical arrow). Both hard and soft models result in non-zero divergence immediately below and above the dipole, i.e., in dual cells centred at (1,1,1) and (1,1,2), respectively. We know from Section II that the propagating S-mode has zero divergence, so dipole radiation fields are physically modelled. A spurious P-mode is invoked to compensate the difference between the S-mode zero divergence and that of the source. However, as shown in Section II, the P-mode does not propagate and remains confined in the proximity of the dipole.

In general, the source divergence varies with time, and so does the P-mode amplitude. A special case is a delta-pulse soft source. It injects unity current at t=0, thus creating unity divergence. At subsequent iterations no further current pulses are applied, and the total divergence remains constant by virtue of the reasoning summarised in Section II. Consequently, the P-mode sets up and remains constant, even after all the radiating fields have been absorbed at the boundaries.

To validate these predictions, we model a cubic region of side 40mm with 2mm mesh resolution and place the dipole in its centre. We excite the dipole with soft delta source. Fig.2 shows the late-time E_z field in the xy-plane of the dipole. This pattern remains stationary.

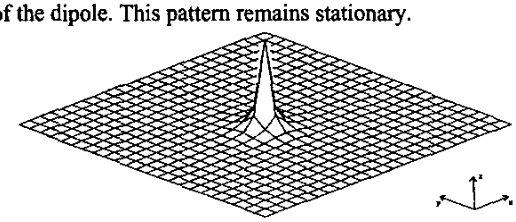

Fig.2. Steady-state static distribution of E_z field in the plane of E_z dipole excited by a soft delta source of 1V/m amplitude. The peak value of E_z is 0.333 V/m.

This experiment also confirms the non-propagating nature of P-modes, which explains why the near-to-far (NTF) transformation filters them out and produces correct *shapes* of radiation characteristics. However, the P-mode may significantly contaminate *absolute values* of antenna directive gain and directivity. To scale the radiation patterns in gain, we need to extract total radiated power as a reference value. Usually we simply integrate the Poynting vector over the NTF box.

Fig.3 shows several radiation patterns, all calculated in steady-state. The steady-state fields on the NTF box are constant but non-zero, which makes the Fourier transform ill-conditioned. Thus, the total power integrated on the NTF box fluctuates with time. The patterns shown in Fig.3 have the correct $\sin^2\theta$ shape but differ in magnitudes. Almost any value of gain and directivity can be snapped from such a simulation.

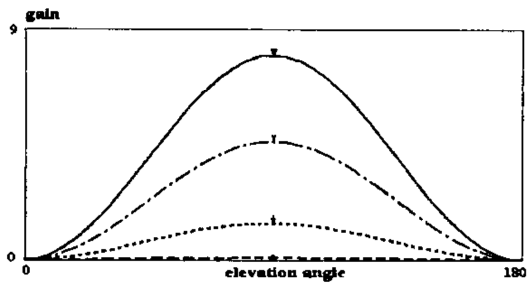

Fig.3. Directive gain of a Hertzian dipole excited by a soft delta source, for different methods of integrating the total radiated power: dotted curve - in the far zone; other curves – on the NTF box, at four different time instants.

As a remedy, an alternative way of power integration is proposed herein. Since the NTF transform filters out the non-propagating fields, we can calculate a full spherical radiation pattern (by NTF transformation for stepped azimuthal and elevation angles), and integrate the power in the far zone. This process is slower but restores the unique values of dipole gain and directivity of 1.5 (see dotted curve in Fig.3). It also provides correct radiation resistance.

IV. Eigenvalue Problems

One of the pioneering papers on FDTD eigenproblem analysis [9] has proposed to start the FDTD simulation with initial field distribution resembling the expected mode. Further papers have been concerned with an alternative approach, namely, introducing auxiliary punctual excitation [10]. With the latter approach, we can also apply sinusoidal waveforms and directly observe the emulation of eigenmodes. Selected 2D cuts through simulated field distributions have been presented previously, but what has not been revealed is field corruption by the P-mode near the source. This is demonstrated in Fig.4. It concerns the TM110 mode in the 10x10x5mm cavity resonator, simulated with 0.5mm mesh resolution, and excited at 21.21 GHz by the hard source located at (3mm, 3mm, 2.25mm). The P-mode content is even better visible and more disturbing when the S-mode passes through zero.

We have shown in previous Section that the P-mode cannot be avoided as it follows directly from the excitation mechanism. However, while for dipoles field distribution around the source is of minor practical importance, as long as we are able to correctly extract the far field data – the knowledge of modal field distributions is crucial for understanding and designing high-frequency resonators.

To develop a method of emulating pure eigenmodes in 3D resonators, we shall start with an earlier concept of a resistive voltage source. It has been originally proposed in [11] for detecting closely-spaced modes in 2D analysis of transmission lines. Basically, we apply excitation from a voltage source via resistance R. Please note that the resistive source reduces to the imposed voltage source for R=0, and to the added current source for R=+INF.

We can now predict that a high but finite R will effectively decouple the auxiliary source from the resonator, and hence reduce the P-mode content. However, we cannot start the analysis with high R because a very long simulation time would be needed to inject sufficient energy into the resonator.

To resolve these conflicting requirements, we develop sources with non-stationary resistance. We start with low R but after the mode has been established, we increase R. Please note that we cannot change R abruptly: this would correspond to instantaneous source disconnection, and excite undesired frequencies. Based on practical simulations, increasing R by 1% per iteration can be recommended. The bottom display of Fig.4 shows the produced pure physical S-mode.

The new capability of eliminating P-modes in eigenvalue analysis opens further possibilities of accurate Q-factor extraction directly from the field distribution. In the considered resonator, we now assume inner air to be lossy ($\tan\delta$=0.01). In steady state we integrate accumulated energy and dissipated power over the volume, detect their average values $\underline{W}$ and $\underline{P}$, and calculate Q from definition: $Q=2\pi f \underline{W} / \underline{P}$.

Please note that the P-mode content increases both $\underline{W}$ and $\underline{P}$. Simulation with a hard source produces the value of Q=90.4. It is important to note that although only one out of 500 FDTD cells has been driven by an auxiliary source, the excited P-mode has caused 9.6% error with respect to the analytical solution of Q=100. Simulation with non-stationary resistance, after eliminating the P-mode as in Fig.4, almost perfectly reproduces the analytical solution giving Q=100.2.

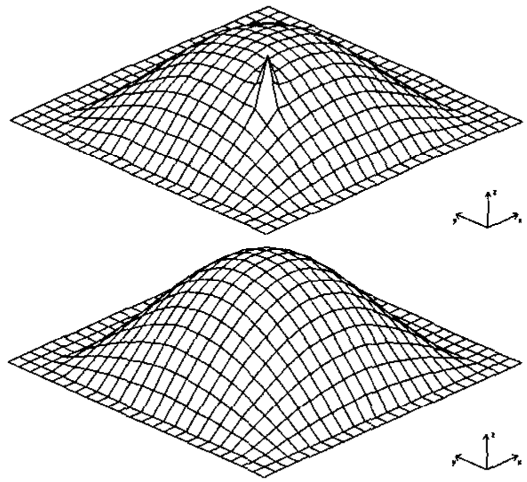

Fig.4. The E_z field in the *xy* plane containing the source: hard (upper) and the one wih non-stationary resistance gradually increased by 1% per iteration over 1000 iterations (lower).

IV. Conclusions

Divergence properties of the FDTD method have been studied from a new perspective of P- and S-eigenmodes. In extension to previous works, which have shown divergence conservation of total FDTD solutions in the absence of any excitation, we have considered practical applications with punctual sources. In a general case, divergence of the total field will then vary with time; in a special case of soft delta sources, the total divergence will be conserved but non-zero. The developed theory indicates that in any case, the total solution can be decomposed into physical S-modes and spurious P-modes. All the divergence induced by the source is confined to the P-modes, which do not propagate.

These theoretical predictions have been confirmed by demonstrating the P-modes invoked by soft and hard sources in Hertzian dipole and cavity resonator simulations. Practical measures for suppressing the parasitic effects of the P-mode on the FDTD results have been proposed and validated. In particular, correct far field characteristics of directive gain, directivity, and radiation resistance have been restored by integrating the reference power in the far zone. The source with non-stationary internal resistance has been developed for emulating pure physical modes in microwave resonators. By suppressing the P-mode it allows to correctly extract dissipated power, energy, and Q-factors directly from the FDTD fields.

The theory of P- and S-modes originated in [7] and validated herein enhances the understanding of the FDTD method fundamentals. It has further been applied to the development of spurious-free excitation of inhomogeneous transmission lines and of higher-order conformal boundary models. Relevant examples will be presented at the Conference.

References

[1] A.Taflove, *Computational Electrodynamics: The Finite-Difference Time-Domain Method*, Chapter 3, Boston-London: Artech House, 1995.

[2] A.C.Cangellaris, "Numerical stability and numerical dispersion of a compact 2-D/FDTD method used for the dispersion analysis of waveguides", *IEEE Microwave and Guided Wave Lett.*, vol.3, no.1, pp.3-5, Jan.1993.

[3] M.Krumpholz, P.Russer, "On the dispersion in TLM and FDTD", *IEEE Trans. Microwave Theory and Tech.*, vol.MTT-42, no.7, pp.1275-1278, July 1994.

[4] J.Van Hese, D.De Zutter, "Modeling of discontinuities in general coaxial structures by the FDTD method", *IEEE Trans. Microwave Theory and Tech.*, vol.MTT-40, no.3, pp.547-556, March 1992.

[5] P.H.Aoyagi, J.F.Lee, R.Mittra, "A hybrid Yee algorithm/scalar wave approach", *IEEE Trans. Microwave Theory and Tech.*, vol.MTT-41, no.9, pp.1593-1600, Sept. 1993.

[6] D.R.Lynch, K.D.Paulsen, "Origin of vector parasites in numericalMaxwell solutions", *IEEE Trans. Microwave Theory and Tech.*, vol.MTT-392, no.3, pp.383-394, March 1991.

[7] M.Celuch-Marcysiak, W.K.Gwarek, "On the nature of solutions produced by finite difference schemes in time domain", *Int.J.Numer.Model.*, vol.12, no.1/2, pp.23-40, Jan.-April 1999.

[8] D.N.Buechler, Daniel H.Roper, C.H.Durney, D.H.Christensen, "Modeling sources in the FDTD formulation and their use in quantifying source and boundary condition errors", *IEEE Trans. Microwave Theory and Tech.*, vol.MTT-43, no.4, pp.810-814, April 1995.

[9] D.H.Choi, W.J.R.Hoefer, "The finite-difference time-domain method and its application to eigenvalue problems", *IEEE Trans. Microwave Theory and Tech.*, vol.MTT-34, no.12, pp.1464-1470, Dec.1986.

[10] P.H.Harms, J.F.Lee, R.Mittra, "A study of the nonorthogonal FDTD method versus the conventional FDTD technique for computing resonant frequencies of cylindrical cavities", *IEEE Trans. Microwave Theory and Tech.*, vol.MTT-40, no.4, pp.741-746, April 1992.

[11] W.Gwarek, M.Celuch-Marcysiak, "Time domain analysis of dispersive transmission lines", Journal de Physique III, pp.581-591, 1993.