Evaluation and Enhancement of Supraconvergence Effects on Nonuniform and Conformal FDTD meshes

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***ABSTRACT* – Numerical errors arising on nonuniform FDTD meshes have been revealed and classified. Formulae for evaluating those errors have been analytically derived and verified in simulations. Simple recipes for suppressing the errors and enhancing their order of supraconvergence with refined discretisation have been proposed. Conformal modelling based on directional and linearised cell merging is introduced and recommended for practical microwave circuit simulations.**

I. INTRODUCTION

A. State of the art

With the proliferation of time-domain electromagnetic solvers throughout microwave research and industry, their convergence properties became an issue of great practical importance. An engineer asked to include an EM solver in his toolkit will typically ask two questions: What level of accuracy can I expect using my computer resources? How will the accuracy improve if I upgrade to a more powerful computer?

The answers to such questions have been sought in many publications including a well-known text book [1]. Two directions of research can be distinguished. The first one considers the characteristic equations of the FDTD method, thus proving its stability [2], energy conservation [3], and immunity to spurious modes [4][5]. Although characteristic equations can be mathematically formulated on arbitrary meshes [1, Ch.11], physically meaningful conclusions are extracted on a uniform mesh, where the only error is the 2nd order phase/frequency error due to numerical dispersion. For a nonuniform [6], conformal [7] or inhomogeneous [8][9] mesh local errors of field approximation are studied instead. Although the 1st order truncation error is then revealed, the overall convergence of phase errors investigated empirically [10] or analytically [11] is found to be of the 2nd order. This phenomenon was for the first time explained by Monk [12] who showed that nonuniform FDTD belongs to the category of the supraconvergent methods [13].

The present paper reveals supraconvergence of amplitude errors caused by numerical reflections or attenuation. It also shows that supraconvergence extends to the case of conformal meshes used for improved PEC boundary approximations, such as those proposed in [14]..[18]. Several concepts for enhancing the supraconvergence effects, and thus improving the accuracy of coarse mesh solutions, are proposed.

B. Original contributions of the present work

We investigate the effects of nonuniform meshes in free space, and then of PEC boundary approximations:

1. We show that in the case of nonuniform meshes there appear two new numerical artifacts: reflection and attenuation/amplification. Formulae describing them are analytically derived and verified in FDTD simulations.
2. We show that each numerical artifact may converge in a different order. We propose a modification, which ensures the 4th order convergence of a numerical reflection error caused by a change in cell size. We also propose recipes for frequency-selective error reduction.
3. We show that the EM fields are amplified or attenuated as the wave propagates over a continuously varying mesh in a lossless and source-free medium.
4. We propose ”linearised merging” of conformal cells, which practically eliminates error function discontinuities investigated analytically in [18] and empirically herein.
5. We combine “linearised” with “directional merging”. Conformal FDTD based on these concepts ensures smooth 2nd order convergence. It is thus recommended for all engineering applications, especially those incorporating an FDTD solver into optimisation loops.

II. STEPPED NONUNIFORM MESH

The simplest nonuniform mesh is created by applying two different cell sizes in the two regions R1, R2:

$$\text{R1: } Dz = Dz_1 \text{ for } z< z_0 \qquad \text{R2: } Dz = Dz_2 \text{ for } z> z_0 \qquad (1)$$

Without the loss of generality we can assume that $z=z_0$ is the plane of tangential E-field nodes updated by:

$$E^{k+1}(z_0)=E^{k}(z_0)+[H^{k+0.5}(z_0+0.5Dz_2)-H^{k+0.5}(z_0-0.5Dz_1)]/C$$
$$\text{where } C=0.5\, e\, (Dz_1+Dz_2) / Dt \qquad (2)$$

We then consider a TEM wave travelling from R1 to R2 and we insert the individual dispersion relations of R1 and R2 into (1). The resulting expression remains contradictory until we allow for a reflected wave in R1. Finally, the numerical reflection coefficient reads:

$$G = (1- \kappa) / (1+ \kappa) \quad (3)$$

with $\kappa = \cos(0.5 b_2 Dz_2) / \cos(0.5 b_1 Dz_1)$

We find that the reflection coefficient is real. It is positive if a wave propagates from fine to coarse mesh, and negative vice versa. These properties have been confirmed by extracting the reflection coefficient from the FDTD simulations (navy blue curve of Fig.1).

The numerical reflection is a supraconvergent effect since it exhibits quadratic reduction, even though the approximation of the *H*-field spatial derivative inherent in (1) includes the 1st order truncation error [1][6]. Several concepts for further limiting the reflection error (enhancing its supraconvergence) are hereby proposed:

1. By inserting a section of cells of an intermediate size (green curve in Fig.1) reflections are reduced to zero when this section is a half-wavelength transformer but reflection maxima follow the original quadratic curve.
2. Frequency-selective enhancement can also be obtained by introducing asymmetry of the stencil (yellow curve in Fig.1):

$$E^{k+1}(z_0)=E^k(z_0)+[a\, H^{k+0.5}(z_0+0.5Dz_2)-b\, H^{k+0.5}(z_0-0.5Dz_1)]/C$$

where $b=1-a$ and $b / a=\kappa$ (4)

3. Wide-band enhancement and the 4th order convergence are obtained by enforcing linearised *E*-field distribution (red curve in Fig.1). We note that if $Dz_1>Dz_2$ then (1) describes the *E*-field locally with the 2nd order but in the plane:

$$z' = z_0 - 0.5(Dz_1-Dz_2) \quad (5)$$

A corrected value of $E(z_0)^*$ is:

$$E(z_0)^* = p\, E^k(z_0+Dz_2) + q\, E^k(z_0') \quad (6)$$

where $p=0.5(Dz_1-Dz_2) / Dz_1$, $q=Dz_2 / Dz_1$

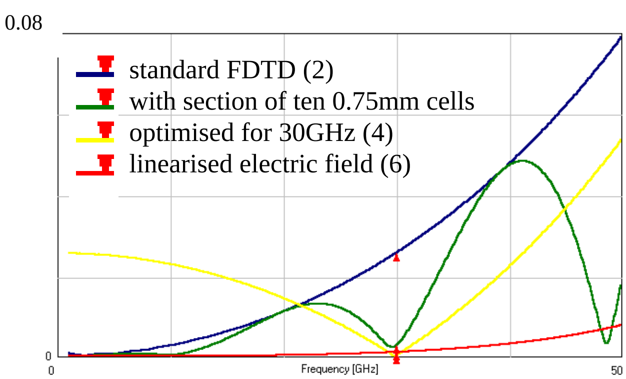

Fig.1: The magnitude of numerical reflections at the boundary between Dz_1=1mm and Dz_2=0.1mm meshes.

III. Continuously Varying Nonuniform Mesh

Let us assume that a transition from input region meshed with cell size Dz_0 to output region meshed with Dz_n is accomplished through a linearly meshed transition region, with consecutive cell sizes given by:

$$Dz_i = Dz_{i-1} + d\,, \quad i=1,..,n \quad (7)$$

Similarly to the previous case of a single-step transition, in the input region we will usually observe numerical reflections. Fig.2 plots the reflection coefficient extracted from the FDTD simulations with pulse excitation when Dz_0=1mm, Dz_n=0.1mm, for several values of step *d* and, consequently, various length *l* of the mesh transition section. Average convergence rates are of the 1.1..1.6 order. Thus the 4th order correction (6) remains the most competitive recipe.

It is however interesting to investigate field behaviour within the linearly varying mesh section. The dispersion relation continuously varies in space, but more importantly – it cannot be satisfied by a real value of ***b***. We must then allow the spatial field dependence to be governed by function:

$$\exp(-gz), \text{ with } g=a+jb. \quad (8)$$

At the boundary between cells Dz_{i+1} and Dz_i the term relating ***a*** and ***b*** takes the form:

$$0.5\cos D \sin(2B) \mathrm{sh}(2A) - \sin D[\mathrm{sh}^2 A \cos^2 B - \sin^2 B\, \mathrm{ch}^2 A]=0 \quad (9)$$

where $A=0.5aDz$, $B=0.5bDz$, $Dz=0.5(Dz_{i+1}+Dz_i)$, $D=0.5b\ d$, and sh, ch denote hyperbolic sine and cosine functions.

Relation (9) between ***a*** and ***b*** is graphically presented in Fig.3. Both *B* and *D* are assumed positive, which means that the wave is travelling from fine to coarse mesh. A negative value of *A*, in view of (8), entails that the fields are numerically amplified. The fields will be numerically attenuated if a wave travels from coarse to fine mesh.

The effect of numerical amplification / attenuation seems to contradict the widely known property of energy conservation in FDTD. However, please note that energy conservation has been proven *versus time* while amplification / attenuation takes place *versus space*. Fig.4 shows the result of FDTD simulation of a 30GHz plane wave travelling between regions meshed with Dz_0=1mm and Dz_n=0.1mm, respectively, through a 9.35mm transition section. This scenario has been previously analysed with a pulse excitation (navy blue curve in Fig.2) and zero reflection coefficient at 30GHz has been detected. Indeed, we now obtain a pure travelling wave in both input and output regions. However, the numerical attenuation in the transition region is visible on the electric field envelope (magenta), and even more clearly on the zoomed fragment of a magnetic field envelope (blue, shown in the inset).

Please note that the numerical attenuation / amplification is another supraconvergent phenomenon in FDTD. While the local truncation error in the transition region is of the 1st order, the curves of Fig.3 reveal quadratic decrease of the attenuation/amplification factor.

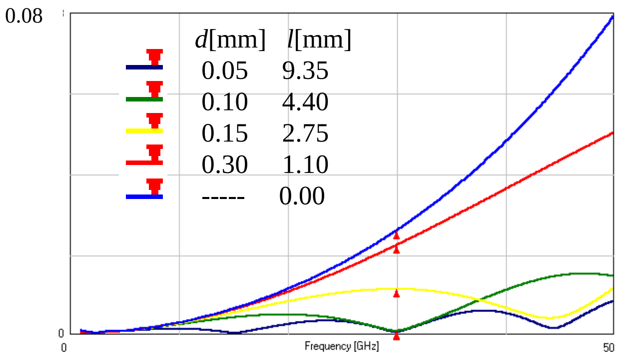

Fig.2: The magnitude of numerical reflections when a transition from mesh Dz_0=1mm to Dz_n=0.1mm is accomplished through a section of linear mesh of length *l*.

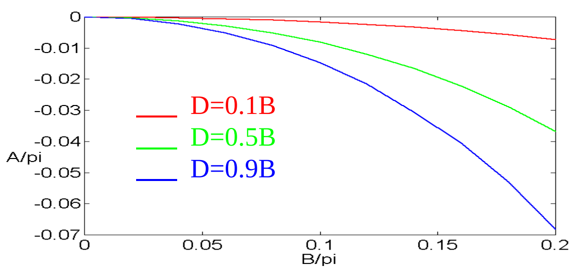

Fig.3: Predicted numerical attenuation of waves propagating over a linearly-meshed region.

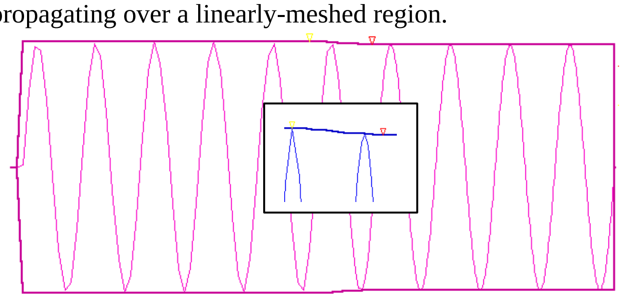

Fig.4: Electric (magenta) and zoomed magnetic (blue) fields of a 30GHz plane wave travelling in air between regions meshed with Dz_0=1mm (left) and Dz_n=0.1mm (right), through a region of *d*=0.1mm linear mesh Attenuation between cursors is 1.0261 (0.224dB).

IV. Offset Metal Boundaries

Imperfect approximation of metal boundaries parallel to, but offset from, the mesh nodes introduces frequency error in eigenvalue problems [5] or, equivalently, phase error in deterministic problems [18]. Error reduction can be obtained by conformal meshing, which in this 1D case reduces to modifications of boundary cells. However, conformal methods used so far exhibit error discontinuities (Fig.5). Therefore, although they provide the 2nd order convergence *with frequency*, convergence *with discretisation* will typically be slower, and the solutions will have discontinuities wherever the mesh topology (number of cells) changes.

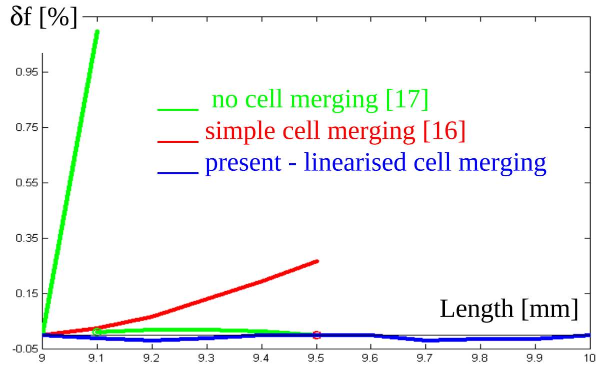

Fig.5: Relative error in fundamental eigenfrequency of a rectangular resonator of length 9..10mm, calculated by conformal FDTD schemes for basic cell size of 1mm.

We hereby put forward the concept of "linearised merging", which incorporates linear variation of tangential *E*-field near PEC into the tangential *H*-field update equation. If PEC boundary is at $z=2d$, a corrected value H^* at the last at $z=-0.5Dz$ node is modified as:

$$H^*(-0.5Dz) = u\, H(-0.5Dz) - v\, H(-1.5Dz) \qquad (10)$$

where $u=(2Dz+d)/(2Dz+2d)$, $v=d/(2Dz+2d)$

As shown in Fig.6, the linearised merging ensures that the errors become practically independent of circuit positioning on the mesh.

V. Curved and Oblique Metal Boundaries

Space limitations of this Summary do not allow for theoretical discussion of the 2D and 3D conformal approximations. This theoretical background will be given in a journal paper, while presently we shall consider an example of Fig.6 pointing to different orders of supraconvergence phenomena on different meshes.

Stair-case approximation is locally of the 0th order, i.e., it amounts to the distortion of resonator dimensions. Convergence of stair-case FDTD with the refined discretisation achieves the 1.5 order (blue line). For conformal methods without cell merging [17] and with simple merging [16] the results at two discretisations are taken from [18]. These results are quite close for both methods, and are thus marked by a common black square.

A competitive conformal approach has been proposed in [7][15]. It divides a small cell with a line perpendicular to the PEC boundary, and adds the two parts to the two cells located in the direction parallel to the PEC boundary. We shall call this approach "directional merging". The convergence of its preliminary implementation of [15] was of the 2.8th order (red line). The improved version combining directional and linearised merging (green line) shows the 3.4th order.

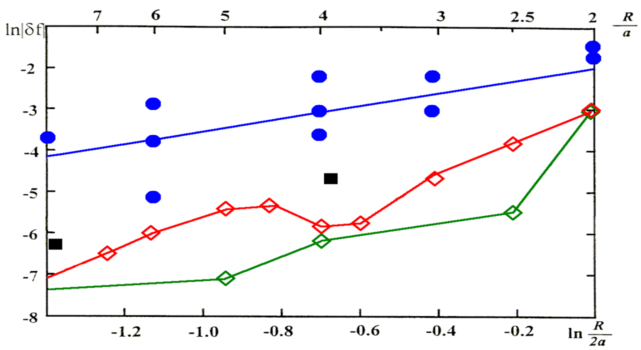

Fig.6: Relative error in fundamental eigenfrequency of a cylindrical resonator calculated by stair-case (blue) and conformal FDTD (black–no merging; red – directional merging, green – linearised directional merging).

VI. Conclusions

Numerical artifacts arising on nonuniform FDTD meshes have been revealed and classified as amplitude errors due to numerical reflections or attenuation/amplification, and phase errors due to imperfect approximation of PEC boundaries. Formulae for evaluating those errors have been analytically derived and verified in simulations. Simple recipes for suppressing the errors and enhancing their order of supraconvergence with refined discretisation have been proposed. Conformal modelling based on directional and linearised cell merging is recommended for practical applications as it is free of error discontinuities and thus ensures smooth and fast convergence.

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