Reduction of late time instabilities of the finite-difference time-domain method in curvilinear co-ordinates

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Abstract: Late time instabilities are always present when applying the finite-difference time-domain (FDTD) method in general curvilinear coordinates. Stability analysis is performed on local non-orthogonal FDTD (LNFDTD) and the result indicates that the source of numerical instability is due to the inherent dissatisfaction of the divergence-free condition for the electric field in a source-free space. An efficient 'time subgridding' scheme is proposed to reduce instabilities so that the full characteristics of electromagnetic structures can be explored. Numerical simulation based on the proposed scheme shows good agreement with theoretical prediction.

1 Introduction

The finite-difference time-domain (FDTD) technique [1] is well suited and widely applied to the computation of electromagnetic problems. Different FDTD schemes have been devised to perform the various electromagnetic computations efficiently. Traditionally, conformal modelling of electromagnetic structures using a staircase finite-difference time-domain method often produces inaccurate results even with the help of powerful computer resources [2]. Thanks to Holland's effort [3], the classic Yee's FDTD algorithm can be expressed in generalised non-orthogonal co-ordinates and it is identified as non-orthogonal FDTD (NFDTD). In NFDTD, the electric and magnetic fields are analysed using their covariant and the contravariant components respectively. Recently, Hao *et al.* [4] modified the conventional NFDTD scheme within the underlying Cartesian co-ordinate system and only those cells close to the curved boundaries are distorted. Namely, it is local-distorted non-orthogonal FDTD (LNFDTD), in which a Cartesian grid is used for the majority of the problem space and therefore less CPU Time and memory are needed than for the NFDTD. However, such a scheme suffers later time numerical instability even when the Courant criterion is satisfied. Gedney [5] and Schuhmann *et al.* [6] demonstrated that the projection operators of the NFDTD scheme must be symmetric positive definite. In this paper, it is shown theoretically that the source of numerical instability in the LNFDTD method is due to the inherent dissatisfaction of the divergence-free condition for the electric field in a source-free space. Conventionally, a unique time step is chosen for NFDTD simulation, and this approach is less efficient, particularly in LNFDTD. An efficient 'time subgridding' scheme is proposed to reduce the late time instability of the LNFDTD method when simulation over a long period is required.

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2 Theoretical analysis of numerical stability of LNFDTD

Stability analysis starts by assuming a plane electromagnetic wave having its usual representation:

$$\boldsymbol{E}(u^1, u^2, u^3, t) = \boldsymbol{\varepsilon}(t)e^{-\mathrm{j}\boldsymbol{k}\cdot\boldsymbol{r}} \tag{1}$$

The electromagnetic field that exists in a region can always be represented with a linear superposition of the above waves, which satisfy the wave equation:

$$-(\nabla \cdot \nabla)\boldsymbol{E} + \nabla(\nabla \boldsymbol{E}) = \frac{-1}{c^2}\frac{\partial^2 \boldsymbol{E}}{\partial t^2} \tag{2}$$

In (1), (u^1, u^2, u^3) are the curvilinear co-ordinates, $\boldsymbol{k}$ is the wave vector, $\boldsymbol{r}$ is the position vector and

$$\boldsymbol{\varepsilon}(t) = \sum_{i=1}^{3} \varepsilon^i(t)\boldsymbol{a}_i$$

is the polarization vector. Both $\boldsymbol{k}$ and $\boldsymbol{r}$ are functions of the curvilinear co-ordinates (u^1, u^2, u^3), which are related to the base vectors $(\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3)$. It is defined as shown in Fig. 1, where $\boldsymbol{a}_i$ $(i = 1, 2)$ are bases of a covariant vector which represents the field flow along the edge of the cells and $\boldsymbol{a}^i$ $(i = 1, 2)$ are bases of a contravariant vector that represents the flux of the fields. The product $\boldsymbol{k} \cdot \boldsymbol{r}$ is equal to $k_1u^1 + k_2u^2 + k_3u^3$ where (k_1, k_2, k_3) are the components of the wavevector with respect to the reciprocal base $(\boldsymbol{a}^1, \boldsymbol{a}^2, \boldsymbol{a}^3)$. It can be proved that:

$$\nabla \cdot \boldsymbol{E} = -2\mathrm{j}\exp(-\mathrm{j}\boldsymbol{kr})\sum_{i=1}^{3}\varepsilon^i(t)\frac{\Delta(k_iu^i)}{2\Delta u^i}$$

$$= -2\mathrm{j}\exp(-\mathrm{j}\boldsymbol{kr})\sum_{i=1}^{3}\varepsilon^i(t)\frac{k_i\Delta(u^i) + u^i\Delta(k_i)}{2\Delta u^i} \tag{3}$$

If the directions of base vectors for each cells in the whole FDTD grid remain constant for a given wave propagation

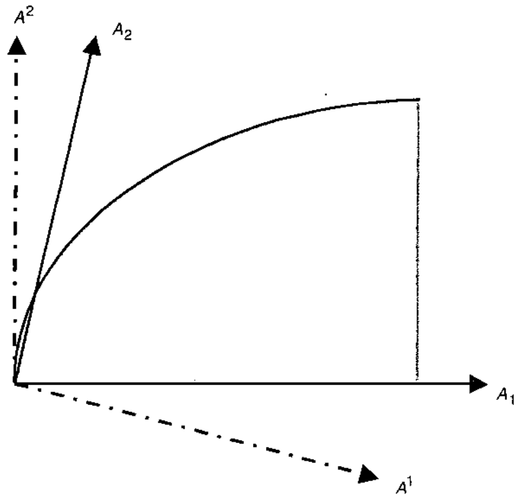

Fig. 1 *Arbitrary vector determined by its contravariant and covariant components*

direction then:

$$\nabla \cdot \boldsymbol{E} = -2\mathrm{j}\exp(-\mathrm{j}\boldsymbol{k}\cdot\boldsymbol{r})\sum_{i=1}^{3}\varepsilon^i(t)\frac{k_i\Delta(u^i)}{2\cdot\Delta u^i}$$
$$= -\mathrm{j}\exp(-\mathrm{j}\boldsymbol{k}\cdot\boldsymbol{r})\sum_{i=1}^{3}\varepsilon^i(t)k_i = 0 \qquad (4)$$

Combining the above expression with (2) one can derive the stability criterion for the time step [7]:

$$\Delta t \leq \frac{1}{c\sqrt{\sum_{i=1}^{3}\sum_{j=1}^{3}\frac{g^{ij}}{\Delta u^j \Delta u^i}}} \qquad (5)$$

where $g^{ij} = \boldsymbol{a}^i \cdot \boldsymbol{a}^j (i, j = 1, 2, 3)$. In the local non-orthogonal FDTD grid, (3) becomes:

$$\nabla \cdot \boldsymbol{E} = -2\mathrm{j}\exp(-\mathrm{j}\boldsymbol{k}\cdot\boldsymbol{r})\left(\sum_{i=1}^{3}\varepsilon^i(t)\cdot\frac{k_i\Delta(u^i)}{2\cdot\Delta u^i}\right)$$
$$-2\mathrm{j}\exp(-\mathrm{j}\boldsymbol{k}\cdot\boldsymbol{r})\sum_{i=1}^{3}\varepsilon^i(t)\frac{u^i\cdot\Delta(k_i)}{2\cdot\Delta u^i}$$
$$= -\mathrm{j}\exp(-\mathrm{j}\boldsymbol{k}\cdot\boldsymbol{r})\cdot\sum_{i=1}^{3}\varepsilon^i(t)u^i\frac{\Delta(k_i)}{\Delta u^i} \neq 0$$

The above non-zero result comes as a result of using the LNFDTD method. This is because the unitary vectors of the local bases in the mixed co-ordinate system used in the LNFDTD scheme, in order to conform to the arbitrary shaped boundary, cannot remain constant throughout the space. Consequently, the introduction of the skew cells within the Cartesian co-ordinate system does not enforce the divergence-free condition for the electric field in a source-free space. In a classic Yee's space lattice, the electric fields present their divergence-free nature, which is not true in the LNFDTD scheme. This phenomenon may be responsible for the late time instabilities that occur in the LNFDTD, even if the Courant criterion is satisfied. It is apparent that a more delicate treatment is needed on the curved cells that conform to the boundary of the electromagnetic structures.

3 Numerical simulation using a 'time subgridding' scheme

It has been demonstrated that the LNFDTD (or irregular non-orthogonal structured FDTD) is a potentially unstable algorithm. However, to ensure a stable solution at the maximum allowed number of iterations, the time step used for LNFDTD simulation could be chosen as

$$\Delta t \leq \frac{1}{c\,\sup\left\{\sqrt{\sum_{i=1}^{3}\sum_{j=1}^{3}\frac{g^{ij}}{\Delta u^j \Delta u^i}}\right\}} \qquad (6)$$

where sup(*) implies the maximum value throughout the grid space [7].

Fig. 2 shows the example structure simulated using the LNFDTD method. This is one quarter of a circular perfect electric conductor (PEC) resonator. A horizontal cut plane through the resonator meshed in the LNFDTD grid is shown in Fig. 2. The generation of a locally conformal grid as well as other details of the resonator modelling are described in [4]. Simulation is performed using an in-house LNFDTD program written in MATLAB™. A single-cycle point source is used to excite the resonator. Fig. 3 demonstrates the time domain signals of the H_y component of the TE mode in the PEC cavity resonator.

Fig. 3 clearly shows that the algorithm becomes unstable above 1400 time steps. To reduce them later time numerical instabilities in LNFDTD, formulations for electric and magnetic field components, iterations for distorted cells are examined (the example is given only for the first component of the E field):

$$e^1(i,j,k)|_{n+1/2} \approx e^1(i,j,k)|_{n-1/2} + \frac{\delta t}{\varepsilon_r\varepsilon_0\sqrt{g}}\left[\frac{h_3(i,j,k)|_n - h_3(i,j-1,k)|_n}{\Delta u^2} - \frac{h_2(i,j,k)|_n - h_2(i,j,k-1)|_n}{\Delta u^3}\right] \qquad (7)$$

$$h_3(i,j,k) \approx g_{3,3}\cdot h^3(i,j,k) + \frac{g_{1,3}}{4}\cdot(h^1(i,j,k) + h^1(i+1,j,k) + h^1(i,j,k-1) + h^1(i+1,j,k-1)) + \frac{g_{2,3}}{4}\cdot(h^2(i,j,k) + h^2(i,j+1,k) + h^2(i,j,k-1) + h^2(i,j+1,k-1)) \qquad (8)$$

where e^i, h^i are the ith contravariant components of the electric and magnetic fields respectively, and h_i is the ith covariant component of the magnetic field ($i = 1$, 2 or 3). g_{mn} ($m, n = 1, 2, 3$) are the elements of metric tensors for the distorted cells and g is the determinant of the metric tensor [4]. Eq. 7 deals with the update of the contravariant components of fields, and (8) shows the transformation between the contravariant components and its corresponding covariant components in space. In many topologies of the conformal FDTD grid, the metric tensor varies significantly from cell to cell (in our case, the number of such variations is over 15). However, even if more sophisticated averaging schemes as in [5, 6] are used instead of (8), the problem of late time instabilities still remains. Conventionally, a unique time step as shown in (6) is chosen for NFDTD simulation, and this approach is less efficient and very time-consuming, particularly in LNFDTD. This is

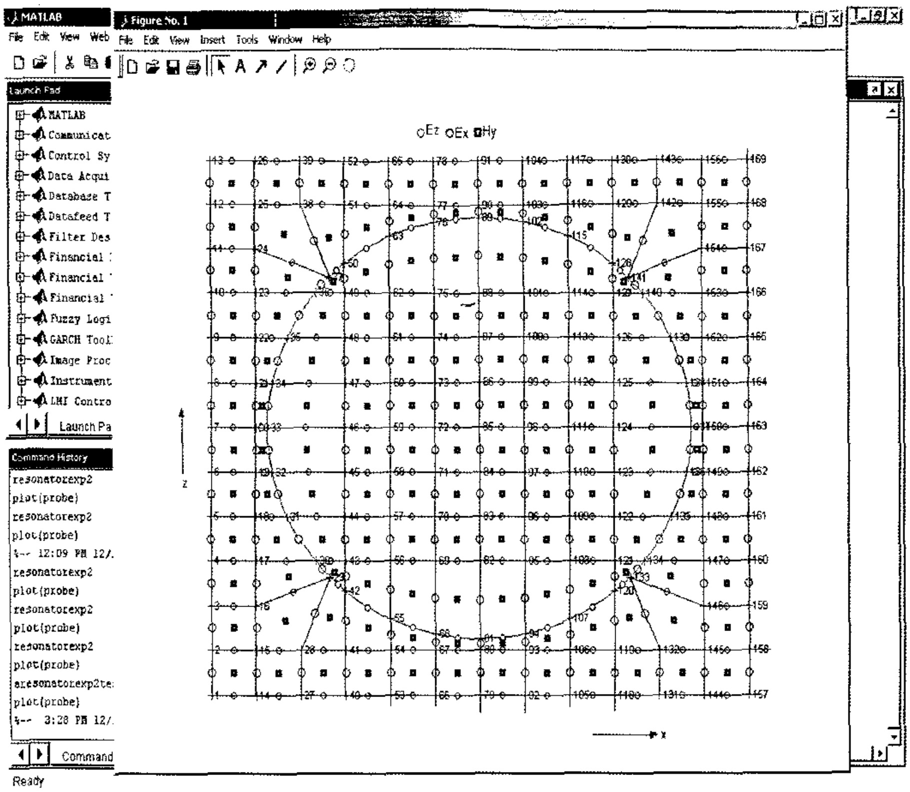

Fig. 2 *Cross section of a cylindrical PEC resonator and its LNFDTD meshes*

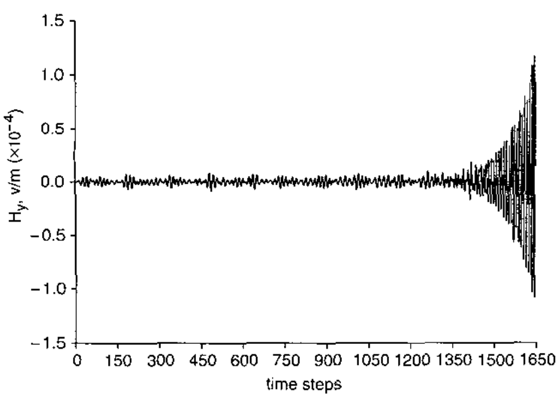

Fig. 3 *Time-domain H field showing instability using conventional time steps*

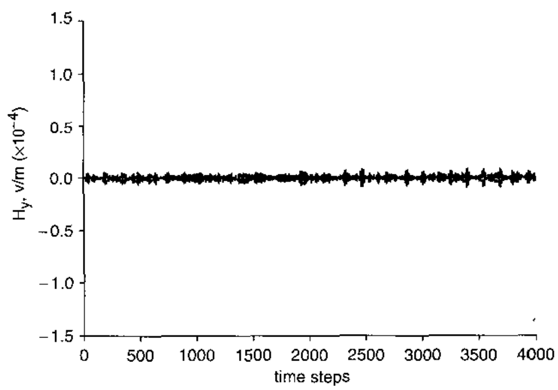

Fig. 4 *Novel time-subgridding shows improved numerical stability*

because, in LNFDTD, the time step required for the distorted cells is considerable smaller than that used for Cartesian cells. The proposed approach is to treat the curvilinear cells in a 'time subgridding' manner, that is to let the algorithm run with a time step that is a fraction of the time step that governs the algorithm outside the non-orthogonal region: $\Delta t_{novel} = \Delta t_{conventional}/n$ (n is an integer). In order to have conformity between the orthogonal and non-orthogonal regions, non-orthogonal electric and magnetic field iteration must be performed n times more inside the curvilinear cells. Fig. 4 shows the time domain signals probed in the PEC resonator.

Even at 4000 time steps (the same Δt as for the previous example: $\Delta t_{conventional}$), the algorithm remains stable; with the conventional LNFDTD method, the algorithm had to stop at about 1500 time steps due to numerical instabilities. The effect of applying the 'time-subgridding' approach to reduce late time instabilities is obvious. The resonant frequencies of the cavities can be determined using a fast fourier transform (*FFT*) algorithm, the results are compared before and after using 'time-subgridding', and are shown in Figs. 5 and 6 respectively. Comparing Figs. 5 and 6, the 'strange' bump that exists in Fig. 5 above 5 GHz is annihilated in Fig. 6. Fig. 6 shows the numerical accuracy improvement in determining the resonant frequencies, because the time-domain field signal with more time steps is taken for the FFT. This can be further proved by comparison of the numerical results using LNFDTD, LNFDTD with 'time-subgridding' and the theoretical results listed in Table 1.

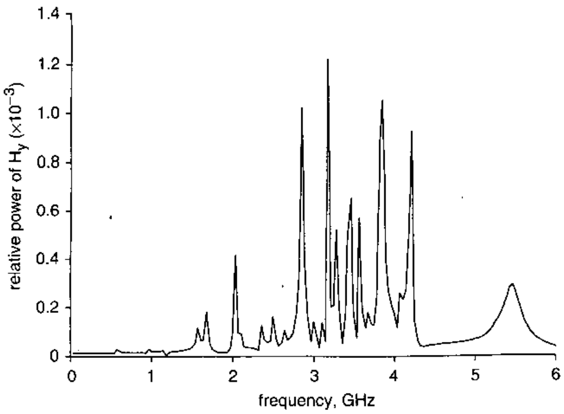

Fig. 5 *Spectrum for TE mode using conventional LNFDTD*

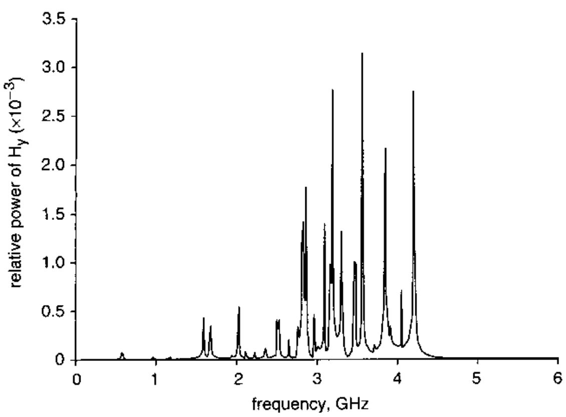

Fig. 6 *Spectrum for TE mode using novel 'time-subgridding' scheme in LNFDTD*

4 Discussion and conclusions

To date, the time sub-gridding scale factor n has been determined experimentally. The effect of n on numerical stability is shown in Fig. 7. As an LNFDTD grid introduces inherently violation of the divergence-free condition, the conventional Courant criterion for such a grid is not

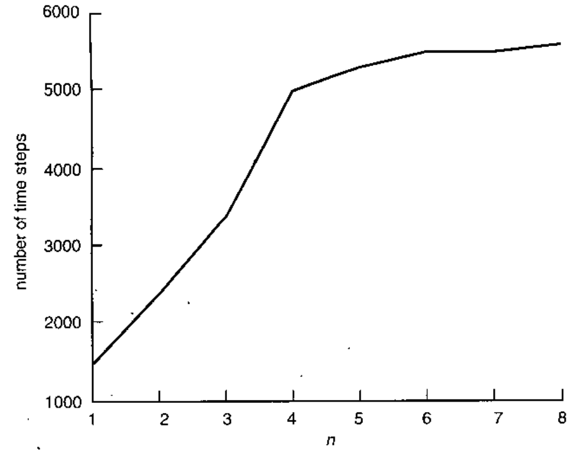

Fig. 7 *'Time-subgridding' scale factor n and its effect on numerical stability*

applicable. A modification of the Courant criterion is necessary for the skew non-orthogonal cells, but a complete theoretical analysis of this is not trivial. Fig. 7 indicates that there is a minimum value of n that gives the most extreme time stability duration for the algorithm. However, even if n is increased above this value, there is no any significant improvement in numerical stability. This implies that the LNFDTD algorithm is unconditionally unstable. In this paper, a 'time-subgridding' method is proposed to reduce such instabilities and to make LNFDTD more efficient. The theoretical analysis indicates that an unconditional stable LNFDTD algorithm is possible if the inherent non-divergence of the fields could be eliminated.

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Table 1: Numerical results using LNFDTD, LNFDTD with time-subgridding and comparison with theoretical results

LNFDTD with time-subgridding, GHz	LNFDTD, GHz	Theoretical results, GHz	LNFDTD with time-subgridding, %	LNFDTD, %
0.588	0.572	0.5863	0.29	−2.44
0.975	0.965	0.9721	0.3	−0.73
1.18	1.14	1.2198	−3.27	−6.56
1.31	–	1.3372	−2.24	–
1.68	1.57	1.693	−0.77	−7.27
–	–	1.7	–	–
2.03	2.04	2.043	−0.64	−0.15
2.11	–	2.136	−1.22	–
2.23	–	2.234	−0.18	–
2.36	2.36	2.389	−1.21	−1.21
2.53	2.5	2.553	−0.9	−2.07
2.65	2.64	2.718	−2.5	−2.87
2.76	2.82	2.732	1.02	3.22
2.96	2.89	2.956	0.14	4.6

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