Optimum time-step size for 2D (2, 4) FDTD method

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The correct choice of time-step size is of crucial importance in the case of the (2, 4) finite-difference time-domain (FDTD) method, as it affects the algorithm’s overall accuracy and convergence rate. A description of the inherent discretisation error is introduced, which is exploited for the derivation of a simple, yet reliable, approximation of the optimum temporal sampling density. As the proposed approach attempts to remedy inaccuracies in a mean-value sense, it is shown that highly efficient calculations can be carried out in this way.

Introduction: Time-domain analysis of electrically-extended electromagnetic problems calls for high-order techniques [1, 2], which can offer more efficient management of computational resources compared to low-order ones. The (2, 4) finite-difference time-domain (FDTD) method [3] is the simplest high-order extension of the classic Yee algorithm [4], combining fourth-order spatial operators with second-order leapfrog updating. However, this co-existence of uneven space-time approximations is not advantageous in practice, unless sufficiently small time steps are selected [3], so that the inadequate performance of temporal integration is compensated for.

In fact, the (2, 4) scheme can attain fourth-order convergence, provided that time steps change by a factor of $r^{-2}$, $r > 1$, when spatial steps are refined by $r$ in all directions. Clearly, such a strategy is necessary to be followed, otherwise, no qualitative improvement over the second-order Yee algorithm can be expected. Yet it is not clear exactly how small the time step should be chosen, so that minimum errors are guaranteed as well. In this Letter, we provide a formula that determines the optimum time-step size for the (2, 4) technique, based on an accuracy criterion. To take into account factors such as grid density and cell shape, a theoretical model of the discretisation flaws is introduced, which is properly corrected to obtain the desired time-step value. Various tests verify the validity of our approach, as well as the anticipated upgrade of the FDTD computational efficiency.

Methodology: Considering the lossless two-dimensional case, time steps in FDTD methods with $\Delta x$, $\Delta y$ space increments can be expressed as

$$\Delta t = \frac{Q\Delta x}{c_0\sqrt{1 + k^2}} = \frac{q\Delta x}{c_0}$$

where $c_0$ is the free-space light speed, and $k = \Delta x/\Delta y$ is characteristic of the cell shape. Stability is ensured by $Q \leq 6/7$ in the case of the (2, 4) scheme. The numerical dispersion relation, obtained by admittance plane-wave solutions, takes the form

$$\frac{1}{q^2} \sin^2 \left( \frac{\pi q}{N} \right) - \sum_{i=1}^{2} u_i^2 \sin \left( \frac{\pi q_i}{u_i N} \right) - \frac{1}{4} \sin \left( \frac{3\pi q_1}{u_1 N} \right)^2 = 0$$

where $u_1 = 1$, $u_2 = k$, $q_1 = \cos \varphi$, $q_2 = \sin \varphi$, $\varphi$ is the propagation angle, $N = \lambda/\Delta x$ denotes grid density along the $x$-direction in cells per wavelength $\lambda$, and $N = \tilde{\lambda}/\Delta x$, where $\tilde{\lambda}$ is the numerical wavelength. Labelling the left-hand side of (2) as $E(N, \varphi)$ and letting $\lambda = \tilde{\lambda}$ produces the non-vanishing quantity $E(N, \varphi)$ that is characteristic of the algorithm’s inherent errors. Considering similar expressions have been used in the past for the foundation of error-controlling FDTD algorithms [5, 6], $E(N, \varphi)$ can serve as an indicator of the method’s reliability.

Given that the type of spatial operators is not to be altered, little can be done for the correction of the method’s numerical anisotropy, which is implied by the $q$-dependence of $E$. On the other hand, it is possible to pursue a zero mean value for $E$ over all propagation angles. The average value of $E$ when $0 \leq \varphi < 2\pi$ is found as

$$E_m(N) = \frac{1}{2\pi} \int_0^{2\pi} E(N, \varphi) d\varphi$$

where $J_0(x)$ denotes zero-order Bessel functions of the first kind. One may determine $q$ by numerically solving $E_m = 0$. Nevertheless, the Maclaurin series of $E_m$ with respect to $q$ can be used to find an explicit time-step approximation. If terms up to second order are computed (hence taking $E_m \approx E_m^{(2)}$, where $E_m^{(2)}$ denotes the corresponding Taylor polynomial), the following estimated value $q_e$ for the optimum $q$ is deduced by solving $E_m^{(2)} = 0$:

$$q_e = \frac{3\pi}{8} \left[ 1 + \frac{1}{k^4} \frac{1}{N^2} + O \left( \frac{1}{N^2} \right) \right]$$

indicating that the proposed Courant numbers depend on the lattice density, in a manner that should suffice for fourth-order behaviour.

To gain further insight, the error $1 - \tilde{c}/c_0$ of the numerical phase velocity $\tilde{c}$ is shown in Fig. 1, when $N = 10$ cells per wavelength and $k = 2$. The optimum value computed from (5) is $Q = 0.26885 (Q = q_e - 1 + k^2)$, while the exact solution of (4) is $Q = 0.268876$. The cases with $Q = 0.6/7$ (stability limit), and $Q = 0.5$ are also considered. As depicted, the proposed time step produces an error curve positioned symmetrically around the zero-error line, while the other choices introduce non-vanishing errors in every direction.

Numerical results: In the first numerical test we examine the effect of our $\Delta t$ choices on the technique’s efficiency, when the TE22 mode is excited in a 6 × 4 cm cavity with perfectly conducting boundaries. The (2, 4) scheme is applied under three different conditions: (a) $Q = 6/7$, (b) $Q = 6/(7r)$, where $r$ indicates the level of refinement of the initial mesh, and (c) the proposed scheme. In all cases the simulated period is 18.87 ns, while the initial mesh consists of $15 \times 10$ cells. As illustrated in Fig. 2, the proposed practice not only guarantees a high rate of convergence, but also exhibits the best tradeoff between accuracy levels and computational burden.

Fig. 1 Error in numerical phase velocity against propagation angle for various time steps

The acquired level of improvement is also revealed by the corresponding average error values: $-2.18 \times 10^{-3}$, $-5.85 \times 10^{-4}$ and $3.11 \times 10^{-7}$.

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The suitability of the proposed approach for broadband simulations is explored in the second example. Here, a 30 cm-long parallel-plate waveguide with 2.5 cm width supporting three different modes at 9, 15 and 20 GHz, is modelled. Fig. 3 plots the evolution of the $L_2$ error in three cases: (a) grid of $652 \times 56$ cells, 7000 time steps with $Q = 6/7$, (b) grid of $480 \times 40$ cells, 12500 time steps with $Q = 0.34286$, and (c) grid of $336 \times 28$ cells, 24498 time steps with $Q = 0.12246$ (optimum value). In the latter case, the optimum $\Delta t$ is obtained considering 17.5 GHz as the design frequency. In all cases the simulated time period is 6.318 ns, while the selected grid sizes are such that the required computational times are similar in the three simulations: 194.5, 189 and 181.2 s, respectively. It becomes clear that the consistency of the proposed approach is again verified. In essence, the increased number of time steps is effectively balanced by the use of coarser grids. In this problem, error reduction by 28.8 and 8 times is ensured, respectively, compared to the first two cases, without additional computational cost.

Conclusions: To guarantee efficient computations, the time-step size of the (2, 4) FDTD scheme should be dictated by accuracy considerations only, rather than stability reasons. A simple formula has been obtained in this Letter, which takes into account grid features and ensures algorithmic performance close to the optimum one. Such an approach can be extended to other (2, 4)-like FDTD techniques, which may also incorporate modified spatial approximations with milder anisotropic features.

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References