A review and comment of the recent FDTD literature from the point of view of the numerical solution fastness

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A Review and Comment of the Recent FDTD Literature from the Point of View of the Numerical Solution Fastness

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Abstract

Since YEE's first introductory work many papers and books have appeared regarding the Finite-Difference Time-Domain (FDTD) Method. This method is a simple and elegant way of solving the time dependent MAXWELL equations, but it has some inherent drawbacks too. The main one is that the stability requires a very strict upper bound for the possible time-steps. This is why this report is devoted to the review and analysis of the recent FDTD literature from the point of view of numerical solution fastness.

1 Introduction

The FDTD method, first described by YEE in 1966 ([41]), is a very efficient and often used method to solve time dependent electromagnetics problems. Despite the simplicity of the method, because of its large computational and storage costs, it generally has been applied only since the end of the eighties. In the past fifteen years the number of publications shows a nearly exponential growth (Figure 1.1). SCHNEIDER and SHLAGER maintain a world wide web page (`www.fdtd.org`), where they have catalogued many publications relating to the FDTD method. Nowadays the number of entries is altogether around 4000. The above authors wrote a selective survey about the FDTD literature in 1995, in which they review 305 papers ([31]). At that time the database consisted of 1000 entries.

The number of FDTD publications shows that this method has a very wide application area. A very important field is the investigation of the interactions between biological bodies and electromagnetic fields. The work [6] studies the electromagnetic energy coupled to the human head due to mobile telephones. The paper [17] investigates the electromagnetic interference between pacemakers and mobile phones. Another widely studied area is the modelling of discrete and integrated microwave circuits (see for instance the papers [16], [25] and [44]). Further applications include (but are not limited to): modelling transmission lines; radar cross section prediction; ionospheric and plasma scattering; integrated optics; electromagnetic compatibility; antenna design; etc. These applications can all be supported by the basic FDTD algorithm, requiring only different pre- and post-processing interfaces to obtain the final results.

In the books [19] and [37] we can find the basics of the FDTD method and some detailed applications of it. A short review of other numerical electromagnetic modelling techniques can be found in [15].

Now we give a brief description of the FDTD method. The FDTD method solves the 3D Maxwell curl equations

$$-\nabla \times \mathbf{H} + \epsilon \partial_t \mathbf{E} = \mathbf{0} \tag{1.1}$$

$$\nabla \times \mathbf{E} + \mu \partial_t \mathbf{H} = \mathbf{0}, \tag{1.2}$$

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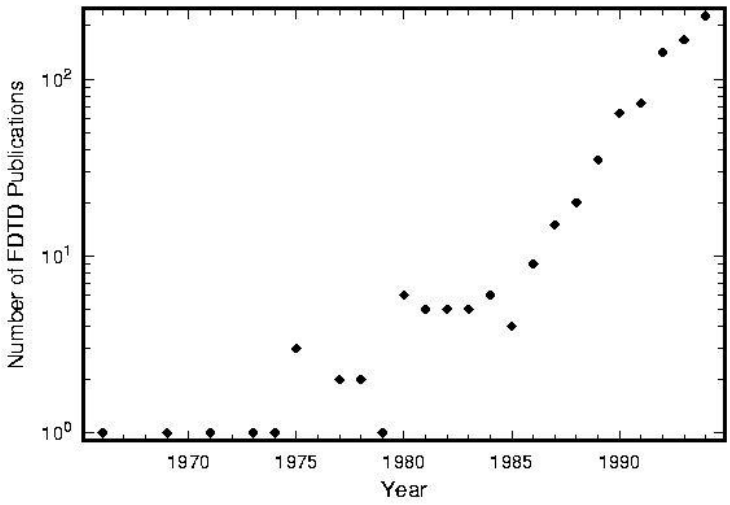

Figure 1.1: *Number of FDTD publications from 1966 till 1995. (Source: [31].)*

numerically, where **E** is the electric field strength, **H** is the magnetic field strength, ϵ is the permittivity and μ is the permeability. The external electric-current density and the external magnetic-current density have been set to zero because they play no role in the stability analysis. The solution of a problem starts with the definition of a generally rectangular mesh (the choice of the step-sizes $\Delta x, \Delta y$ and Δz) for the electric field and another staggered grid for the magnetic field around the objects in question (human head and mobile phones, antennas, wires, microwave circuits, etc.). The building blocks of this mesh are the so-called YEE-cells (Figure 1.2, Figure 1.3). Defining the approximations of the field strengths at the points shown in Figure 1.2 we calculate the first spatial derivatives using central differences. Choosing a time-step Δt and applying the so-called leap-frog algorithm we update the field quantities as follows:

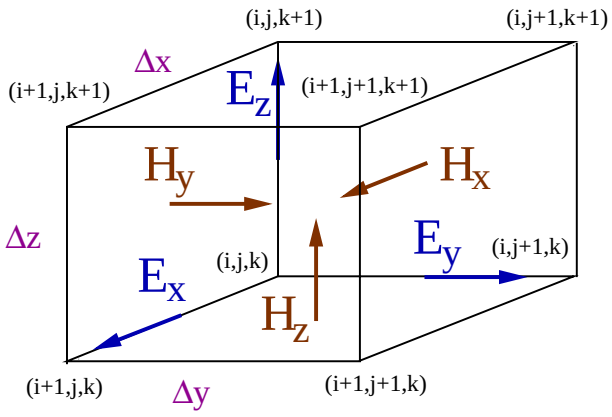

Figure 1.2: *Standard* YEE *cell.*

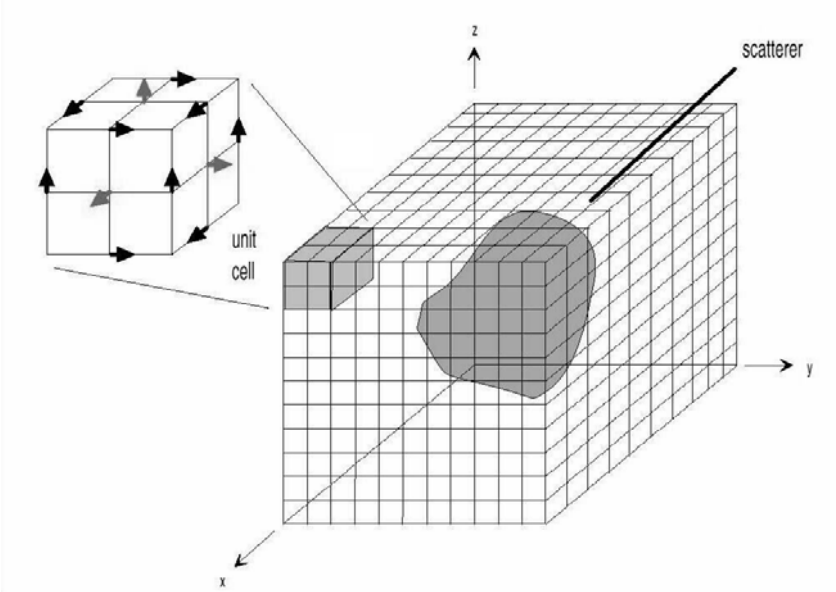

Figure 1.3: *Scatterer in the computational space. (Source: [15].)*

$$\mathbf{E}_{n+1} = \mathbf{E}_n + \Delta t \mathbf{M}_\epsilon^{-1} \mathbf{D} \mathbf{H}_{n+1/2}, \tag{1.3}$$

$$\mathbf{H}_{n+1/2} = \mathbf{H}_{n-1/2} - \Delta t \mathbf{M}_\mu^{-1} \mathbf{D} \mathbf{E}_n, \tag{1.4}$$

where $\mathbf{E}_n$ and $\mathbf{H}_{n-1/2} \in \mathbb{R}^{3N}$ are the approximations of the $\mathbf{E}$ and $\mathbf{H}$ fields at the time levels $n\Delta t$, $(n-1/2)\Delta t$, respectively, $\mathbf{M}_\epsilon, \mathbf{M}_\mu \in \mathbb{R}^{3N \times 3N}$ are diagonal matrices of the material parameters, $\mathbf{D} \in \mathbb{R}^{3N \times 3N}$ is the finite difference approximation of the curl operator including the boundary conditions, and N denotes the number of YEE-cells in the computational domain.

The main advantages of the method are as follows:

- Because of the special discretization method of the MAXWELL curl equations, the divergence equations are fulfilled automatically.
- Using the leap-frog algorithm, no system of linear equations must be solved.
- At each time step, the equations used to update the field components are fully explicit.
- The material parameters (μ, ϵ) can have different values for different field orientations permitting anisotropic or nonlinear materials to be handled.

The drawbacks of the FDTD method can be summarized in three points:

- numerical dispersion,
- staircased boundaries, consequence of the Nyquist sampling theorem
- strict stability conditions,

which are detailed in the next paragraphs.

Numerical dispersion: The phase velocity of numerical wave modes can differ from the speed of light by an amount varying with the wavelength, direction of propagation in the grid and grid discretization. For large computational domains, e.g., ones that have at least in one dimension forty wavelengths or larger, phase errors from dispersion and grid anisotrophy can be significant unless a

small spatial discretization is used. TAFLOVE has derived the dispersion relation for homogeneous waves in the FDTD grid ([36], [37]). The equation he derived is correct, but the assumption that some coarsely resolved fields have a phase velocity of zero is not. SCHNEIDER and WAGNER show in papers [32] and [30] that the FDTD dispersion relation even for homogeneous waves permits solutions with complex wave numbers. These complex (numerical) waves experience exponential decay as they propagate and their speed can be greater than the speed of light. The dispersion errors associated with these waves are maximum along the grid axes and minimum along the grid diagonal.

Staircased boundaries, Nyquist sampling theorem: Because the basic elements are cubes, curved surfaces on a scatterer must be staircased. For configurations with sharp, acute edges, an adequately staircased approximation may require a very small grid size. At the same time, the volume of the grid must be large enough to encompass the entire object and most of the near field (Figure 1.3). Another restriction for the choice of the step-size in spatial dimension comes from the Nyquist sampling theorem. This theorem says that at least two samples per wavelength are needed in order for the spatial information to be adequately sampled. Usually the step size $\lambda/10$ is used, where λ is the smallest wavelength in the model.

Strict stability conditions: In paper [26] the author presents an elegant one-step vector iteration form for the FDTD method, and analyses the stability properties of the FDTD method. The iteration has the form

$$\mathbf{F}_{n+1} = \mathbf{G}\mathbf{F}_n, \tag{1.5}$$

where

$$\mathbf{F}_n = \begin{bmatrix} \mathbf{M}_\epsilon^{1/2} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_\mu^{1/2} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{M}_\epsilon^{1/2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{M}_\mu^{1/2} \end{bmatrix} (\mathbf{E}_n\ \mathbf{0}\ \mathbf{0}\ \mathbf{H}_{n-1/2})^\top \in \mathbb{R}^{3N+3N+3N+3N}, \tag{1.6}$$

$$\mathbf{G} = \begin{bmatrix} \mathbf{I} + (\Delta t \mathbf{A})^2 & -\Delta t \mathbf{A} \\ -\Delta t \mathbf{A} & \mathbf{I} \end{bmatrix} \in \mathbb{R}^{12N \times 12N}, \tag{1.7}$$

$$\mathbf{A} = \begin{bmatrix} \mathbf{M}_\epsilon^{-1/2} & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_\mu^{-1/2} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{0} & -\mathbf{D} \\ \mathbf{D} & \mathbf{0} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{M}_\epsilon^{-1/2} & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_\mu^{-1/2} \end{bmatrix} \in \mathbb{R}^{6N \times 6N}, \tag{1.8}$$

and $\mathbf{I} \in \mathbb{R}^{6N \times 6N}$ denotes the unit matrix. In this setting the FDTD method is said to be stable if the iteration (1.5) is stable, that is if the matrix $\mathbf{G}$ is a stable matrix. The main result of the paper is as follows.

Theorem 1.1 *The FDTD method is stable if and only if the condition*

$$\Delta t < \frac{2}{\varrho(\mathbf{A})} \tag{1.9}$$

is fulfilled ($\varrho(\mathbf{A})$ is the spectral radius of the matrix $\mathbf{A}$).

The above theorem practically means that the upper bound for the time-step Δt is

$$\Delta t < \frac{1}{c\sqrt{1/\Delta x^2 + 1/\Delta y^2 + 1/\Delta z^2}}, \tag{1.10}$$

which produces a very small time-step in electromagnetics real life models, because c generally means the speed of light in the electromagnetic applications and we have to choose the spatial step-sizes to be very small to decrease the dispersion and the effects of staircasing.

If we solve a problem with 10^6 cells, where $\Delta x = \Delta y = \Delta z = 10^{-6}(m)$ with the YEE-algorithm (9 operations are needed to update each variable) the upper bound for the time-step

would be $\Delta t \leq 2 \times 10^{-15}(s)$. This means that we have to execute 2.7×10^{19} operations to evaluate the field quantities after 1 microsecond. Using a fast computer with 10^{12} operations per second this procedure would take 6×10^7 seconds, that is 7.44 hours. This huge computational time is unacceptable in real-life problems.

This report is devoted to the review of the recent FDTD literature. Our aim is to trace the possibilities to accelerate the speed of numerical calculations. To measure the advance of a numerical scheme we introduce the relative advancing speed (RAS). We define this number as

$$RAS = \frac{n(T) \cdot \Delta t_{max}}{T}, \tag{1.11}$$

where T is an arbitrary time-period, $n(T)$ denotes the number of time-iterations in the numerical solution, which can be executed during the period T, and Δt_{max} is the maximal time-step allowed by the stability conditions. For the classical YEE-algorithm we have (setting $\Delta x = \Delta y = \Delta z = h$)

$$RAS = \frac{(1/2) \cdot h/(c\sqrt{3})}{3 \cdot 9 \cdot N \cdot t_{op}} = \frac{1}{15\sqrt{3}} \frac{h}{c \cdot N \cdot t_{op}} \approx 0.038 \frac{h}{c \cdot N \cdot t_{op}}, \tag{1.12}$$

where t_{op} is the time of one operation (addition or multiplication) on our computer. Let us observe that choosing a time-step $\Delta t = \Delta t_{max}/2$ the relative advancing speed changes like $RAS' = RAS/2$, but if the step-size h goes halves, then $RAS' = RAS/16$ because $N' = 2^3 N$. This means that a change of the spatial step-size has much more effect on the RAS number than a change of the time-step.

Our investigation is devided into two parts. In Section 2 we list the possibilities of the increase of the spatial cell size, while in Section 3 we examine the properties of the time integration.

2 Increase of the spatial step-sizes

In this section we study the possibilities of discretization schemes which differ from the original second-order in space finite difference YEE-scheme. The first idea is the application of higher order schemes. Higher-order discretization could be done both in spatial and time dimension ([4]), but application to the temporal derivatives requires storage of more temporal values than the YEE-method. FANG has developed a fourth-order in time and space algorithm that does not require additional temporal values but requires additional field values ([5]). In paper [20] MANRY, BROSCHAT and SCHNEIDER approximate the fields by four- or six-point LAGRANGE interpolating polynomials. These algorithms reduced both numerical dispersion and grid anisotrophy, permitting a smaller number of points per wavelength to be used and thus saving computer memory and reducing the total number of operation needed. They present Table 2.1 for 2D problems. We compare the methods from the stability point of view. Let us calculate the RAS number for the methods described in this paper. The number of operations are 12, 36 and 52 per time-step for the YA, $2-4$ and $2-6$ methods, respectively. The upper bounds for the time-steps are $\Delta t \leq h/(c\sqrt{2})$, $\Delta t \leq 6h/(7c\sqrt{2})$ and $\Delta t \leq 120h/(149c\sqrt{2})$. We obtain Table 2.2. The table shows that on a fixed mesh the higher-order methods advance more slowly than the YEE-algorithm. This means that if the spatial discretization is given (for example to avoid the effects of staircasing), then there is no reason to use higher-order methods. If the mesh is not fixed, then from the phase error point of view the YEE-algorithm with $PPW = 160$, the 2-4-algorithm with $PPW = 20$ and the 2-6-algorithm with $PPW = 10$ are equivalent. For these methods the RAS numbers are

$$RAS_{YA} = \frac{0.059\lambda}{160^3 \cdot N_x \cdot N_y \cdot c \cdot t_{op}} = \frac{1.44 \times 10^{-8}\lambda}{N_x \cdot N_y \cdot c \cdot t_{op}}, \tag{2.13}$$

$$RAS_{2-4} = \frac{0.017\lambda}{20^3 \cdot N_x \cdot N_y \cdot c \cdot t_{op}} = \frac{2.13 \times 10^{-6}\lambda}{N_x \cdot N_y \cdot c \cdot t_{op}}, \tag{2.14}$$

PPW	YA	2-4	2-6	Memory
10	7.18λ	119.13λ	1801.95λ	$N_xN_y \cdot 5.47KB$
20	29.98λ	1846.54λ	108666.0λ	$N_xN_y \cdot 21.86KB$
40	121.17λ	29288.3λ	$6.85107 \times 10^6\lambda$	$N_xN_y \cdot 87.5KB$

Table 2.1: *Distance to produce $\pi/8$ phase error due to grid anisotrophy and the required memory for an $N_x\lambda$-by-$N_y\lambda$ (λ is the wavelength) problem discretized at a given points per wavelength (PPW) value. YA=*YEE*-algorithm, 2-4 and 2-6 denote the fourth and sixth order spatial discretization. (Source: [20].)*

	YA	2-4	2-6
RAS	$0.059h/(c \cdot N \cdot t_{op})$	$0.017h/(c \cdot N \cdot t_{op})$	$0.011h/(c \cdot N \cdot t_{op})$

Table 2.2: *RAS numbers of the 2D* YEE*-algorithm and the fourth and sixth order methods.*

$$RAS_{2-6} = \frac{0.011\lambda}{10^3 \cdot N_x \cdot N_y \cdot c \cdot t_{op}} = \frac{1.1 \times 10^{-5}\lambda}{N_x \cdot N_y \cdot c \cdot t_{op}}, \tag{2.15}$$

which means that the use of the $2-6$-method is the best solution. This method is 1000 times faster than the YEE-method.

TURKEL has presented a fourth-order scheme in [39]. This scheme has the name Ty(2,4). On the base of this method he has considered fourth-order accurate compact implicit schemes for the numerical solutions of the 2D MAXWELL equations in papers [40], [43], which were joint works with YEFET. The same mesh stencil is used as in the standard YEE-scheme. In particular extra information over the wider stencil is not required. This has several advantages. First, it is relatively easy to modify an existing code based on the YEE-algorithm. Second, a staggered mesh, without additional mesh location, makes the boundary treatment easier since some of the quantities are located inside the domain rather than on the boundary. In their scheme an inversion of an "almost" tridiagonal matrix is needed, but the inverse is never evaluated, rather the LU-decomposition is calculated once in each direction. The scheme is second-order accurate in time and fourth-order accurate in space. As usual, the temporal accuracy can be improved by choosing a smaller time-step. This increases the work only linearly and does not increase the storage. This is why the authors write that one should choose a time-step based on accuracy conditions and not on stability grounds.

Numerical tests have shown that the application of higher order discretizations on staggered grids are more accurate than on unstaggered grids ([7]). But the main drawback of a staggered scheme is that it makes difficult to model metal boundaries and dielectric interfaces. In paper [42] the fourth order scheme of [5] has been modified near the boundaries to get a scheme which does not degrade the convergence rate of the original higher order scheme. Moreover, the stability analysis shows that if metal boundaries are present then the necessary stability bound of [5] holds for the modified scheme too. Problems with dielectric boundaries require a slightly smaller stability bound.

One of the problems of the FDTD method is that we have to choose a very fine mesh to avoid the drawbacks of staircasing. This implies a very small upper bound for the possible time-steps. There are several suggested remedies to circumvent the effects of the errors introduced by the staircase approximations. They include Cartesian subgridding, conformal modelling, multiblock body fitted structured grids, structured grids and overlapping grids. However, none of these methods combine stability, second-order accuracy and efficiency (in time spent on implementation, grid generation and computation). This is why some authors suggest that different methods must be used on the boundaries and inside the regions.

In paper [1] the classical FDTD solver is combined by two unstructured solvers, by an explicit Finite Volume solver and an Implicit Finite Element solver. The method uses unstructured grids

around small geometrical details but revert to structured grids as quickly as possible for the rest of the computational domain. They achieve a very efficient and flexible second-order scheme. The calculated stability bounds are smaller than in the YEE-method, but because of the unstructured grid no staircasing is needed. The authors demonstrate that this scheme can be used for 3D problems too.

FEM-FDTD hybrids have been constructed, but all suffer from weak instability, referred to as late time growth, which limits their usefulness. The method of RYLANDER and BONDESON in [27] combines the efficiency of the FDTD with the ability of the FEM to model complex geometry. The advantage of the method is that it is completely stable for the time-steps up to the stability limit for the FDTD without added dissipation and produces no spurious solution. The space is discretized by cubes for FDTD and by tetrahedrons for FEM. In the transition region pyramids are used. The edge elements of the pyramids produce a continuous tangential component for the electric field, which is necessary for a curl-conforming FEM formulation. The crucial step for achieving stability is to apply the GALERKIN-method in a way that matches the finite difference algorithm. This leads to a discretization with a completely symmetric spatial operator.

In the papers [14], [22] finite volume methods are used to avoid the staircasing. In the second one the elliptical constraints of the MAXWELL equations are approximated by hyperbolic conditions starting from the so-called Generalized Lagrange Multiplier Maxwell model. Using high-resolution finite volume scheme an efficient and flexible parallel MAXWELL solver can be obtained for explicit field calculation in time. We notice that in this procedure a divergence recovery step is added, which does not require the solution of a POISSON equation.

A new approach to the numerical handling of electromagnetics problems is investigated in papers [2], [8] and [9]. The essence of the method looks as follows: The authors start with the MAXWELL equations in the frequency domain, and introduce the magnetic and electric potentials satisfying the COULOMB gauge condition. Then the original equations are rewritten for potentials and are discretized on rectangular (staggered) meshes. The same authors describe a fast finite volume simulation in 3D. The main steps of the methods are as follows: First the HELMHOLTZ decomposition is applied to $\mathbf{E}$; then a stabilizing term is added, resulting in a strongly elliptic system; the system is written in first order form to allow flexibility in the ensuing discretization; and finally, the divergence-free COULOMB gauge condition is eliminated. The resulting weakly coupled system of partial differential equations enables an efficient preconditioner for the large, sparse algebraic system which results from the discretization. Then the equations are discretized using staggered grid, where the stabilizing term vanishes at the exact solution of the discrete equation. The resulting linear system is solved using fast preconditioned KRYLOV methods.

3 Temporal discretization schemes

In the papers [3], [18] and [38] the authors investigate the conservative system of hyperbolic partial differential equations

$$\partial_t \mathbf{u} = \mathbf{R}\mathbf{u} = -\sum_i \partial_i \mathbf{F}_i(\mathbf{u}) + \mathbf{S}(\mathbf{u}, \partial_i \mathbf{u}, \partial_i \partial_j \mathbf{u}, \mathbf{x}, t), \tag{3.16}$$

where t is the time coordinate, i and j run over 1, 2 or 3 components of the spatial coordinate $\mathbf{x}$, $\mathbf{u}$ denotes the vector of conservative variables, and the right hand side contains the source terms $\mathbf{S}$ and the derivatives of the fluxes $\mathbf{F}_i$. The above equation is applied for problems of magnetohydrodynamics by the authors, but the MAXWELL equation can be also written in conservative form. The explicit approach can be very inefficient especially for the solution of steady state problems. The usual strategy is to solve the time dependent equations and march towards the steady state solution. If the convergence stagnates, the physical time corresponding to the final solution is huge relative to the time-step allowed by the strict stability conditions. Therefore, an excessive number of explicit time steps are needed.

If we treat the problem with an implicit solver, then we can lift the most severe stability restrictions on the time-step, or can even allow to take arbitrarily large time-steps. But in these

cases we have to perform much more work than in the explicit case, because we have to solve sequences of linear algebraic equations. The cited papers state that the solution of the stability problem could be the so-called semi-implicit schemes, where certain variables or terms in the equations, which give stricter upper bound for the step-size, are treated implicitly and the others explicitly.

In paper [18] the implicit and semi-implicit schemes are defined and discussed. The implicitly treated variables are denoted by $\mathbf{u}_{impl}$ and the implicitly treated part of $\mathbf{R}$ by $\mathbf{R}_{impl}$. The discretization

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t_n \mathbf{R}(\mathbf{u}^n) + \alpha \Delta t_n \left[\frac{\mathbf{u}^n - \mathbf{u}^{n-1}}{\Delta t_{n-1}} - \mathbf{R}(\mathbf{u}^n) \right] + \tag{3.17}$$

$$+ \beta \Delta t_n \left[\mathbf{R}_{impl}(\mathbf{u}^{n+1}) - \mathbf{R}_{impl}(\mathbf{u}^n) \right]$$

is used (the parameters α and β may vary between zero and one) and to solve it the linearization

$$\mathbf{R}_{impl}(\mathbf{u}^{n+1}) = \mathbf{R}_{impl}(\mathbf{u}^{n+1}_{exp}, \mathbf{u}^n_{impl}) + \frac{\partial \mathbf{R}_{impl}}{\partial \mathbf{u}_{impl}} (\mathbf{u}^{n+1}_{impl} - \mathbf{u}^n_{impl}) + \mathcal{O}(\Delta t^2) \tag{3.18}$$

is applied.

In paper [38] the authors implemented semi-implicit schemes in the software package Versatile Advection Code (VAC, see `http://www.phys.uu.nl/ toth/`), and they have compared the methods on several test problem. These tests illustrate the obtainable efficiency gain of the methods.

Applying an implicit method is an efficient tool when stability is more of concern than accuracy. However for very large systems the solution of the involved linear system may be very expensive. Botchev, Sleijpen and van der Vorst have developed a method in [3] where they use a moderate number of the minimum residual iterations. Of course, this puts limits to the step-size since these approximate schemes may be viewed as explicit schemes and they are never unconditionally stable. They apply different schemes for each time step. The advantage of this metod is that it is much more stable than each of them separately. A convenient way is proposed to control the stability and adjust the step-size adaptively.

Physical or chemical processes, in which dissipation does not play a significant role may be modelled by means of Hamiltonian systems of ordinary differential equations. A Hamiltonian system is known to have favorable properties concerning long-time integrations. In the simplest case the Hamilton-function gives the total energy of the process to be modelled. A so-called symplectic integrator will exactly conserve the energy in the discrete Hamiltonian that is an approximation to the true energy of the system. The difference between the discrete and continuum Hamiltonians can be viewed as a small perturbation given by the truncation error, but the error is also Hamiltonian. Thus, almost all orbits that are stable in the real system will continue to be stable in the numerical system. An elegant summary of the symplectic methods can be found in the book [29]. In paper [21] the numerical integration of a wide class of Hamiltonian partial differential equations are discussed, discretizing the Hamiltonian and the Poisson structure separately. The author describes the circumstances under which the best results can be obtained; in particular, when the Hamiltonian can be split into linear and nonlinear terms. In [34] the authors present a one-parameter family of schemes, which include the leapfrog, implicit midpoint, trapezoid, Störmer-Verlet and Cowell-Numerov schemes. The symplecticness is proved and stability and accuracy analysis is presented.

In the paper [28] the authors develop and test variable step symplectic Runge-Kutta-Nyström algorithm. They have observed that for symplectic formulae, moving from constant to variable step-sizes results in a marked decrease in efficiency. In these cases these methods are no longer superior to standard non-symplectic methods. Stoffer has given an argument, why symplectic integrators should not be used with variable step-size ([35]): integrating a system of ordinary differential equations with variable step-size is equivalent to integrating another system with constant step-size, but this system is not Hamiltonian, even if the original system is. Despite this the articles [10] and [11] the authors present a "meta-algorithm" which allows us to combine the use of variable steps with symplectic integrators, without destroying their favorable properties.

In the early eighties [12] and [13] achieved promising results in getting an unconditionally stable scheme for two-dimensional models. However, using the techniques mentioned in the above papers, it proved difficult to demonstrate the required numerical stability for the general three-dimensional case and research in this area was largely discontinued. Recently, there has been a revival of interest of the use of the so-called Alternating-Direction Implicit methods (ADI) because these methods ensure an unconditionally stable numerical solution for the MAXWELL equations. In paper [23] the numerial formulation of the ADI FDTD method for a two dimensional TE wave is presented. The numerical stability is derived and the numerical dispersion of the formulation is studied analytically. In paper [24] the author generalizes his previous results for 3D problems. The unconditional stability of the method is verified numerically and the method is compared with the conventional 3D FDTD method. In September of 2000 the paper of ZHENG, CHEN and ZHANG appeared wherein for the first time unconditional numerical stability is derived for the full three-dimensional MAXWELL equations ([45]). This method is different from the conventional ADI procedures. In the usual methods the alternations in the computation directions are made with respect to the three spatial coordinate directions: In the 3D case the computations are broken up into three substeps for each cycle since there are three spatial coordinates x, y and z. In the method proposed by the paper the ADI is applied in terms of the sequence of the term of the curl discretization. It then leads to only two alternations in the computation directions. We demonstrate the essence of the method by the discretization of the first component

$$\frac{\partial E_x}{\partial t} = \frac{1}{\epsilon}\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}\right) \tag{3.19}$$

of the equation (1.1). For the first half time-step (from the nth to the $n+1/2$th) the derivative $\partial H_z/\partial y$ is replaced with an implicit difference approximation of its unknown pivotal values at $n+1/2$th time step; while the derivative $\frac{\partial H_y}{\partial z}$ is replaced with an explicit finite difference approximation in its known values at the previous nth time step. In expressions

$$\frac{E^{n+1/2}_{x,(i+1/2,j,k)} - E^{n}_{x,(i+1/2,j,k)}}{\Delta t/2} = \tag{3.20}$$

$$= \frac{1}{\epsilon}\left[\frac{H^{n+1/2}_{z,(i+1/2,j+1/2,k)} - H^{n+1/2}_{z,(i+1/2,j-1/2,k)}}{\Delta y} - \frac{H^{n}_{y,(i+1/2,j,k+1/2)} - H^{n}_{y,(i+1/2,j,k-1/2)}}{\Delta z}\right].$$

For the second half time-step (from the $n+1/2$th to the $n+1$th) is done the same, but in reverse order, that is

$$\frac{E^{n+1}_{x,(i+1/2,j,k)} - E^{n+1/2}_{x,(i+1/2,j,k)}}{\Delta t/2} = \tag{3.21}$$

$$= \frac{1}{\epsilon}\left[\frac{H^{n+1/2}_{z,(i+1/2,j+1/2,k)} - H^{n+1/2}_{z,(i+1/2,j-1/2,k)}}{\Delta y} - \frac{H^{n+1}_{y,(i+1/2,j,k+1/2)} - H^{n+1}_{y,(i+1/2,j,k-1/2)}}{\Delta z}\right].$$

The authors rewrite their method in a one-step vector-iteration form, and investigate the stability of the iteration. They prove, applying MAPLE V5.2 in the calculations of the eigenvalues, that the generated method is unconditionally stable. Thus the time-step can be chosen arbitrarily, however, the numerical calculations show that to guarantee the same accuracy like in the classical FDTD method, we can reduce the computational time only with a factor 0.6.

4 Summary

The need for calculating fast, accurate solutions of the three-dimensional electromagnetic equations arises in many important application areas. This is why a lot of effort has recently been invested

in finding appropriate numerical algorithms. Unfortunately, we can establish that the choice of numerical techniques to solve the MAXWELL equations depends on the parameter ranges and various other restrictive assumptions, and as a such is to a significant degree application dependent. Now we summarize the possibilities for the numerical solution depending on the problems at hand.

- In general, the number of computations is more dependent on the measure of the grid cells than the time-step. This means that our goal must be the increase of the spatial cells during the constructions of numerical methods. We can raise the step-size applying finite volume or finite element discretization schemes to model the curved surfaces. With the so-called hybrid methods we can avoid the unnecessarily small step-sizes, which are necessitated by the avoidance of the staircased boundaries. Applying higher order methods we can also enlarge the step-size keeping the accuracy.

- Because the MAXWELL-equations have a non-stiff property, it is generally solved by explicit numerical methods, like the FDTD method. As we have seen, FDTD has a stability restriction $\Delta t \leq \text{const.} \cdot h$, where the constant is relatively small. This restriction is consistent with what we would choose anyway based on accuracy consideration, because the $FDTD$ method has a local approximation error of order $\mathcal{O}(\Delta t^2 + h^2)$ (it applies central differences both in spatial and time dimension). It is known that for implicit schemes there are no upper bounds for the choice of the time-step, thus the restriction for the time-step comes from accuracy investigations and has the form $\Delta t \leq \mathcal{O}(h)$. This means that we cannot choose arbitrarily large time-steps even constructing an unconditionally stable scheme. We can generally say that if we would like a very accurate solution then we should apply explicit methods (the method is slow), while if we would like the solution after a relatively large time-period, then the best possibility is to apply an unconditionally stable method with a suitable large time-step (the method is relatively inaccurate). This is why we have to find the balance between the accuracy and an acceptable relative advancing speed in case of each application.

  The methods which apply implicit or semi-implicit integration in time are very remarkable, especially when stability is more important than accuracy. The result of the paper [45] is very notable, because here we can increase the time-step up to the bound coming from the accuracy restrictions. For that matter we notice that the accuracy of the classical FDTD method is high enough, in most of cases greater approximation error is also satisfactory.

- The methods based on potentials are developing, and they can hold new possibilities for an efficient numerical simulation of the MAXWELL equations (see [2, 8, 9]).

- If there are acute angels at the boundaries of the scatterers, then the cell-size must be small to model adequately the curved surface. In these cases Finite Element or Finite Volume methods are suggested to apply. It could be very efficient the use of hybrid methods, where inside the computational domain we apply a structured grid with the original FDTD method and an unstructured grid at the boundaries with Finite Element or Finite Volume Method.

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