Solving the Maxwell Equations by the Chebyshev Method: A One-Step Finite-Difference Time-Domain Algorithm

Hans De Raedt, Kristel Michielsen, J. Sebastiaan Kole, and Marc Thilo Figge

***Abstract*—We present a one-step algorithm that solves the Maxwell equations for systems with spatially varying permittivity and permeability by the Chebyshev method. We demonstrate that this algorithm may be orders of magnitude more efficient than current finite-difference time-domain (FDTD) algorithms.**

***Index Terms*—Electromagnetic propagation, finite-difference time-domain (FDTD) methods, Maxwell equations.**

I. Introduction

MOST finite-difference time-domain (FDTD) methods solve the time-dependent Maxwell equations using algorithms based on a proposal by Yee [1]–[3]. The Yee algorithm is flexible, fast, and easy to implement. A limitation of Yee-based FDTD techniques is that their stability is conditional, meaning that their numerical stability depends on the mesh size used for the spatial discretization and on the time step of the time integration [2], [3]. In practice, the amount of computational work required to solve the time-dependent Maxwell equations by present FDTD techniques [2]–[10] prohibits applications to a class of important fields such as bioelectromagnetics and VLSI design [2], [11], [12]. The basic reason for this is that the time step in the FDTD calculation has to be relatively small in order to maintain a reasonable degree of accuracy in the time integration.

In this paper, we describe a one-step algorithm, based on Chebyshev polynomial expansions [13]–[19], to solve the time-dependent Maxwell equations for arbitrarily long times. We demonstrate that the computational efficiency of this one-step algorithm can be orders of magnitude larger than of other FDTD techniques.

II. Algorithm

We consider electromagnetic (EM) fields in linear, isotropic, nondispersive and lossless materials. The time evolution of EM fields in these systems is governed by the time-dependent Maxwell equations [20]. Some important physical symmetries of the Maxwell equations can be made explicit by introducing the fields

$$\mathbf{X}(t) \equiv \sqrt{\mu}\mathbf{H}(t) \quad \text{and} \quad \mathbf{Y}(t) \equiv \sqrt{\varepsilon}\mathbf{E}(t). \tag{1}$$

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Here, $\mathbf{H}(t) = (H_x(\mathbf{r},t), H_y(\mathbf{r},t), H_z(\mathbf{r},t))^T$ denotes the magnetic and $\mathbf{E}(t) = (E_x(\mathbf{r},t), E_y(\mathbf{r},t), E_z(\mathbf{r},t))^T$ the electric field vector, while $\mu = \mu(\mathbf{r})$ and $\varepsilon = \varepsilon(\mathbf{r})$ denote, respectively, the permeability and the permittivity. The velocity of light in vacuum is given by $c = 1/\sqrt{\varepsilon_0\mu_0}$ (in MKS units), where ε_0 denotes the permittivity and μ_0 the permeability in vacuum. In the absence of electric charges, Maxwell's curl equations [2] read

$$\frac{\partial}{\partial t}\begin{pmatrix}\mathbf{X}(t)\\ \mathbf{Y}(t)\end{pmatrix} = \mathcal{H}\begin{pmatrix}\mathbf{X}(t)\\ \mathbf{Y}(t)\end{pmatrix} - \frac{1}{\sqrt{\varepsilon}}\begin{pmatrix}0\\ \mathbf{J}(t)\end{pmatrix} \tag{2}$$

where $\mathbf{J} = (J_x(\mathbf{r},t), J_y(\mathbf{r},t), J_z(\mathbf{r},t))^T$ represents the source of the electric field and $\mathcal{H}$ denotes the operator

$$\mathcal{H} \equiv \begin{pmatrix} 0 & -\frac{1}{\sqrt{\mu}}\nabla\times\frac{1}{\sqrt{\varepsilon}} \\ \frac{1}{\sqrt{\varepsilon}}\nabla\times\frac{1}{\sqrt{\mu}} & 0 \end{pmatrix}. \tag{3}$$

Writing $\mathbf{Z}(t) = (\mathbf{X}(t), \mathbf{Y}(t))^T$ it is easy to show that $\mathcal{H}$ is skew symmetric, i.e., $\mathcal{H}^T = -\mathcal{H}$, with respect to the inner product $\langle \mathbf{Z}|\mathbf{Z}'\rangle \equiv \int_V \mathbf{Z}^T\cdot\mathbf{Z}'d\mathbf{r}$, where V denotes the system's volume. In addition to (2), the EM fields also satisfy $\nabla\cdot(\sqrt{\mu}\mathbf{X}(t)) = 0$ and $\nabla\cdot(\sqrt{\varepsilon}\mathbf{Y}(t)) = 0$. If we measure distances in units of the wave length λ, time and frequency are expressed in units of λ/c and c/λ, respectively. The Maxwell equations take a dimensionless form if we replace $\varepsilon(\mu)$ by its value relative to $\varepsilon_0(\mu_0)$ and express $\mathbf{H}$ and $\mathbf{E}$ in units of A/m and V/m, respectively. In the following we adopt this dimensionless form and use the dimensionless quantities $\mathbf{H}$, $\mathbf{E}$, ε, μ, t, and $\mathbf{r}$.

A numerical algorithm that solves the time-dependent Maxwell equations necessarily involves some discretization procedure of the spatial derivatives in (2). As we explain later, the rigorous mathematical justification of the one-step algorithm is very simple if the discretization procedure does not change the basic symmetries of the Maxwell equations, meaning that the matrix correspondig to the operator $\mathcal{H}$ should also be skew symmetric. Any of the many different discretization procedures (for an overview see [2]) can be used as long as it preserves this fundamental physical symmetry (for explicit examples also see [10]). In our numerical examples we adopt the standard Yee-lattice discretization scheme [2] and fix the mesh size $\delta = 0.1$. We will use the term **exact solution** as an abbreviation for **rigorous solution of the discretized Maxwell equations on a grid with a fixed mesh size δ and a fixed discretization method**. Of course, the rigorous solution on the grid with mesh size $\delta > 0$ will differ from the rigorous solution of the original continuum problem because of numerical dispersion [2]. The accuracy of the solution on the grid

can be improved by reducing δ and/or using a more accurate discretization scheme [2], [10]. In this paper, we do not discuss this (important) aspect of spatial discretization as it is not essential to the construction of the one-step algorithm (assuming the basic physical symmetry of the Maxwell equations is not changed). Thus, we focus entirely on the time integration of the problem defined on the Yee grid.

On a spatial grid Maxwell's curl equations (2) can be written in the compact form [9], [10]

$$\frac{\partial}{\partial t}\mathbf{\Psi}(t) = H\mathbf{\Psi}(t) - \mathbf{\Phi}(t). \tag{4}$$

The vector $\mathbf{\Psi}(t)$ is a representation of $\mathbf{Z}(t)$ on the grid. The skew-symmetric matrix H is the discrete analogue of the operator (3), and the vector $\mathbf{\Phi}(t)$ contains all the information on the current source $\mathbf{J}$. The formal solution of (4) is given by

$$\mathbf{\Psi}(t) = U(t)\mathbf{\Psi}(0) - \int_0^t U(t-u)\mathbf{\Phi}(u)du \tag{5}$$

where $U(t) = e^{tH}$ denotes the time-evolution matrix. The underlying physical symmetries of the time-dependent Maxwell equations are reflected by the fact that the matrix H is real and skew symmetric [9], implying that $U(t)$ is orthogonal [21]. In practice it is trivial to check whether H is skew-symmetric or not.

Numerically, the time integration is carried out by using a time-evolution operator $\overline{U}(t)$ that is an approximation to $U(t) = e^{tH}$. We denote the approximate solution by $\overline{\mathbf{\Psi}}(t)$. First we use the Chebyshev polynomial expansion to approximate $U(t)$ and then show how to treat the source term in (5). We begin by "normalizing" the matrix H. The eigenvalues of the skew-symmetric matrix H are pure imaginary numbers. In practice H is sparse so it is easy to compute $\|H\|_1 \equiv \max_j \sum_i |H_{i,j}|$. Since $B \equiv -iH/\|H\|_1$ is real and symmetric, it is diagonalizable (i.e. it has a complete set of orthonormal eigenvectors), all its eigenvalues are real and lie in the interval [−1,1] [21], [22]. Expanding the initial value $\mathbf{\Psi}(0)$ in the (unknown) eigenvectors $\mathbf{b}_j$ of B, we find from (5) with $\mathbf{\Phi}(t) = 0$

$$\mathbf{\Psi}(t) = e^{tH}\mathbf{\Psi}(0) = e^{izB}\mathbf{\Psi}(0) = \sum_j e^{izb_j}\mathbf{b}_j \langle \mathbf{b}_j | \mathbf{\Psi}(0) \rangle \tag{6}$$

where the b_j denote the (unknown) eigenvalues of B and $z = t\|H\|_1$. Although there is no need to know the eigenvalues and eigenvectors of B explicitly, it is important to note that in writing down (6), we implicitly assumed that the matrix H has a complete set of eigenvectors. A sufficient condition for this assumption to be true is that H is normal, i.e. $HH^T = H^T H$ [21], [22] (note that this would extend the range of applicability to include nondispersive electric and magnetic losses). On the other hand, if the eigensystem of H is ill-conditioned and/or H's departure from normality is large, the difference between e^{izB} and some matrix polynomial approximation may be considerably larger than the maximum of the difference between e^{izx} the corresponding scalar polynomial approximation over all $x \in [-1, 1]$ [22], [23]. Thus, unless H is normal, the mathematical justification of the Chebyshev polynomial approach requires additional conditions and a much more complicated analysis [24].

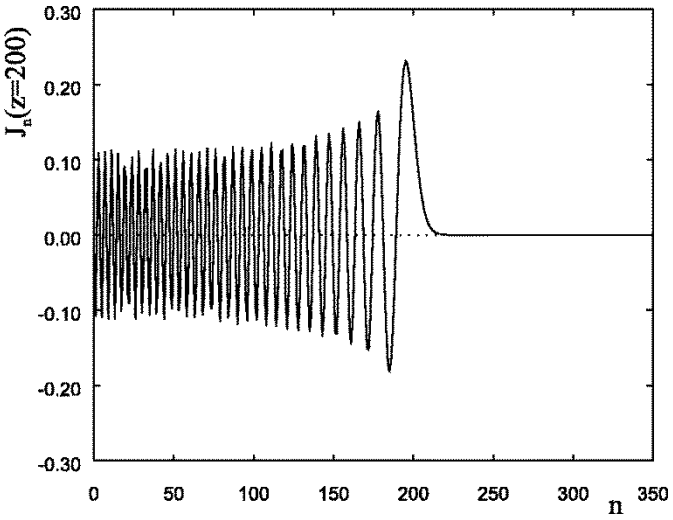

Fig. 1. Dependence of the Bessel function $J_n(z = 200)$ on the order n.

For the case at hand we find the Chebyshev polynomial expansion of $\mathbf{\Psi}(t)$ by computing the Fourier coefficients of the function $e^{iz\cos\theta}$ [25]. Alternatively, since $-1 \le b_j \le 1$, we can use the expansion [25] $e^{izb_j} = J_0(z) + 2\sum_{k=1}^{\infty} i^k J_k(z) T_k(b_j)$, where $J_k(z)$ is the Bessel function of integer order k, to write (6) as

$$\mathbf{\Psi}(t) = \left[J_0(z)I + 2\sum_{k=1}^{\infty} J_k(z)\widetilde{T}_k(B) \right] \mathbf{\Psi}(0). \tag{7}$$

Here, I is the identity matrix and $\widetilde{T}_k(B) = i^k T_k(B)$ is a matrix-valued modified Chebyshev polynomial that is defined by the recursion relations

$$\widetilde{T}_0(B)\mathbf{\Psi}(0) = \mathbf{\Psi}(0), \quad \widetilde{T}_1(B)\mathbf{\Psi}(0) = iB\mathbf{\Psi}(0) \tag{8}$$

and

$$\widetilde{T}_{k+1}(B)\mathbf{\Psi}(0) = 2iB\widetilde{T}_k(B)\mathbf{\Psi}(0) + \widetilde{T}_{k-1}(B)\mathbf{\Psi}(0) \tag{9}$$

for $k \ge 1$. From numerical analysis it is known that for fixed K, the Chebyshev polynomial is very nearly the same polynomial as the minimax polynomial [26], i.e., the polynomial of degree K that has the smallest maximum deviation from the true function, and is much more accurate than for instance a Taylor expansion of the same degree K [23].

In practice we (will have to) truncate the sum in (7), i.e., to obtain the approximation $\overline{\mathbf{\Psi}}(t)$ we will sum only the contributions with $k \le K$. The procedure to find K is most easily understood by looking at the plot of the expansion coefficients as a function of k. From Fig. 1 it is clear that $|J_k(z)|$ vanishes rapidly if k becomes larger than z. For instance, $|J_k(z = 200)| < 10^{-10}$ for all $k > z+100$. Thus we can fix the number K by requiring that $|J_k(t\|H\|_1)| > \kappa$ for all $k \le K$. Here κ is a small number that determines the accuracy of the approximation. In our numerical experiments we use conventional 14–15 digit floating-point arithmetic and we have taken $\kappa = 10^{-10}$. Once we have found the smallest K such that $|J_k(t\|H\|_1)| > \kappa$ for all $k \le K$, there is no point of taking more than K terms in the expansion. Indeed, since $\|\widetilde{T}_k(H/\|H\|_1)\| \le 1$ by construction of the modified Chebyshev polynomials, it follows from Fig. 1 that such contributions would only add to the noise. However, taking less

than z terms has considerable negative impact on the accuracy of the results. Hence, in practice the choice of K is rather limited (e.g., $K \in [z, z+100]$ if $z = 200$). In any case, for fixed κ, K increases linearly with $t\|H\|_1$.

Performing one time step amounts to repeatedly using recursion (9) to obtain $\widetilde{T}_k(B)\mathbf{\Psi}(0)$ for $k = 2, \ldots, K$, multiply the elements of this vector by $J_k(z)$ and add all contributions. This procedure requires storage for two vectors of the same length as $\mathbf{\Psi}(0)$ and some code to multiply such a vector by the sparse matrix H. The result of performing one time step yields the solution at time t, hence, the name one-step algorithm. In contrast to what (8) and (9) might suggest, the algorithm does not require the use of complex arithmetic.

We now turn to the treatment of the current source $\mathbf{J}(t)$. The contribution of the source term to the EM field at time t is given by the last term in (5). One approach might be to use the Chebyshev expansion (7) for $U(t-u) = e^{(t-u)H}$ and to perform the integral in (5) numerically. However, that is not efficient as for each value of $t-u$ we would have to perform a recursion of the kind (9). Thus, it is better to adopt another strategy. For simplicity, we first consider a sinusoidal source

$$\mathbf{J}(\mathbf{r}, t) = \Theta(T-t)\mathbf{s}(\mathbf{r})\sin(\Omega t) \tag{10}$$

where $\mathbf{s}(\mathbf{r})$ specifies the spatial distribution and Ω the angular frequency of the source. The step function $\Theta(T-t)$ indicates that the source is turned on at $t = 0$ and is switched off at $t = T$.

The formal solution for the contribution of the sinusoidal source (10) reads

$$\begin{aligned}\int_0^t e^{(t-u)H}\mathbf{\Phi}(u)du &= (\Omega^2 + H^2)^{-1}e^{t-T'H} \\ &\quad \times \left(\Omega e^{T'H} - \Omega\cos\Omega T' - H\sin\Omega T'\right)\mathbf{\Xi} \\ &\equiv f(H, t, T', \Omega)\mathbf{\Xi}\end{aligned} \tag{11}$$

where $T' = \min(t, T)$ and $\mathbf{\Phi}(u) \equiv \Theta(T-t)\sin(\Omega t)\mathbf{\Xi}$ with $\mathbf{\Xi}$ a vector of the same length as $\mathbf{\Psi}(0)$ that represents the time-independent, spatial distribution $\mathbf{s}(\mathbf{r})$. The coefficients of the Chebyshev polynomial expansion of the formal solution (11) are calculated as follows. First we repeat the scaling procedure described earlier and substitute in (11) $H = ix\|H\|_1$, $t = z/\|H\|_1$, $T' = Z'/\|H\|_1$, and $\Omega = \omega\|H\|_1$. Then, we compute the (Fast) Fourier Transform with respect to $x = \cos\theta$ of the function $f(\cos\theta, z, Z', \omega)$ (which is nonsingular on the interval $0 \le \theta \le \pi$). By construction, the Fourier coefficients $S_k(t\|H\|_1)$ are the coefficients of the Chebyshev polynomial expansion [25].

Taking into account all contributions of the source term with k smaller than K' (determined by a procedure similar to the one for K), the one-step algorithm to compute the EM fields at time t reads

$$\begin{aligned}\overline{\mathbf{\Psi}}(t) = &\left[J_0\left(t\|H\|_1\right)I + 2\sum_{k=1}^{K} J_k\left(t\|H\|_1\right)\widetilde{T}_k(B)\right]\mathbf{\Psi}(0) \\ &- \left[S_0\left(t\|H\|_1\right)I + 2\sum_{k=1}^{K'} S_k\left(t\|H\|_1\right)\widetilde{T}_k(B)\right]\mathbf{\Xi}.\end{aligned} \tag{12}$$

Other types of sources can be treated in the same manner but, in order to reduce the computational work to obtain the coefficients $S_k(t\|H\|_1)$, it is expedient to choose the time dependence of the source term such that the convolution integral in (5) can be found in closed form. For instance, for the modulated Gaussian pulsed source defined by [2]

$$\mathbf{J}(\mathbf{r}, t) = \mathbf{s}(\mathbf{r})e^{-\alpha(t-t_0)^2}\cos(\Omega t + \varphi) \tag{13}$$

where α, t_0, Ω, and φ are the source parameters. The coefficients $S_k(t\|H\|_1)$ are obtained by (Fast) Fourier transformation with respect to the angle θ of the function

$$\begin{aligned}p(\cos\theta) = &\frac{\sqrt{\pi}e^{i(z-z_0)\cos\theta}}{4\|H\|_1\sqrt{\beta}} \\ &\times \left\{e^{-\frac{(\cos\theta-\omega)^2}{4\beta+i(\omega z_0+\varphi)}}\left[\operatorname{erf}\left(\frac{2\beta(z-z_0)+i(\cos\theta-\omega)}{2\sqrt{\beta}}\right)\right.\right. \\ &\left.+\operatorname{erf}\left(\frac{2\beta z_0 - i(\cos\theta-\omega)}{2\sqrt{\beta}}\right)\right] + e^{-\frac{(\cos\theta+\omega)^2}{4\beta-i(\omega z_0+\varphi)}} \\ &\times \left[\operatorname{erf}\left(\frac{2\beta(z-z_0)+i(\cos\theta+\omega)}{2\sqrt{\beta}}\right)\right. \\ &\left.\left.+\operatorname{erf}\left(\frac{2\beta z_0 - i(\cos\theta+\omega)}{2\sqrt{\beta}}\right)\right]\right\}\end{aligned} \tag{14}$$

where $\beta = \alpha/\|H\|_1^2$ and $z_0 = t_0/\|H\|_1$. Note that in our one-step approach the time dependence of the source is taken into account exactly, without actually sampling it. Furthermore, from the derivation of (11) or (14) it is clear that from a mathematical point of view there is no restriction on Ω. However, it is easy to see from (11) [or (14)] that the functional dependence on $\cos\theta$ changes character if $|\omega|$ becomes larger than one. This reflects the fact that the numerical values on nodes of the grid may not yield a physically meaningful representation of the solution unless $|\Omega|$ is (much) smaller than the maximum frequency ($\le \|H\|_1 \propto 1/\delta$) supported by the grid with mesh size δ.

III. Results

The following two examples illustrate the efficiency of the one-step algorithm. First we consider a system in vacuum ($\varepsilon = \varepsilon_0$ and $\mu = \mu_0$) which is infinitely large in the y and z direction, hence, effectively one dimensional (1-D), and subject to perfectly reflecting boundary conditions [2]. The current source (10) is placed at the center of a system of length 250.1 and oscillates with angular frequency $\Omega = 1$ during the time interval $0 \le t \le T = 8\pi$. In Table I, we present results of numerical experiments with two different FDTD algorithms. The time step used is denoted by τ and the mesh size $\delta = 0.1$ of the Yee-type grid is kept fixed. We define the error of a solution $\widetilde{\mathbf{\Psi}}(t)$ obtained by the FDTD algorithm of Yee [1], [2] or the unconditionally stable FDTD algorithm $T4S2$ [9], [10] by $\Delta(t) \equiv \|\widetilde{\mathbf{\Psi}}(t) - \overline{\mathbf{\Psi}}(t)\|/\|\overline{\mathbf{\Psi}}(t)\|$, where $\overline{\mathbf{\Psi}}(t)$ denotes the vector of the EM fields as obtained by the one-step algorithm. The error on the Yee-algorithm result vanishes as τ^2 for sufficiently small τ [1], [2]. However, as Table I shows, unless τ is made sufficiently small ($\tau \le 0.0125$ in this example), the presence of the source term changes the quadratic behavior to almost linear.

The rigorous bound on the error between the exact and $T4S2$ results tells us that this error should vanish as τ^4 [9], [27]. This knowledge can be exploited to test if the one-step algorithm

TABLE I
ERROR $\Delta(t)$ AFTER SIMULATION TIME $t = 100$ AS A FUNCTION OF THE TIME STEP τ FOR TWO FDTD ALGORITHMS. THE NUMBER OF MATRIX-VECTOR OPERATIONS REQUIRED TO COMPUTE THE SOLUTION IS $K' = 2080, t/\tau$, AND $6t/\tau$ FOR THE ONE-STEP, YEE, AND $T4S2$ ALGORITHM, RESPECTIVELY

τ	Yee	$T4S2$
$0.10000 \times 10^{+0}$	0.75×10^{-1}	0.51×10^{-1}
0.50000×10^{-1}	0.25×10^{-1}	0.33×10^{-2}
0.25000×10^{-1}	0.12×10^{-1}	0.21×10^{-3}
0.12500×10^{-1}	0.66×10^{-2}	0.13×10^{-4}
0.62500×10^{-2}	0.24×10^{-2}	0.91×10^{-6}
0.31250×10^{-2}	0.63×10^{-3}	0.30×10^{-6}
0.15625×10^{-2}	0.16×10^{-3}	0.15×10^{-7}
0.78125×10^{-3}	0.39×10^{-4}	0.60×10^{-8}

yields the exact numerical answer for the problem defined on the grid. Using the triangle inequality, we can write

$$\left\|\boldsymbol{\Psi}(t) - \overline{\boldsymbol{\Psi}}(t)\right\| \le \left\|\boldsymbol{\Psi}(t) - \widetilde{\boldsymbol{\Psi}}(t)\right\| + \left\|\widetilde{\boldsymbol{\Psi}}(t) - \overline{\boldsymbol{\Psi}}(t)\right\|$$
$$\le \tau^4 t C \left(\|\boldsymbol{\Psi}(0)\| + \int_0^t \|\mathbf{J}(u)\|\, du \right) + \Delta(t) \left\|\overline{\boldsymbol{\Psi}}(t)\right\| \quad (15)$$

where C is a positive constant [27]. The numerical data in Table I (third column) show that $\Delta(t) \to 0$ as τ^4 and, therefore, we can be confident that the one-step algorithm yields the correct answer within rounding errors. Furthermore, since the results of the one-step algorithm are exact within almost machine precision, in general the solution also satisfies $\nabla \cdot (\sqrt{\mu}\mathbf{X}(t)) = 0$ and $\nabla \cdot (\sqrt{\varepsilon}\mathbf{Y}(t)) = 0$ within the same precision.

In a strict mathematical sense we can only prove that $\|\boldsymbol{\Psi}(t) - \overline{\boldsymbol{\Psi}}(t)\| \le \epsilon_K \|\boldsymbol{\Psi}(0)\| + \epsilon_{K'} \int_0^t \|\mathbf{J}(u)\| du$, leaving open the possiblity that using the one-step algorithm for genuine time-stepping may yield a numerically unstable procedure. However, in practice, the errors ϵ_K and $\epsilon_{K'}$ of the Chebyshev polynomial approximations are very small, almost zero within machine precision. It is this high precision that allows the use of the one-step algorithm as a genuine time-stepping algorithm with (very) large time steps.

From Table I it follows that if one finds an error of more than 2.5% acceptable, one could use the Yee algorithm, though we recommend to use the one-step algorithm because then the time-integration error is neglegible. The Yee algorithm is no competition for the $T4S2$ algorithm if one requires an error of less than 1%, but the $T4S2$ algorithm is not nearly as efficient as the one-step algorithm with respect to the number of required matrix-vector operations.

A more general quantitative analysis of the efficiency can be made using the fact that for an nth-order algorithm ($n = 2$ for the Yee algorithm and $n = 4$ for the $T4S2$ algorithm), the error $\Delta(t)$ vanishes no faster with τ than $\tau^n t$. Each time step takes a number $W(n)$ of matrix-vector operations (of the type $\boldsymbol{\Psi}' \leftarrow M\boldsymbol{\Psi}$), e.g., for a 3-D system we have $W(2) = 1$ and $W(4) = 10$ for the Yee algorithm and the $T4S2$ algorithm, respectively. In practice, the actual number of floating point operations carried out by our algorithms agrees with these estimates. The total number of matrix-vector operations it takes to obtain the solution at a reference time t_r with error $\Delta_r(t_r)$ is then given by $N_r = W(n)t_r/\tau_r$ and thus $\Delta_r(t_r) \propto W(n)^n t_r^{n+1}/N_r^n$. The number of operations N that it will take to compute the EM fields at time t with accuracy $\Delta(t)$ is then calculated from

$$N = N_r \left(\frac{\Delta_r(t_r)}{\Delta(t)} \right)^{\frac{1}{n}} \left(\frac{t}{t_r} \right)^{\frac{(n+1)}{n}}. \quad (16)$$

We note that one numerical reference experiment per n th-order algorithm is sufficient to determine the parameters N_r, $\Delta_r(t_r)$, and t_r. While these parameters may be different for different systems, the scaling of N with $t^{3/2}$ and with $t^{5/4}$, respectively, for second- and fourth-order algorithms, will not be affected. Most importantly, since the number of matrix-vector operations required by the one-step algorithm scales linearly with t, it is clear that for long enough times t, the one-step algorithm will be orders of magnitude more efficient than the current FDTD methods. In Fig. 2 we show the required number of operations as a function of time t taking, as an example, simulation data of 3-D systems (discussed later) to fix the parameters N_r, $\Delta_r(t_r)$, and t_r. We conclude that for longer times none of the FDTD algorithms can compete with the one-step algorithm in terms of efficiency. For $t = 20$, the one-step algorithm is a factor of 10 faster than the Yee algorithm. Thereby, we have disregarded the fact that the Yee algorithm yields results within an error of 0.1% while the one-step algorithm gives the numerically exact solution.

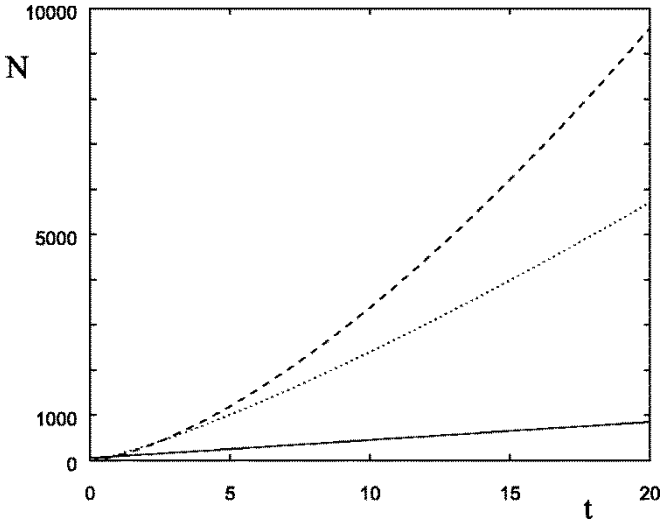

Fig. 2. The number of $\boldsymbol{\Psi}' \leftarrow M\boldsymbol{\Psi}$ operations N needed to compute the solution of the 3-D Maxwell equation at time t for systems like those shown in Fig. 3. Solid line: One-step algorithm; dashed line: Yee algorithm [1]–[3] yielding a solution within 0.1% error; dotted line: T4S2 algorithm [9], [10] yielding a solution within 0.1% error.

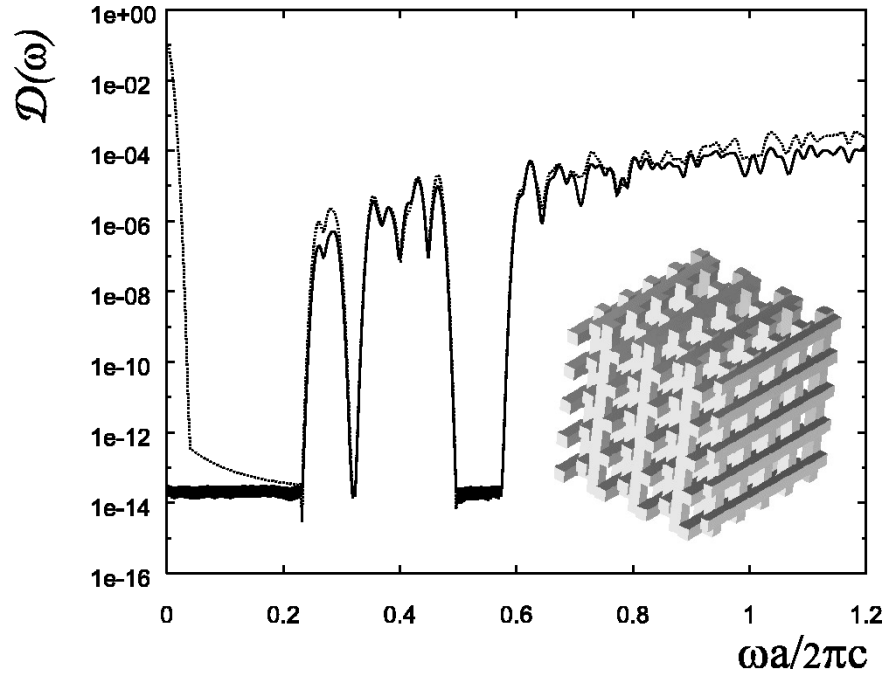

Fig. 3. Frequency spectrum of a 3-D photonic woodpile (inset) [28] as obtained by $T4S2$ (dashed line) and the one-step algorithm (solid line). The width, height, and period (a) of the rods are 0.55, 0.7, and 2, respectively. The dielectric constant of the rods is 12.96 and the simulation box measures $6 \times 6 \times 5.6$, subject to periodic boundary conditions.

For $t \rightarrow \infty$ and for a fixed accuracy, (16) shows that the one-step algorithm will be more efficient than any FDTD algorithm (for which $n < \infty$). However, this does not mean that the one-step algorithm is computationally more efficient than FDTD algorithms for all cases of interest. First of all, the asymptotic long-time behavior and/or very high accuracy of the time integration is not always of interest. In terms of computational work, the one-step algorithm becomes (much) less competitive if the application requires knowledge of the EM fields at many intermediate times (recall that intermediate results generated during the recursion (9) have no physical significance). Moreover, the present mathematical justification of the one-step algorithm limits the range of applications. For instance, FDTD methods can easily handle absorbing boundary conditions [2] but at present, there is no guarantuee that the Chebyshev polynomial approximation will still be accurate in these circumstances. As with most numerical algorithms, also in this case the method of choice depends on the application but it is a good practice to use several completely different methods to solve the same problem.

As the second example we use the one-step algorithm to compute the frequency spectrum of a 3-D photonic woodpile [28]. This structure, shown in the inset of Fig. 3, possesses a large infrared bandgap and is under current experimental and theoretical investigation [28], [29]. To determine all eigenvalues of the corresponding matrix H we follow the procedure described in [9], [30], [31]. We use random numbers to initialize the elements of the vector $\mathbf{\Psi}(0)$. Then we calculate the inner product $F(t) = \langle \mathbf{\Psi}(0) | \mathbf{\Psi}(t) \rangle$ as a function of t and average $f(t) = F(t)/F(0)$ over several realizations of the initial vector $\mathbf{\Psi}(0)$. The full eigenmode distribution $\mathcal{D}(\omega)$ is obtained by Fourier transformation of $f(t)$. In Fig. 3 we show $\mathcal{D}(\omega)$, as obtained by $T4S2$ and the one-step algorithm, with a time step $\tau = 0.075$ (set by the largest eigenvalue of H), a mesh size $\delta = 0.1$, and 8192 time steps. For this choice of parameters, the Yee algorithm would be unstable [2], [3] and would yield meaningless results. The $T4S2$ calculation shows a peak at $\omega = 0$. This reflects the fact that, in a strict sense, the $T4S2$ algorithm does not conserve $\nabla \cdot (\sqrt{\mu}\mathbf{X}(t))$ and $\nabla \cdot (\sqrt{\varepsilon}\mathbf{Y}(t))$ [9], [10]. However, the peak at $\omega = 0$ vanishes as τ^4. Repeating the $T4S2$ calculation with $\tau = 0.01$ yields a $\mathcal{D}(\omega)$ (not shown) that is on top of the result of the one-step algorithm (see Fig. 3) and is in good agreement with band-structure calculations [28]. For $\tau = 0.01$ the one-step algorithm is 3.5 times more efficient than $T4S2$. Note that in this example, the one-step algorithm is used for a purpose for which it is least efficient (time-stepping with relatively small time steps). Nevertheless, the gain in efficiency is still substantial. In simulations of the scattering of the EM fields from the same woodpile (results not shown), the one-step algorithm is one to two orders of magnitude more efficient than current FDTD algorithms, in full agreement with the error scaling analysis given earlier.

IV. Conclusion

We have described a one-step algorithm, based on the Chebyshev polynomial expansions, to solve the time-dependent Maxwell equations with spatially varying permittivity and permeability and current sources. In practice, this algorithm is as easy to implement as FDTD algorithms. Our error scaling analysis shows and our numerical experiments confirm that for long times the one-step algorithm can be orders of magnitude more efficient than current FDTD algorithms. This opens possibilities to solve problems in computational electrodynamics that are currently intractable.

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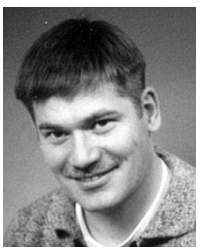

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