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Abstract. We present a one-step algorithm to solve the time-dependent Maxwell equations for systems with spatially varying permittivity and permeability. We compare the results of this algorithm with those obtained from unconditionally stable algorithms and demonstrate that for a range of applications the one-step algorithm may be orders of magnitude more efficient than multiple time-step, finite-difference time-domain algorithms. We discuss both the virtues and limitations of this one-step approach.

1 Introduction

Many applications in physics and engineering require numerical methods to solve the time-dependent Maxwell equations (TDME) [1]. A popular approach is the finite-difference time-domain (FDTD) method [1] based on a proposal by Yee [2]. It is flexible, fast and easy to implement. A limitation of Yee-based FDTD techniques is that their stability is conditional, depending on the mesh size of the spatial discretization and the time step of the time integration [1].

Recently we have introduced a family of unconditionally stable algorithms to solve the TDME [3–5]. The operator that governs the time evolution of the electromagnetic (EM) fields is orthogonal and can be written as the matrix exponential of a skew-symmetric matrix [3, 5]. Orthogonal approximations to the time-evolution operator yield unconditionally stable algorithms by construction [13]. Details of the construction of such algorithms can be found elsewhere [3, 5].

A limitation of both the Yee-based [1] and our unconditionally stable algorithms [3, 5] is that the amount of computational work required to propagate the EM fields for long times may be prohibitive for a class of important applications, such a bioelectromagnetics and VLSI design [1, 6, 7]. The basic reason for this is that in order to maintain a reasonable degree of accuracy during the time integration, the time step has to be relatively small. In addition, in the Yee-based approach the time step is also limited by the Courant number [1].

A well-known alternative to time-stepping is to use Chebyshev polynomials to construct approximations to the time-evolution operator [8–10, 12]. In this paper we make use of these rapidly converging polynomial approximations to construct a one-step algorithm that solves the TDME. Also in this case the orthogonality of the time-evolution operator plays a key role in the construction of the algorithm.

2 One-step algorithm

In the absence of charges and currents, the TDME can be written as [3, 5]

$$\frac{\partial}{\partial t}\Psi(t) = \mathcal{H}\Psi(t), \tag{1}$$

where $\Psi(t)$ is a vector that contains all information on the magnetic fields $\mathbf{H} = (H_x(\mathbf{r},t), H_y(\mathbf{r},t), H_z(\mathbf{r},t))^T$ and electric fields $\mathbf{E} = (E_x(\mathbf{r},t), E_y(\mathbf{r},t), E_z(\mathbf{r},t))^T$. The operator $\mathcal{H}$ is a compact representation for the curl operators that appear in the Maxwell equations [3]. Its precise form is not important for what follows. We will only use the fact that $\mathcal{H}$ is skew-symmetric, i.e. $\mathcal{H}^T = -\mathcal{H}$, with respect to the inner product $\langle\Psi|\Psi'\rangle \equiv \int_V \Psi^T \cdot \Psi'\, d\mathbf{r}$, where V denotes the volume of the enclosing, perfectly conducting box. The formal solution of Eq. (1) is given by $\Psi(t) = U(t)\Psi(0) = e^{t\mathcal{H}}\Psi(0)$ where $\Psi(0)$ represents the initial state of the EM fields.

A numerical procedure that solves the TDME involves a discretization of the spatial derivatives. This maps the continuum problem described by $\mathcal{H}$ onto a lattice problem defined by a (sparse) matrix H. The underlying symmetry of the TDME suggests to use matrices H that are real and skew-symmetric. The discretization procedure itself is not essential for what follows as long as H is skew symmetric. We omit these technicalities here and refer the reader to Ref. [3].

The time evolution of the EM fields on the lattice is given by $\Psi(t+\tau) = U(\tau)\Psi(t) = e^{\tau H}\Psi(t)$. The final step in the construction of the numerical procedure to solve the Maxwell equation is to choose a (good) approximation of the time-evolution operator $U(\tau)$. In the case of the Chebyshev approach we proceed as follows.

First we "normalize" the matrix H. The eigenvalues of the skew-symmetric matrix H are pure imaginary numbers. Hence the eigenvalues of the Hermitian matrix $A = -iH$ are real and if a is one of these eigenvalues so is $-a$. The eigenvalues of A lie in the interval $[-\|A\|_2, \|A\|_2]$ where $\|A\|_2$ is the largest (in absolute value) eigenvalue of A [14]. Obviously $\|A\|_2$ is hard to find. However for our purposes we only need an upperbound to $\|A\|_2$. Since A is sparse it is easy to compute $\|A\|_1 \equiv \max_j \sum_i |A_{i,j}|$ and the upperbound follows from $\|A\|_2 \leq \|A\|_1$ [14]. Note that $\|A\|_1 = \|H\|_1$. By construction the eigenvalues of $B \equiv A/\|A\|_1 = -iH/\|H\|_1$ all lie in the interval $[-1, 1]$. The time-evolution operator then reads $U(t) = e^{tH} = e^{izB}$ where $z = t\|A\|_1$.

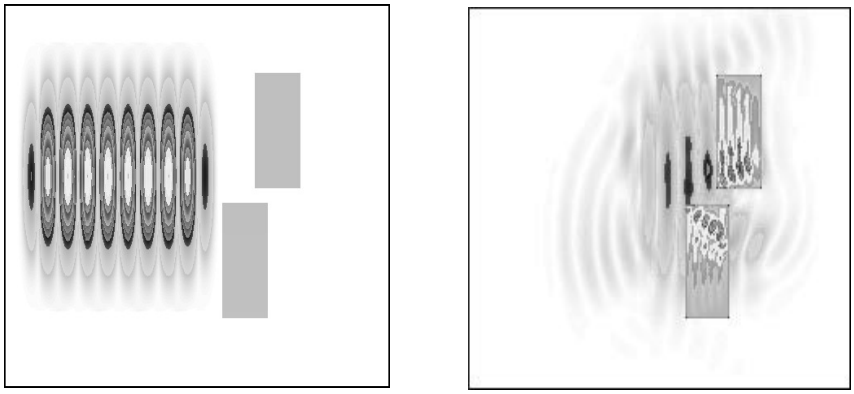

Fig. 1. Initial (left) and final distribution of the EM field intensity at $t = 5$ of the TM mode, as obtained from the numerical solution of the Maxwell equations by the one-step algorithm (5) with $K = 194$. The fourth-order unconditionally stable algorithm $T4S2$ [3, 4] yields the same pictures (not shown).

Expanding the initial value $\Psi(0)$ in the (unknown) eigenvectors $\mathbf{b}_j$ of B we have $\Psi(t) = U(t)\Psi(0) = e^{izB}\Psi(0) = \sum_j e^{izb_j}\mathbf{b}_j\langle\mathbf{b}_j|\Psi(0)\rangle$ where the b_j denote the (unknown) eigenvalues of B. Using $e^{izx} = J_0(z)+2\sum_{k=1}^{\infty} i^k J_k(z)T_k(x)$ where $J_n(z)$ is the Bessel function of integer order n and $T_n(x) = \cos(n \arccos x)$ is the n-th Chebyshev polynomial of the first kind [15], we obtain

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

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

$$\widetilde{T}_0(B)\Psi(0) = \Psi(0) \quad , \quad \widetilde{T}_1(B)\Psi(0) = iB\Psi(0), \tag{3}$$

$$\widetilde{T}_{k+1}(B)\Psi(0) = 2iB\widetilde{T}_k(B)\Psi(0) + \widetilde{T}_{k-1}(B)\Psi(0) \quad \text{for} \quad k \geq 1. \tag{4}$$

From Eqs.(3),(4) it is clear that $\widetilde{T}_k(B)\Psi(0)$ is real valued, as it should be in the case of the Maxwell equations.

In practice we will have to truncate the sum in Eq.(2), i.e. we will use only the first $K + 1$ contributions to approximate $U(t)\Psi(0)$:

$$\Psi(t) = e^{tH}\Psi(0) \approx \left[J_0(t\|H\|_1)I + 2\sum_{k=1}^{K} J_k(t\|H\|_1)\widetilde{T}_k(B)\right]\Psi(0). \tag{5}$$

As $\|T_k(B)\|_1 \leq 1$ by construction and $|J_k(z)| \leq |z|^k/2^k k!$ for z real [15], we may expect that the error of this approximation vanishes (exponentially) fast with increasing K if K is sufficiently large.

Table 1. Performance of the one-step algorithm that solves the TDME for three different times t as obtained from simulations of the two-dimensional system depicted in Fig.1. The fourth-order unconditionally stable algorithm $T4S2$ [3, 4] with a time step τ was used to compute $\Psi(t,\tau)$. The vector $\Psi(t)$, obtained by the Chebyshev method, was taken as reference for the calculation of the error $e = \|\Psi(t) - \Psi(t,\tau)\|$. N_H is the number of times the operation $H\Psi$ was carried out.

	$t=2$		$t=5$		$t=20$	
τ	e	N_H	e	N_H	e	N_H
0.100	2.5×10^{-3}	200	5.3×10^{-3}	500	1.8×10^{-2}	2000
0.010	4.0×10^{-7}	2000	8.5×10^{-7}	5000	2.9×10^{-6}	20000
0.001	4.0×10^{-11}	20000	8.5×10^{-11}	50000	2.9×10^{-10}	200000
Chebyshev	0	96	0	194	0	649

According to Eq.(5), performing one time step amounts to repeatedly using recursion (4) to obtain $\widetilde{T}_k(B)\Psi(0)$ for $k = 2, \ldots, K$, to multiply the elements of this vector by $J_k(t\|H\|_1)$ and to add all contributions. This procedure requires storage for two vectors of the same length as $\Psi(0)$ and some code to multiply such a vector by the sparse matrix H. The coefficients $J_k(t\|H\|_1)$ should be calculated to sufficiently high precision. The number K is fixed by requiring that $|J_k(t\|H\|_1)| < \kappa$ for all $k > K$. Here κ is a control parameter that determines the accuracy of the solution. Keeping κ fixed, it is evident that the larger $t\|H\|_1$, the larger K will have to be in order to keep the accuracy the same.

3 Simulation Results

In our simulations we measure distances in units of the wavelength λ and time in units of λ/c where c is the speed of light in vacuum. In Fig.1 we present numerical results for a two-dimensional system of size 12×10, with mesh size $\delta = 0.1$. The number of lattice sites in the x and y-direction is $L_x = 239$ and $L_y = 199$ respectively. The shape of the initial wave (see Fig.1, left) is $\exp(-((x-x_0)/\sigma_x)^{10} - ((y-y_0)/\sigma_y)^2)\sin(q(x-x_0))$ with a spread $\sigma_x = 2.75$ and $\sigma_y = 2$, is centered at $(x_0, y_0) = (3.5, 5.5)$ and has energy $\omega = q = 5$. Initially this wavepacket approaches the two rectangular blocks of dielectric material (permittivity $\varepsilon = 5$, permeability $\mu = 1$) from the left.

In Table I we present the results of an error analysis and arithmetic-operation count. The calculations have been carried out for the same system as in Fig.1. The fourth-order unconditionally stable algorithm $T4S2$ [3, 4] with a time step τ was used to compute $\Psi(t,\tau)$. From Table I we see that the error of T4S2 decreases as τ^4, as it should [13]. For $\tau = 0.001$ the result of T4S2 and of the one-step algorithm are about the same to working precision. Depending on the desired accuracy of the T4S2 calculation, the comparison of the N_H's of the one-step and T4S2 algorithm shows that the former can be orders of magnitude more

efficient. Also the Yee FDTD algorithm is no match for the one-step algorithm from the point of view of efficiency.

Although we have not yet made serious efforts to optimize the code, typically the one-step algorithm is more than an order of magnitude faster than FDTD algorithms [16]. This roughly matches our expectations based on a count of the number of arithmetic operations for the two methods, taking as input the value of K on the one hand, and the number of time steps and the order of the FDTD algorithms on the other. Our general conclusions are in concert with those drawn on the basis of numerical experiments with the Schrödinger equation [9].

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