Solving the Time-Dependent Maxwell Equations by Unconditionally Stable Algorithms

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Abstract. We present a family of unconditionally stable algorithms, based on the Suzuki product-formula approach, that solve the time-dependent Maxwell equations in systems with spatially varying permittivity and permeability. Salient features of these algorithms are discussed. As an illustration we compute, as a function of cluster size, the spectrum of electromagnetic modes in a cluster of photonic bandgap material.

1 Introduction

The Maxwell equations describe the evolution of electromagnetic (EM) fields in space and time [1]. They apply to a wide range of different physical situations and play an important role in a large number of engineering applications. In many cases, numerical methods are required to solve Maxwell's equations, either in the frequency or time domain. For the time domain, a well-known class of algorithms is based on a method proposed by Yee [2] and is called the finite-difference time-domain (FDTD) method. These algorithms owe their popularity mainly due to their flexibility and speed while at the same time they are 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 [3].

In this paper we describe a family of unconditionally stable algorithms that solve the time-dependent Maxwell equations (TDME) [4]. The key to the construction of these algorithms is the observation that orthogonal approximations to the (orthogonal) time evolution operator automatically yield unconditionally stable algorithms. The Lie-Trotter-Suzuki product formulae [5–7] provide the mathematical framework to construct orthogonal approximations to the time-evolution operator of the Maxwell equations.

2 Theory

We consider EM fields in a three-dimensional medium with spatially varying permittivity and/or permeability, surrounded by a perfectly conducting box. In

the absence of free charges and currents, the EM fields in such a system satisfy Maxwell's equations [3]

$$\frac{\partial}{\partial t}\,\mathbf{B} = -\nabla \times \mathbf{E} \quad \text{and} \quad \frac{\partial}{\partial t}\,\mathbf{D} = \nabla \times \mathbf{H}\,, \tag{1}$$

$$\operatorname{div}\mathbf{B} = 0 \quad \text{and} \quad \operatorname{div}\mathbf{D} = 0\,, \tag{2}$$

where $\mathbf{H} = (H_x(\mathbf{r},t), H_y(\mathbf{r},t), H_z(\mathbf{r},t))^T = \mu\mathbf{B}$ denotes the magnetic field, $\mu = \mu(\mathbf{r})$ is the permeability, $\mathbf{E} = (E_x(\mathbf{r},t), E_y(\mathbf{r},t), E_z(\mathbf{r},t))^T = \mathbf{D}/\varepsilon$ the electric field, and $\varepsilon = \varepsilon(\mathbf{r})$ denotes the permittivity. For simplicity of notation, we will omit the spatial dependence on $\mathbf{r} = (x,y,z)^T$ unless this leads to ambiguities. On the surface of the perfectly conducting box the EM fields satisfy the boundary conditions $\mathbf{n} \times \mathbf{E} = 0$ and $\mathbf{n} \cdot \mathbf{H} = 0$, with $\mathbf{n}$ denoting the vector normal to a boundary of the surface [1].

Some important symmetries of the Maxwell equations (1)-(2) can be made explicit by introducing the fields $\mathbf{X}(t) = \sqrt{\mu}\mathbf{H}(t)$ and $\mathbf{Y}(t) = \sqrt{\varepsilon}\mathbf{E}(t)$. In terms of the fields $\mathbf{X}(t)$ and $\mathbf{Y}(t)$, the TDME read

$$\frac{\partial}{\partial t}\begin{pmatrix}\mathbf{X}(t)\\ \mathbf{Y}(t)\end{pmatrix} = \begin{pmatrix} 0 & -\frac{1}{\sqrt{\mu}}\nabla \times \frac{1}{\sqrt{\varepsilon}} \\ \frac{1}{\sqrt{\varepsilon}}\nabla \times \frac{1}{\sqrt{\mu}} & 0 \end{pmatrix}\begin{pmatrix}\mathbf{X}(t)\\ \mathbf{Y}(t)\end{pmatrix} \equiv \mathcal{H}\begin{pmatrix}\mathbf{X}(t)\\ \mathbf{Y}(t)\end{pmatrix}. \tag{3}$$

Writing $\Psi(t) = (\mathbf{X}(t), \mathbf{Y}(t))^T$, Eq. (3) becomes $\frac{\partial}{\partial t}\Psi(t) = \mathcal{H}\Psi(t)$ It is easy to show that $\mathcal{H}$ is skew-symmetric, i.e. $\mathcal{H}^T = -\mathcal{H}$, with respect to the inner product $\langle\Psi|\Psi'\rangle \equiv \int_V \Psi^T \cdot \Psi'\, d\mathbf{r}$, where V denotes the volume of the enclosing box. The formal solution of the TDME 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. The operator $U(t) = e^{t\mathcal{H}}$ determines the time evolution. By construction $\|\Psi(t)\|^2 = \langle\Psi(t)|\Psi(t)\rangle = \int_V \left[\varepsilon\mathbf{E}^2(t) + \mu\mathbf{H}^2(t)\right]\, d\mathbf{r}$, relating the length of $\Psi(t)$ to the energy density $w(t) \equiv \varepsilon\mathbf{E}^2(t) + \mu\mathbf{H}^2(t)$ of the EM fields [1]. As $U(t)^T = U(-t) = U^{-1}(t) = e^{-t\mathcal{H}}$ it follows that $\langle U(t)\Psi(0)|U(t)\Psi(0)\rangle = \langle\Psi(t)|\Psi(t)\rangle = \langle\Psi(0)|\Psi(0)\rangle$. Hence the time-evolution operator $U(t)$ is an orthogonal transformation, rotating the vector $\Psi(t)$ without changing its length $\|\Psi\|$. In physical terms this means that the energy density of the EM fields does not change with time, as expected on physical grounds [1].

3 Unconditionally Stable Algorithms

A numerical procedure that solves the TDME necessarily starts by discretizing the spatial derivatives. This maps the continuum problem described by $\mathcal{H}$ onto a lattice problem defined by a matrix H. Ideally, this mapping should not change the basic symmetries of the original problem. The underlying symmetry of the TDME suggests to use matrices H that are real and skew-symmetric. Adopting the staggered Yee grid and central differences for the spatial derivatives [2, 3], the resulting matrix H is indeed skew-symmetric and the EM fields satisfy the

required boundary conditions [4]. As the discretization procedure is not essential for what follows, we omit these technicalities here and refer the reader to Ref. [4].

Formally the time evolution of the EM fields on the lattice is given by $\Psi(t+\tau) = U(\tau)\Psi(t) = e^{\tau H}\Psi(t)$. In practice, a numerical procedure solves the TDME by making use of an approximation $\tilde{U}(t)$ to the true time evolution $U(t)$. A necessary and sufficient condition for an algorithm to be unconditionally stable is that $\|\tilde{U}(t)\Psi(0)\| \leq \|\Psi(0)\|$. In other words, the length of $\Psi(t)$ should be bounded, for arbitrary initial condition $\Psi(t=0)$ and for any time t [8]. By choosing for $\Psi(0)$ the eigenvector of $\tilde{U}(t)$ that corresponds to the largest eigenvalue of $\tilde{U}(t)$, it follows that the algorithm will be unconditionally stable by construction if and only if the largest eigenvalue of $\tilde{U}(t)$ (denoted by $\|\tilde{U}(t)\|$) is less or equal than one [8]. If the approximation $\tilde{U}(t)$ is itself an orthogonal transformation, then $\|\tilde{U}(t)\| = 1$ and the numerical scheme will be unconditionally stable.

A systematic approach to construct orthogonal approximations to matrix exponentials is to make use of the Lie-Trotter-Suzuki formula [5, 6] and generalizations thereof [7, 9]. For instance if $H = \sum_{i=1}^{p} H_i$

$$U_1(\tau) = e^{\tau H_1} \dots e^{\tau H_p}, \tag{4}$$

might be a good approximation to $U(\tau)$ if τ is sufficiently small and, most importantly, if all the H_i are real and skew-symmetric, $U_1(\tau)$ is orthogonal by construction. Therefore, by construction, a numerical scheme based on Eq. (4) will be unconditionally stable. The Taylor series of $U(\tau)$ and $U_1(\tau)$ are identical up to first order in τ. The product-formula approach provides simple, systematic procedures to improve the accuracy of the approximation to $U(\tau)$ without changing its fundamental symmetries. For example the orthogonal matrix

$$U_2(\tau) = U_1(-\tau/2)^T U_1(\tau/2) = e^{\tau H_p/2} \dots e^{\tau H_1/2} e^{\tau H_1/2} \dots e^{\tau H_p/2}, \tag{5}$$

is correct up to second-order in τ [7, 9]. Suzuki's fractal decomposition approach [7] gives a general method to construct higher-order approximations based on $U_1(\tau)$ or $U_2(\tau)$. A particularly useful approximation, correct up to fourth-order in τ, is given by [7]

$$U_4(\tau) = U_2(a\tau)U_2(a\tau)U_2((1-4a)\tau)U_2(a\tau)U_2(a\tau), \tag{6}$$

where $a = 1/(4-4^{1/3})$. The approximations Eqs. (4), (5), and (6) have proven to be very useful in many applications [6, 9–18] and turn out to be equally useful for solving the TDME. In practice, an efficient implementation of the first-order scheme is all that is needed to construct the higher-order algorithms Eqs. (5) and (6).

4 Simulation Results

Numerically the existence of photonic bandgaps is most easily studied by adopting periodic boundary conditions. However, in nature periodic boundary conditions are very hard to realize. Therefore it is of interest to study the dependence

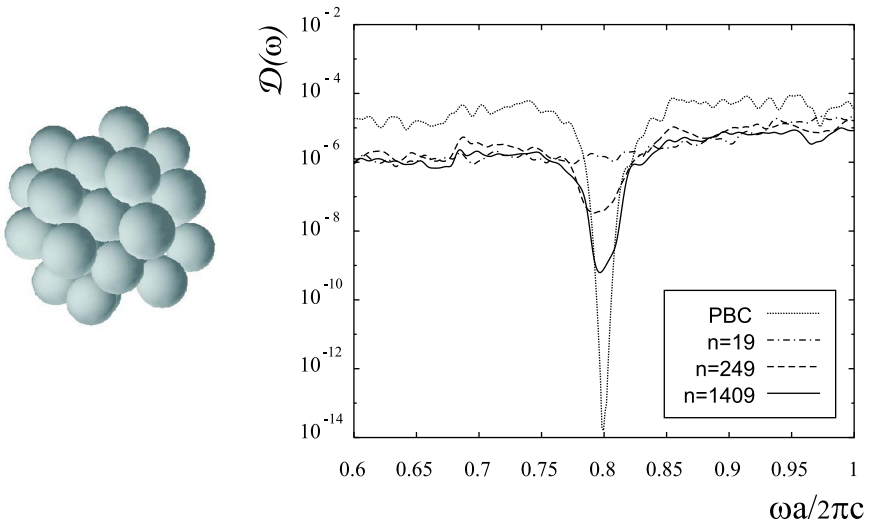

Fig. 1. Left: The 3D system: group of connected spheres of air (grey) in a dielectric background (white). The centers of the spheres form an FCC structure Right: Local density of states as function of frequency for 3D systems consisting of n spheres. PBC denotes the reference system with periodic boundary conditions.

of photonic bandgaps as a function of system size with physically realizable boundary conditions. The method we outline above is well-suited for this purpose. It does not rely on periodic boundary conditions nor on the use of the Fourier transform of the unit cell. We consider three-dimensional clusters of touching spheres filled with air in a dielectric background. The centers of the spheres form an FCC lattice, see Fig.1. The procedure we use to compute the (Local) Density of States (L)DOS is described in detail in Ref. [19].

First we compute the DOS for the system with periodic boundary conditions for a reference system containing 8 x 8 x 8 FCC unit cells of linear size λ. The FCC lattice constant is set at $a = 3\lambda$ and, combined with a mesh size $\delta = 0.1\lambda$, ensures that the spheres of air are discretized with sufficient detail. The permittivity of the dielectricum $\epsilon = 11.9\epsilon_0$, where ϵ_0 is the dielectric constant of vacuum. The DOS of this system clearly exhibits one photonic bandgap, see Fig.1 (dashed line) at $\omega a/2\pi c = 0.8$ where c is the speed of light in vacuum. Then we compute the LDOS of the FCC cluster of n spheres filled with air (without periodic boundary conditions) by using as an initial state, a random wave localized within the central sphere. In Fig.1 we also show the results for $n = 19, 249, 1409$. It is clear that the finite-sized clusters also exhibit a photonic bandgap and that the strength of the bandgap strongly depends on n (note the logarithmic scale of the y-axis). Roughly speaking the minimum of the LDOS approaches its limiting value as $e^{-\alpha\sqrt{n}}$ where α is a material specific constant.

5 Conclusion

We have described a new family of algorithms to solve the time-dependent Maxwell equations. Salient features of these algorithms are [4, 20]:

- rigorously provable unconditional stability for 1D, 2D and 3D systems with spatially varying permittivity and permeability,
- the order of accuracy in time and space can be systematically increased without affecting the unconditional stability,
- the exact conservation of the energy density of the electromagnetic field,
- easy to implement in practice.

In view of the generic character of the approach discussed in this paper, it can be used to construct unconditionally stable algorithms that solve the equations for e.g. sound, seismic and elastic waves as well.

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