A Frequency-Dependent PSTD Algorithm for General Dispersive Media

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***Abstract*— Based on the Fourier representation of spatial derivatives, the recursive convolution approaches, and the perfectly matched layer (PML), we develop a pseudospectral time-domain (PSTD) algorithm for electromagnetic problems involving general dispersive media. As a result of the accurate representation of spatial derivatives, the PSTD algorithm for dispersive media requires only a small number of cells per minimum wavelength, significantly reducing the number of unknowns. Multidimensional numerical results confirm the efficacy of the PSTD algorithm for large-scale inhomogeneous media.**

***Index Terms*— Dispersive media, FDTD, perfectly matched layer (PML), plasma, pseudospectral time-domain (PSTD) method.**

I. Introduction

DISPERSIVE media such as biological tissues, soil, and plasma are encountered in many microwave and guided wave applications. The interaction of electromagnetic waves with inhomogeneous dispersive media is often simulated by the frequency-dependent finite-difference time-domain (FDTD) method (e.g., [1] and [2]). Although the FDTD method is versatile and has found widespread applications, a high sampling density of at least ten cells per minimum wavelength is required, significantly limiting its applications in large-scale problems. Further improvements are possible with higher order or spectral schemes. As one of the improvements, the pseudospectral time-domain (PSTD) algorithm has been recently developed for nondispersive media, and proves to provide high accuracy and efficiency for large-scale problems [3]. The efficiency of the PSTD method is due to the accurate approximation of spatial derivatives using the fast Fourier transform (FFT). In this work, we further extend the PSTD algorithm to multidimensional problems involving general dispersive media. We use the recursive convolution approaches [1], [2] to simplify the temporal convolution. The wraparound effect in the pseudospectral method is eliminated by extending the perfectly matched layer (PML) [5] to dispersive media [4], [6], [7]. The frequency-dependent PSTD algorithm for dispersive media allows a coarse grid close to the Nyquist sampling density, significantly reducing the number of unknowns.

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II. Formulation

Consider an inhomogeneous conductive electrically dispersive medium with magnetic permeability μ and conductivity σ. The perfectly matched layer (PML) originally proposed by Berenger [5] can be further extended to conductive and dispersive medium, as in [4], [6], and [7]. Following the formulation of [4] using the complex stretched coordinates, we can arrive at the PML modified Ampere's law as

$$\frac{\partial}{\partial \eta}(\hat{\eta} \times \mathbf{H}) = a_\eta \frac{\partial \mathbf{D}^{(\eta)}}{\partial t} + \omega_\eta \mathbf{D}^{(\eta)} + a_\eta \sigma \mathbf{E}^{(\eta)} + \omega_\eta \sigma \int_{-\infty}^{t} \mathbf{E}^{(\eta)}\, dt + \mathbf{J}^{(\eta)} \tag{1}$$

where a_η and ω_η are PML parameters, and the split components are denoted by the superscript, as defined in [4], and $\mathbf{J}$ is the electric current density. The PML modified Faraday's law remains the same as for a nondispersive medium [3]. Note that all medium parameters may be space dependent for an inhomogeneous medium.

With appropriate boundary conditions, the modified Ampere's law in (1), the modified Faraday's law, and the constitutive equation together give the solution for the electromagnetic fields. Noting that the constitutive relations take the same form for all split components, we can omit the superscript (η) in the discussion on the constitutive relation. The time-domain constitutive relation is

$$\mathbf{D}(t) = \epsilon_0 \epsilon_\infty \mathbf{E}(t) + \epsilon_0 \int_{-\infty}^{t} \mathbf{E}(\tau)\, \chi(t-\tau)\, d\tau \tag{2}$$

where ϵ_∞ is the relative dielectric constant at $\omega \to \infty$ and $\chi(t)$ is the dispersive susceptibility function whose frequency spectrum is denoted by $\tilde{\chi}(\omega)$.

The straightforward implementation of the temporal convolution in (2) is very inefficient as it requires the storage of the history of $\mathbf{E}$. This issue has been addressed using several different methods, including the recursive convolution and piecewise recursive convolution methods [1], [2] and their improved forms [4]. Here, we first approximate a general susceptibility function in the frequency domain as a sum of simple functions

$$\tilde{\chi}(\omega) = \sum_{q=1}^{M} \frac{\Gamma_q}{-i\omega - s_q} \tag{3}$$

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where s_q and Γ_q are the complex poles and the corresponding residues. The corresponding time-domain expression is

$$\chi(t) = \sum_{q=1}^{N} \mathrm{Re}[\hat{\chi}_q(t)] = \sum_{q=1}^{N} \mathrm{Re}[R_q e^{s_q t} U(t)] \tag{4}$$

where $N = M$, $R_q = \Gamma_q$ when all s_q and Γ_q are real, and $N = M/2$, $R_q = 2\Gamma_q$ when there are $M/2$ complex-conjugate pole pairs. The expressions of s_q and Γ_q for the commonly encountered dispersive media of Debye, Lorentz, and plasma can be easily derived.

We now use a unified piecewise approximation for the field for $t \in [m\triangle t, (m+1)\triangle t]$

$$\mathbf{E}(t) \approx \mathbf{E}(m+1) + K_a \frac{[\mathbf{E}(m+1) - \mathbf{E}(m)]}{\triangle t}[t - (m+1)\triangle t] \tag{5}$$

where $K_a = 0$ for recursive convolution (RC) [1] and $K_a = 1$ for piecewise linear recursive convolution (PLRC) [2].

Introducing an auxiliary function

$$\mathbf{\Psi}_q(n) = \sum_{m=0}^{n-1} \Big\{ \Big[\hat{\chi}_q(0) - \hat{\xi}_q(0)\Big]\mathbf{E}(n-m) + \hat{\xi}_q(0)\mathbf{E}(n-m-1)\Big\} e^{s_q m \triangle t}$$

and using (4) and (5), we can derive from (2) the following recursive relations:

$$\mathbf{\Psi}_q(n+1) = \Big[\hat{\chi}_q(0) - \hat{\xi}_q(0)\Big]\mathbf{E}(n+1) + \hat{\xi}_q(0)\mathbf{E}(n) + \mathbf{\Psi}_q(n) e^{s_q \triangle t} \tag{6}$$

$$\mathbf{D}(n+1) = \epsilon_0 \Big\{ \epsilon_\infty + \sum_{q=1}^{N} \mathrm{Re}\Big[\hat{\chi}_q(0) - \hat{\xi}_q(0)\Big] \Big\} \mathbf{E}(n+1) + \epsilon_0 \sum_{q=1}^{N} \mathrm{Re}\Big[\hat{\xi}_q(0)\Big]\mathbf{E}(n) + \epsilon_0 \sum_{p=1}^{N} \mathrm{Re}\big[\mathbf{\Psi}_q(n) e^{s_q \triangle t}\big] \tag{7}$$

where the expressions of $\hat{\chi}_q(0)$ and $\hat{\xi}_q(0)$ are given in [4].

In the PSTD algorithm [3], instead of using a conventional Yee grid, we use a centered grid where all field components and material properties are located at the center of the unit cell. Spatial derivatives are approximated by FFT's instead of finite differences. Using (6) and (7) in the PML modified Ampere's law (1), we arrive at the time-stepping equation for the electric field in the PSTD algorithm

$$c_1^{(\eta)} \mathbf{E}^{(\eta)}(n+1) = \mathcal{F}_\eta^{-1}\big\{ik_\eta \mathcal{F}_\eta\big[\hat{\eta} \times \mathbf{H}\big(n + \tfrac{1}{2}\big)\big]\big\} + c_0^{(\eta)} \mathbf{E}^{(\eta)}(n) - \sigma \omega_\eta \triangle t \mathbf{E}_I^{(\eta)}(n) + \mathbf{\Phi}^{(\eta)}(n) - \mathbf{J}^{(\eta)}\big(n + \tfrac{1}{2}\big) \tag{8}$$

where function $\mathbf{\Phi}^{(\eta)}$ and coefficients $c_0^{(\eta)}$ and $c_1^{(\eta)}$ are given in [4]. The time-stepping equation for the magnetic field remains the same as for nondispersive media [3]. In (8), $\mathcal{F}_\eta$ and $\mathcal{F}_\eta^{-1}$ denote the forward and inverse FFT, respectively, and k_η is the Fourier variable in the η direction. This treatment of spatial derivatives is exact up to the Nyquist sampling density, significantly reducing the number of unknowns [3].

TABLE I
PARAMETERS FOR DEBYE MEDIA

Medium I	Medium II
$\epsilon_\infty = 4$, $\epsilon_s = 12$ $\sigma = 0.002$ S/m $\tau = 2.0 \times 10^{-10}$ s	$\epsilon_\infty = 9$, $\epsilon_s = 16$ $\sigma = 0.004$ S/m $\tau = 6.4 \times 10^{-11}$ s
$\Gamma_1 = 40$ GHz $s_1 = -5.0$ GHz	$\Gamma_1 = 109.37$ GHz $s_1 = -15.625$ GHz

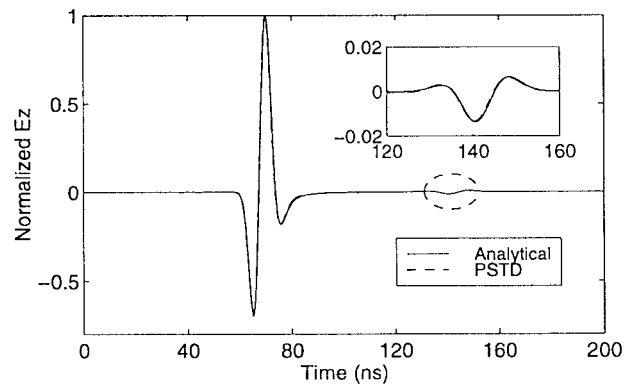

Fig. 1. The PSTD and analytical results for a line electric current source at the center of a cylinder (Debye medium I) in a background Debye medium II. The inset shows the magnified second transmitted wave after the reflection from the back of the cylinder.

III. NUMERICAL RESULTS

First we validate the two-dimensional (2-D) PSTD results for a cylinder (Debye medium I) of radius 3.2 m in another background medium (Debye medium II). The material parameters of the dispersive Debye media are listed in Table I. A parallel electric line source, with a Blackman–Harris window time function at the center frequency $f_c = 300$ MHz, is located at the center of the cylinder (also the origin). The discretization is $\Delta x = \Delta y = 5.0$ cm, and $\Delta t = 50$ ps. In Fig. 1 the PSTD and analytical results for the E_z component at the observation point $\boldsymbol{\rho} = (50\Delta x, 96\Delta y)$ show the high accuracy of the PSTD algorithm. Note that the coarse grid used here corresponds to only two cells per minimum wavelength at the highest frequency $f_{\max} = 2.5 f_c$. Moreover, the RC and PLRC approaches have a similar accuracy.

Next we show the application of the PSTD algorithm for laser pulses propagating in a 2-D plasma hollow waveguide. The plasma hollow acts as an optical fiber and can be used as a particle-accelerating medium [8]. Fig. 2(a) shows such a plasma hollow waveguide with air in the center. The waveguide wall consists of six unmagnetized plasma layers. In these layers the collision frequency $\nu_c = 2 \times 10^{13}$ Hz is constant, while the values of the plasma frequency ω_p change linearly from 1.3442×10^{15} (the innermost layer) to 3.5565×10^{15} rad/s. The source at the left side of the waveguide excites a 10-period sinusoidal wave at a frequency of 1.8868×10^{14} Hz. The discretization is $\Delta x = 0.21307$ μm, $\Delta y = 0.05327$ μm, and $\Delta t = 6.25 \times 10^{-17}$ s. Fig. 2(b) displays the snapshots of the laser wave field at four different time steps ($n = 2000, 3000, 4000,$ and 5000). It clearly confirms that the

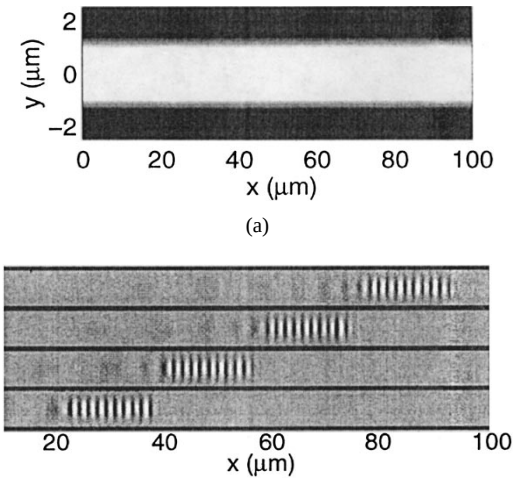

Fig. 2. (a) Geometry of a plasma slab waveguide. The waveguide walls consist of six layers of unmagnetized plasma. (b) Laser pulse propagation in the plasma hollow waveguide. From bottom to top, snapshots at time step $n = 2000, 3000, 4000,$ and 5000.

plasma hollow can guide the laser pulses without significant distortion over a relatively long distance.

IV. Conclusions

We have developed a PSTD algorithm for general dispersive media. In this algorithm, an arbitrary dispersive medium is modeled by the sum of functions with simple poles, and temporal convolution integrals are simplified by RC and PLRC. The FFT algorithm is used to approximate spatial derivatives, while the PML is used to eliminate the wraparound effects. As a result of the spectral representation of spatial derivatives, a coarse sampling close to the Nyquist density becomes possible while maintaining the accuracy. Future work will address the nonuniform sampling in space to make the algorithms more flexible.

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