Time-Domain Finite-Difference Beam Propagation Method

Husain M. Masoudi, Muhammad A. AlSunaidi, and John M. Arnold

Abstract— **A new technique to model the behavior of pulsed optical beams in waveguides is proposed and analyzed. The technique is an extension of the traditional continuous-wave beam propagation method (BPM) to include time dependence, therefore called the time-domain BPM (TD-BPM). The method was tested using different waveguide examples and it is concluded that the technique is simple and accurate. Compared with the finite-difference TD method, the new TD-BPM is more efficient in terms of computer memory and execution time especially for large optical devices.**

Index Terms— **Beam propagation method, finite-difference analysis, modeling, numerical analysis, optical waveguide theory, partial differential equation, pulse propagation.**

I. Introduction

LARGE-SCALE modeling of guided-wave optical devices is becoming more important as optical circuits became more complicated. Many of these devices exploit nonlinear optical interactions. Most previous analyzes have concentrated on continuous-wave (CW) operation, and less progress has been made to model time-domain (TD) problems. Pulse propagation in optical structures can be analyzed, in principle at least, by the finite-difference TD (FDTD) [1]. However, this method requires enormous computer resources (execution time and memory) even for simple two-dimensional (2-D) structures, and is at present still impractical for the three-dimensional (3-D) modeling of parametric interactions in guided-wave devices, which may require lengths of 10^4 wavelengths or more, over time scales which may be 10^3–10^4 times larger than the optical carrier period even for picosecond pulse envelopes. Recently, slow-wave simulators have been proposed which depend on a slowly varying envelope variation [2]. These techniques are not suitable for modeling pulse propagation. Another approach uses the beam propagation method (BPM) style in writing the wave equation in the spectral domain, wherein each frequency of the pulsed beam is propagated to the desired distance and the final pulse shape is reconstructed using the inverse fast Fourier transform (FFT) [3]. This is only feasible for linear propagation problems.

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In this letter, we derive and solve a paraxial wave equation including time dependence directly in the TD, extending the classical explicit finite-difference BPM approach. In its simplest form the method involves separating the real-valued scalar wavefunction ψ into a product of the carrier frequency oscillation and a complex modulating envelope, in the form $\psi(\mathbf{x}, t) = \Psi(\mathbf{x}, t)e^{i\kappa z}e^{-i\omega t} + \Psi^*(\mathbf{x}, t)e^{-i\kappa z}e^{i\omega t}$, obtaining the wave equation for the complex envelope Ψ without approximation, then applying a paraxial approximation to the wave equation by neglecting derivatives with respect to z higher than the first derivative. In this way, the time dependence of the complex envelope is treated as though it was just a further transverse variable in addition to the two spatial dimensions. It is implicit in this approximation that the wave propagation is essentially in one direction, toward $z = +\infty$, but the complex envelope is not necessarily assumed to be slowly varying in time t.

To test the validity of this method we apply it to dispersive linear guided-wave problems in two dimensions where the correct behavior of the wave can be predicted analytically, and we find excellent agreement with the theoretical predictions. An essential feature of the method is that it requires the computational window to be adjusted in time at each propagation step so as to effectively move at the group velocity of the pulse envelope, otherwise a compact pulse eventually disappears from the window after a certain number of propagation steps.

II. Paraxial Approximation and Discretization

We begin with the scalar TD wave equation $\nabla^2\psi - n^2/c_0^2\partial_t^2\psi = 0$, where $n = n(\mathbf{x})$ is the position-dependent refractive index variation and c_0 is the wave velocity in free space. A carrier frequency ω and a propagation coefficient $\kappa = \kappa_0 n_0$ in the direction of propagation are extracted from ψ, as $\psi = \Psi e^{i\kappa z}e^{-i\omega t}+$ c.c. where $\kappa_0 = \omega/c_0$, n_0 is a reference refractive index, and c.c. means the complex conjugate of the expression preceding it. Under the standard parabolic approximation, obtained by neglecting second derivatives of the wavefunction with respect to the axial coordinate z, the scalar wave equation becomes

$$2i\left(\kappa\partial_z\Psi + \frac{n^2}{c_0^2}\kappa_0\partial_t\Psi\right) + (n^2\kappa_0^2 - \kappa^2)\Psi - \frac{n^2}{c_0^2}\partial_t^2\Psi + \nabla_\perp^2\Psi = 0. \quad (1)$$

The substitution of a moving time coordinate $\tau = t - z/v_g$ with arbitrary v_g changes (1) to

$$2i\left\{\kappa\partial_z\Psi + \kappa_0\left(\frac{1}{c} - \frac{1}{v_g}\right)\partial_\tau\Psi\right\} + (n^2\kappa_0^2 - \kappa^2)\Psi - \frac{n^2}{c_0^2}\partial_\tau^2\Psi + \nabla_\perp^2\Psi = 0. \qquad (2)$$

Using the central finite-difference approximations

$$\partial_\alpha\Psi \rightarrow \frac{1}{2\Delta\alpha}(\Psi(\alpha+\Delta\alpha) - \Psi(\alpha-\Delta\alpha)), \qquad \alpha = z, \tau$$
$$\partial_\delta^2\Psi \rightarrow \frac{1}{\Delta\delta^2}(\Psi(\delta+\Delta\delta) + \Psi(\delta-\Delta\delta) - 2\Psi(\delta)), \qquad \delta = x, y, \tau \qquad (3)$$

to replace the partial derivatives in (1) leads to the second-order accurate explicit finite-difference time-domain BPM (TD-BPM)

$$\vec{\Psi}_{s+1} = \vec{\Psi}_{s-1} + L_s\vec{\Psi}_s \qquad (4)$$

where Ψ_s is a vector formed by samples of the field $\Psi(x, y, s\Delta z, \tau)$ at the 3-D mesh of points $x = m_x\Delta x$, $y = m_y\Delta y$, $\tau = m_\tau\Delta\tau$, and L is a sparse matrix which effects the finite-difference arithmetic (3) on this mesh. The index $s \rightarrow s+1$ steps the vector Ψ_s forward along z by one mesh period $z \rightarrow z + \Delta z$. The discretized (4) is very similar to the classical CW equation given in [4] and [5], but with an additional transverse variable τ; if the field ψ is time independent, then the TD-BPM reverts to the CW case. The explicit propagation of the optical field using the TD-BPM is straightforward since the computation of Ψ_{s+1} involves a multiplication of the input field Ψ_s with a very sparse matrix, which makes the method very efficient and highly parallel [4]. Stability analysis of the algorithm is carried out as in [5], by searching for discretized plane wave solutions of (4) under the condition of a uniform medium, and determining conditions under which these plane waves can have real propagation coefficients. The characteristic equation for the propagation coefficient β of such a discretized plane wave, $\Psi = \exp(i\beta s\Delta z)\exp(i\gamma_x m_x\Delta x)\exp(i\gamma_y m_y\Delta y)\exp(-i\Omega m_\tau\Delta\tau)$ assuming that n is independent of position $\mathbf{x}$, $n\kappa_0 = \kappa$, and $v_g = c$, is

$$-2\left(\kappa\frac{\sin\beta\Delta z}{\Delta z}\right) - \frac{4\sin^2\frac{1}{2}\Omega\Delta\tau}{c^2\Delta\tau^2} + \frac{4\sin^2\frac{1}{2}\gamma_x\Delta x}{\Delta x^2} + \frac{4\sin^2\frac{1}{2}\gamma_y\Delta y}{\Delta y^2} = 0 \qquad (5)$$

and it is required that this equation have solutions for which $-1 < \sin\beta\Delta z < 1$ to permit real values of β; this shows that the algorithm is stable under the condition

$$-\frac{\kappa}{\Delta z} < -\frac{2\sin^2\frac{1}{2}\Omega\Delta_\tau}{c^2\Delta\tau^2} + \frac{2\sin^2\frac{1}{2}\gamma_x\Delta x}{\Delta x^2} + \frac{2\sin^2\frac{1}{2}\gamma_y\Delta y}{\Delta y^2} < \frac{\kappa}{\Delta z}. \qquad (6)$$

This is satisfied for all Ω, γ_x, and γ_y if $[2/\Delta x^2 + 2/\Delta y^2] < \kappa/\Delta z$, and $2/(c^2\Delta\tau^2) < \kappa/\kappa\Delta z$.

III. Numerical Examples

In this section we apply the TD-BPM algorithm to two different problems in order to characterize the technique rigorously. A temporal pulse of the form $\Psi(x, y, z = 0, \tau) = \Psi_0(x, y)\exp(-\tau^2/\sigma^2)$ is assumed as initial condition at $z = 0$ in all simulations, where σ scales the duration of the initial pulse. Boundary conditions for the field are necessary in the two transverse spatial variables and in the TD. It is also necessary to compensate for the displacement of the pulse in the time window as z advances, due to the motion of the envelope Ψ at the group velocity. For simplicity we have chosen spatial boundary conditions $\Psi(\pm M_x\Delta x, \pm M_y\Delta y, s\Delta z, m_\tau\Delta\tau) = 0$ on a rectangular boundary surrounding the structure. We have investigated two simple methods of applying temporal boundary conditions. The first method involves applying the boundary conditions $\Psi = 0$ at $\tau = \pm M_\tau\Delta\tau$ in the relative time window (coordinate τ), moving in the absolute time frame (coordinate t) with the velocity of the pulse, so that the relative motion of the pulse in the time window is eliminated. However, the required velocity v_g is not necessarily known in advance of the calculation, and has to be generated dynamically as the computation progresses. An alternative technique is the application of periodic boundary conditions at the ends of the relative time window, so that a pulse leaving the window at one side simply re-enters at the other side even if the correct velocity is not known precisely. Both of these techniques were tested and proved quite workable; they both permit the time window to be of a finite extent $2M_\tau\Delta\tau$, of the order of a few pulsewidths.

A. Metallic Waveguide

The first example involves a 2-D (x and z) metallic waveguide containing empty space with refractive index $n = 1$; x is the transverse direction and z is the propagation direction. The cutoff frequency of this waveguide depends on the width of the waveguide as [7] $\omega_c = m\pi c_0/a$ where $m = 1, 2, \cdots$. Consider a pulsed first ($m = 1$) guided mode propagating in the structure. The temporal pulsewidth at a distance z is given by $\sigma^2(z) = \sigma^2(0) + (2z\beta'')^2$ [7], where the dispersion parameter $\beta'' = d^2\beta/d\omega^2$ can be calculated analytically from the modal dispersion relation $\beta = (\omega/c_0)(1 - (\omega/\omega_c)^2)^{1/2}$. For a waveguide width of $a = 1.0$ μm, the cut-off wavelength is $\lambda_c = 2$ μm and the first guided mode in the transverse direction x can be written as $\Psi = \sin(\pi x/a)$. Tests on the TD-BPM showed that the reference propagation coefficient κ should be chosen to be equal to the propagation coefficient β of the guided mode in order that the pulse travel with the correct velocity and hence be stationary in the relative time window. Fig. 1 shows the relative error of the pulsewidth *versus* the carrier wavelength for two different initial pulsewidths. Increasing the carrier wavelength increases the propagation angle $\theta = \arcsin(\lambda/\lambda_c)$, with respect to the axial direction, of the two plane waves forming the mode inside the waveguide, making the mode less paraxial, and also decreases the number of carrier cycles under the pulse. The figure shows that, as the angle θ increases, the relative error of the TD-BPM increases, due to the loss

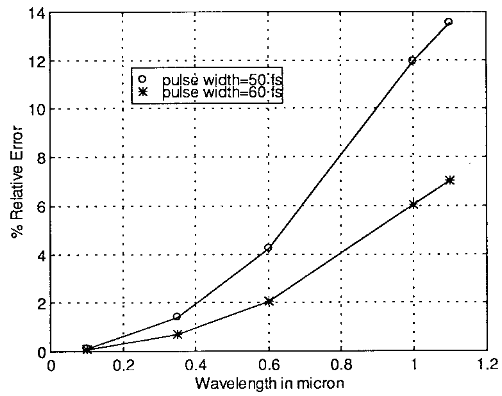

Fig. 1. The percentage relative error of the pulsewidth versus the working wavelength for two different initial pulsewidths. The calculations were performed at $z = 332$ μm, $\Delta t = 1$ fs, $\Delta x = 0.04$ μm.

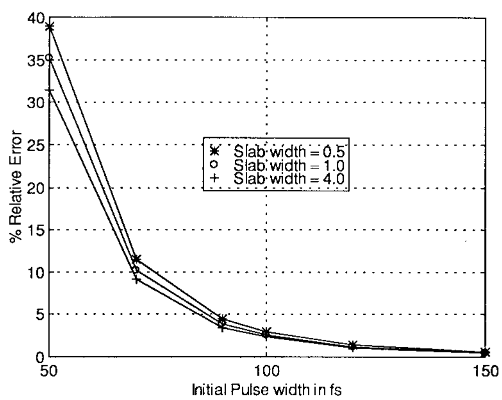

Fig. 2. The percentage relative error of the pulsewidth as a function of the initial pulsewidth $\sigma(0)$ for three different slab thickness a in μm. n_o was taken to be the effective index of the guided mode.

of paraxiality. On the other hand, the figure also shows that increasing the initial pulsewidth decreases the error.

B. Dielectric Waveguide

In this example, we have considered a symmetric dielectric slab waveguide with refractive indexes of $n = 1.2$ (guiding layer), $n = 1.0$ (cladding layers) and $\lambda = 1.0$ μm. A pulsed first guided mode was initiated at $z = 0$ and propagated to a distance of $z = 500$ μm, and the pulsewidth was compared with the theoretical value of $\sigma^2(z) = \sigma^2(0) + (2z\beta'')^2$. The initial modal distribution at $z = 0$ and the dispersion parameter β'' that appears in this formula were computed numerically from the dispersion relation for a dielectric slab [8]. Fig. 2 shows the relative error as a function of the initial pulsewidth $\sigma(0)$ for three different waveguide widths a. Changing the width of the waveguide again changes the angle of the guided mode. The three slab widths were 0.5, 1.0, and 4.0 μm corresponding to mode angles of 23.7°, 16.1°, and 5.3°, respectively. It is clear from Fig. 2 that the mode angle has little effect on the error, but the initial pulsewidth plays a very important role. This example shows that the technique can handle easily pulses as small as 100 fs for half a millimeter distance with a relative error of less than 3%.

IV. Conclusion

A new technique for modeling pulsed optical beams has been proposed and examined. The TD-BPM, which solves the paraxial wave equation for time-domain problems, was introduced using the explicit finite difference method. Tests on the TD-BPM showed that the technique accurately reproduces correct behavior in simple problems which can be studied analytically. In this work, the method was applied to two classes of problems: propagation of pulsed guided modes in metallic waveguides, and pulsed guided modes in dielectric waveguides. We have concluded that the technique is simple, efficient and accurate. This method is particularly well suited to the study of unidirectional propagation of compact temporal pulses over long distances in a guided-wave environment. Work is under way to extend the method to wide-angle propagation that removes the paraxial limit imposed on the method. In addition, the technique will be examined in the presence of material dispersion and nonlinear parametric optical interactions mediated through $\chi^{(2)}$ and $\chi^{(3)}$ nonlinear susceptibilities, where the TD method is essential in order to study the propagation of intense ultrashort pulses.

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