Full-Vectorial Beam-Propagation Method Based on the McKee–Mitchell Scheme with Improved Finite-Difference Formulas

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***Abstract*—The alternating-direction implicit method proposed by McKee–Mitchell is applied to full-vectorial paraxial wave equations. The high computational efficiency of the present method is demonstrated in comparison with an iterative solver. Novel finite-difference formulas that take into account discontinuities of the fields are proposed and employed to ensure second-order accuracy. Calculations regarding the effective index of rib waveguides show that the present results remarkably agree with values obtained from the modal transverse resonance method.**

***Index Terms*—Finite-difference methods, optical beam propagation, optical waveguides.**

I. Introduction

CONSIDERABLE effort has been directed to improving a full-vectorial beam-propagation method (VBPM) from various viewpoints. The VBPM's developed so far have often caused problems in terms of stability and/or accuracy. This is due to the existence of mixed derivatives in coupled wave equations. Since vectorial treatment is absolutely necessary to simulate polarization-dependent and coupling devices, accurate and stable numerical methods should be developed.

Pioneer work on a VBPM has been made by Huang and Xu [1] using finite-difference (FD) techniques with an iterative solver. Since the iterative solver is somewhat time-consuming, Mansour *et al.* [2] introduced the alternating-direction implicit (ADI) technique into the VBPM. Their formulation was based on the Peaceman–Rachford scheme. Although the Peaceman–Rachford splitting is effective in scalar [3] and semivectorial calculations [4], [5], the application to the full-vectorial case often causes instability in numerical results. Yevick *et al.* [6] introduced the ADI technique using lines at $\pm 45^\circ$ to the principal axis. This technique, the so-called Douglas–Gunn splitting, yields stable results but is extremely complicated. On the other hand, McKee–Mitchell [7] have developed an ADI process for parabolic equations with a mixed derivative, which is known to yield reasonable results with simpler splitting. However, no attempt has been made to apply the McKee–Mitchell scheme to a VBPM.

One should also note that inaccuracy in previous VBPM's stems from improper treatment of the mixed derivatives. Since the field and its derivatives are often discontinuous, the conventional FD formulas severely deteriorate the numerical results. In the case of a semivectorial analysis, several improved FD formulas have been proposed, which attain considerable accuracy [8], [9]. This fact encourages us to develop improved FD formulas even for the mixed derivatives in the VBPM.

In this paper, we propose a novel VBPM based on the McKee–Mitchell (MM) scheme [7], and demonstrate its better stability than the VBPM based on the well-known Peaceman–Rachford (PR) scheme, while maintaining high computational efficiency. Special attention is paid to evaluation of mixed derivatives as well as second derivatives. We propose new FD formulas taking into account discontinuities of refractive indexes. The new FD formulas ensure second-order accuracy even in full-vectorial calculations. The present VBPM can also be used in imaginary-axis propagation. We assess the accuracy of the present VBPM in the eigenmode analysis in a rib waveguide as a classical benchmark test, since reliable data on propagation constants are available [10]. Calculation shows how appropriate evaluation of the mixed derivatives improves convergence behavior. Negligence of discontinuities of the first derivative in previous works results in poor convergence. Remarkable agreement not obtainable in previous works is observed with the results derived by the modal transverse resonance method [10], [11].

II. McKee–Mitchell Scheme

Assuming that the refractive index varies slowly along z, we solve the following paraxial vector wave equations [1]:

$$2jkn_0 \frac{\partial E_x}{\partial z} = (\tilde{D}_{xx} + D_{yy} + \nu)E_x + \tilde{D}_{xy}E_y \tag{1}$$

$$2jkn_0 \frac{\partial E_y}{\partial z} = (D_{xx} + \tilde{D}_{yy} + \nu)E_y + \tilde{D}_{yx}E_x \tag{2}$$

where

$$\tilde{D}_{\alpha\alpha}E_\alpha = \frac{\partial}{\partial \alpha}\left[\frac{1}{n^2}\left(\frac{\partial}{\partial \alpha}\left(n^2 E_\alpha\right)\right)\right] \tag{3}$$

$$D_{\alpha\alpha}E_\beta = \frac{\partial^2 E_\beta}{\partial \alpha^2} \tag{4}$$

$$\tilde{D}_{\alpha\beta}E_\beta = \frac{\partial}{\partial \alpha}\left[\frac{1}{n^2}\left(\frac{\partial}{\partial \beta}\left(n^2 E_\beta\right)\right) - \frac{\partial E_\beta}{\partial \beta}\right] \tag{5}$$

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with $\alpha, \beta \in \{x, y\}$, and $\nu = k^2[n^2(x, y, z) - n_0^2]$, in which k is the free-space wavenumber, $n(x, y, z)$ is the index profile, and n_0 is the reference refractive index.

Based on the MM scheme, which is known to yield reasonable results with simpler splitting than the Douglas–Gunn scheme [7], we derive FD equations from the coupled paraxial wave equations. Since (1) and (2) have a similar form, we only treat (1) in the following. After integrating (1) over an interval of Δz, we get

$$2jkn_0[E_x^{n+1} - E_x^n] = \frac{\Delta z}{2}\,[(\tilde{\delta}_x^2 + \delta_y^2 + \nu)(E_x^{n+1} + E_x^n) + \tilde{\delta}_{xy}^2(E_y^{n+1} + E_y^n)] \tag{6}$$

where the differential operators $\tilde{D}_{xx}$, D_{xx}, and $\tilde{D}_{xy}$ are replaced by difference operators $\tilde{\delta}_x^2$, δ_x^2, and $\tilde{\delta}_{xy}^2$, respectively. Using the assumption of $E_y^{n+1} \simeq E_y^n$, we obtain

$$\left[1 - \frac{\Delta z}{4jkn_0}\,(\tilde{\delta}_x^2 + \delta_y^2 + \nu)\right]E_x^{n+1} = \left[1 + \frac{\Delta z}{4jkn_0}\,(\tilde{\delta}_x^2 + \delta_y^2 + \nu)\right]E_x^n + \frac{\Delta z}{2jkn_0}\,\tilde{\delta}_{xy}^2 E_y^n. \tag{7}$$

The ADI process, derived by McKee–Mitchell, is in unsplit form

$$\left[1 - \frac{\Delta z}{4jkn_0}\left(\tilde{\delta}_x^2 + \frac{1}{2}\,\nu\right)\right]\left[1 - \frac{\Delta z}{4jkn_0}\left(\delta_y^2 + \frac{1}{2}\,\nu\right)\right]E_x^{n+1} = \left[1 + \frac{\Delta z}{4jkn_0}\left(\tilde{\delta}_x^2 + \frac{1}{2}\,\nu\right)\right]\left[1 + \frac{\Delta z}{4jkn_0}\left(\delta_y^2 + \frac{1}{2}\,\nu\right)\right]E_x^n + \frac{\Delta z}{2jkn_0}\,\tilde{\delta}_{xy}^2 E_y^n. \tag{8}$$

Now we introduce the Douglas–Rachford type splitting, so that we obtain

$$\left[1 - \frac{\Delta z}{4jkn_0}\left(\tilde{\delta}_x^2 + \frac{1}{2}\,\nu\right)\right]E_x^{n+*} = \left[1 + \frac{\Delta z}{4jkn_0}\left(\tilde{\delta}_x^2 + \frac{1}{2}\,\nu\right) + \frac{\Delta z}{2jkn_0}\left(\delta_y^2 + \frac{1}{2}\,\nu\right)\right]E_x^n + \frac{\Delta z}{2jkn_0}\,\tilde{\delta}_{xy}^2 E_y^n \tag{9a}$$

$$\left[1 - \frac{\Delta z}{4jkn_0}\left(\delta_y^2 + \frac{1}{2}\,\nu\right)\right]E_x^{n+1} = E_x^{n+*} - \frac{\Delta z}{4jkn_0}\left(\delta_y^2 + \frac{1}{2}\,\nu\right)E_x^n. \tag{9b}$$

Equation (9) involves the solution of only two tridiagonal sets of equations at each propagation step. This is in contrast to the Douglas–Gunn splitting, which requires the solution of four tridiagonal sets of equations at each propagation step.

III. Improved FD Formulas

We treat three consecutive mesh points with a discontinuity between points i and $i+1$ and derive FD formulas when the interface between different media is located midway between two mesh points.

We first express the fields ϕ_{i-1} and ϕ_{i+1} using Taylor-series expansions. ϕ_{i-1} is given by

$$\phi_{i-1} = \phi_i - \Delta x\,\frac{\partial \phi_i}{\partial x} + \frac{\Delta x^2}{2}\,\frac{\partial^2 \phi_i}{\partial x^2} - \frac{\Delta x^3}{6}\,\frac{\partial^3 \phi_i}{\partial x^3} + O(\Delta x^4). \tag{10}$$

With respect to ϕ_{i+1}, the continuity relations at the interface should be satisfied. Let ϕ_R and ϕ_L refer to the fields at the infinitesimally right and left of the interface, respectively. When ϕ_R is used, ϕ_{i+1} can be written as

$$\phi_{i+1} = \phi_R + \frac{\Delta x}{2}\,\frac{\partial \phi_R}{\partial x} + \frac{\Delta x^2}{8}\,\frac{\partial^2 \phi_R}{\partial x^2} + \frac{\Delta x^3}{48}\,\frac{\partial^3 \phi_R}{\partial x^3} + O(\Delta x^4). \tag{11}$$

On the other hand, using ϕ_i, ϕ_L can be expressed as

$$\phi_L = \phi_i + \frac{\Delta x}{2}\,\frac{\partial \phi_i}{\partial x} + \frac{\Delta x^2}{8}\,\frac{\partial^2 \phi_i}{\partial x^2} + \frac{\Delta x^3}{48}\,\frac{\partial^3 \phi_i}{\partial x^3} + O(\Delta x^4). \tag{12}$$

Since the relation between ϕ_R and ϕ_L [8], [9]

$$\begin{aligned}
\phi_R &= \theta\phi_L \\
\frac{\partial \phi_R}{\partial x} &= \frac{\partial \phi_L}{\partial x} \\
\frac{\partial^2 \phi_R}{\partial x^2} &= \theta\left[\frac{\partial^2 \phi_L}{\partial x^2} + k^2(n_i^2 - n_{i+1}^2)\phi_L\right] \\
\frac{\partial^3 \phi_R}{\partial x^3} &= \frac{\partial^3 \phi_L}{\partial x^3} + k^2(n_i^2 - n_{i+1}^2)\,\frac{\partial \phi_L}{\partial x}
\end{aligned}$$

ϕ_{i+1} can be rewritten in the form

$$\phi_{i+1} = \theta(1 + m\Delta x^2)\phi_i + \left[1 + \theta + m\Delta x^2\left(\theta + \frac{1}{3}\right)\right] \cdot \frac{\Delta x}{2}\,\frac{\partial \phi_i}{\partial x} + (1+\theta)\,\frac{\Delta x^2}{4}\,\frac{\partial^2 \phi_i}{\partial x^2} + (1+\theta)\,\frac{\Delta x^3}{12}\,\frac{\partial^3 \phi_i}{\partial x^3} + O(\Delta x^4) \tag{13}$$

where $\theta = n_i^2/n_{i+1}^2$ and $m = k^2(n_i^2 - n_{i+1}^2)/8$.

The FD formula for the second derivative can be obtained by eliminating the first derivative from (10) and (13) [9]

$$\frac{\partial^2 \phi_i}{\partial x^2} = \frac{2(a_2\phi_{i-1} + b_2\phi_i + \phi_{i+1})}{d\Delta x^2} + O(\Delta x^2) \tag{14}$$

where $a_2 = (\theta + 1)/2 + m\Delta x^2\Gamma$, $b_2 = -(3\theta + 1)/2 - m\Delta x^2(\theta + \Gamma)$, and $d = 1 + \theta + m\Delta x^2\Gamma$, in which $\Gamma = \theta/2 + 1/6$. The coefficient d can be approximated by $1 + \theta$ without significant effects. Equation (14), regarded as an extension of Stern's formula [12], is a special case of (6) in our previous paper [9]. Note that recently Vassallo [13] also developed similar improved FD formulas for the second derivative.

Consideration is now given to the treatment of the mixed derivative. No attempt has been made to evaluate the mixed derivatives accurately. Direct discretization of the mixed derivative results in poor convergence behavior, as will be shown in Fig. 5. To evaluate the mixed derivative correctly, we consider the first derivative, since the mixed derivative is composed of the combination of the first derivatives. As in the case of derivation of (14), we can derive the following

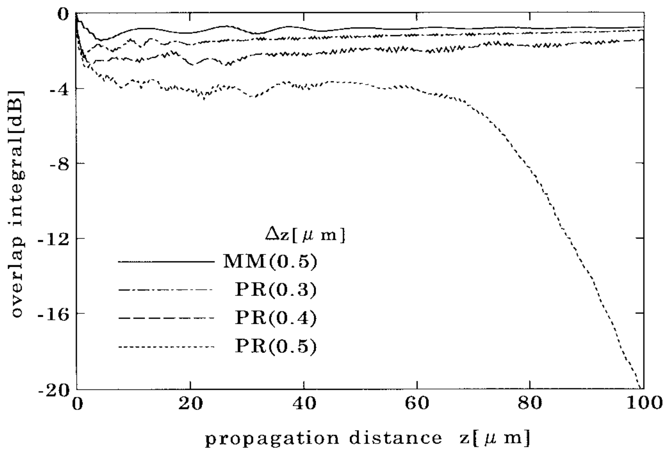


Fig. 1. Overlap integral between the numerical and exact fields for a minor component of HE_{11} mode of a step-index fiber as a function of propagation distance z.

three-point FD formula for the first derivative by eliminating the second derivative from (10) and (13):

$$\frac{\partial \phi_i}{\partial x} = \frac{a_1\phi_{i-1} + b_1\phi_i + \phi_{i+1}}{d\Delta x} + O(\Delta x^2) \tag{15}$$

where $a_1 = -(\theta+1)/2$ and $b_1 = (1-\theta)/2 - m\Delta x^2\theta$. Equations (14) and (15) are utilized to evaluate the first and second derivatives in (9). For example, (14) is applied to $\tilde{\delta}_x^2$ or (3), and to δ_x^2 or (4) with $\theta = 1$. Equation (15) is used for $\partial E_\beta/\partial\beta$ and $\partial E_\beta/\partial\alpha$ in $\tilde{\delta}_{xy}^2$ [see (5)] with $\theta = 1$. $(\partial/\partial\beta)(n^2 E_\beta)$ may be evaluated by another FD formula, in which the interface conditions of electric flux density are satisfied. Following the similar procedure mentioned above, we obtain

$$\frac{\partial \tilde{\phi}_i}{\partial x} = \frac{a_1\tilde{\phi}_{i-1} + b_1\tilde{\phi}_i + \theta\tilde{\phi}_{i+1}}{d\Delta x} + O(\Delta x^2). \tag{16}$$

Corresponding formulas similar to (14)–(16) are also derived when the discontinuity lies between points $i-1$ and i (see the Appendix).

IV. Results

We first compare the MM scheme with the PR scheme in propagation behavior of HE_{11} mode of a step-index fiber. Fig. 1 shows the overlap integral between the numerical and exact fields for the minor component as a function of propagation distance. The exact fields are chosen as input fields. The transverse mesh size is taken to be $\Delta(= \Delta x = \Delta y) = 0.071$ μm. The total number of mesh points is $N_x \times N_y = 160 \times 160$. The configuration parameters are as follows. The core radius is $\rho = 0.71$ μm, and the refractive indexes of the core and cladding are $n_{co} = 1.3$ and $n_{cl} = 1.0$. A wavelength of $\lambda = 1.55$ μm is used, so that the normalized frequency is $V = 2.4$. This fiber is not realistic, but is considered to investigate sensitivity of the schemes in a strongly guiding structure. It is found that the MM scheme allows a larger propagation step length Δz than that in the PR scheme. Further calculation shows similar tendency in the major component. The PR scheme is efficient only for scalar [3] and semivectorial cases [4], [5].

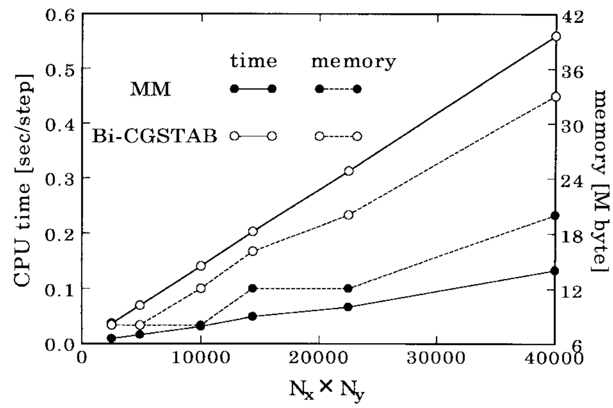


Fig. 2. Comparison in computational effort between the McKee–Mitchell scheme and the iterative solver.

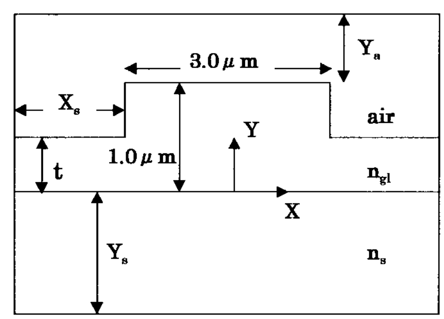


Fig. 3. Rib waveguide geometry.

High computational efficiency of the MM scheme is demonstrated in Fig. 2, in which comparison with the VBPM using an iterative solver (Bi-CGSTAB) [14] is made. The computing time in the Bi-CGSTAB depends on a tolerance factor for convergence. The tolerance factor is chosen in such a way that the results obtained by the Bi-CGSTAB are comparable to those obtained by the MM scheme. In the MM scheme, the standard Thomas algorithm can be used, leading to less CPU time and memory.

For a step-index fiber, we cannot correctly assess the accuracy of FD formulas due to discretization error of a circular core. Hence, we next consider a rib waveguide (shown in Fig. 3) used as a classical benchmark [10]. The configuration parameters are $n_s = 3.40$, $n_{gl} = 3.44$, $\lambda = 1.15$ μm, rib width $= 3.0$ μm, central rib height $= 1.0$ μm, and lateral height $= t$ varying from 0.1 to 0.9 μm. The computational domain parameters are $Y_a = 0.5$ μm above the top of the rib, $Y_s = 3.0$ μm below the guiding layer, and $X_s = 2.5$ μm (or 5.5 μm for $t = 0.9$ μm) aside from the rib lateral side.

The fundamental mode can be calculated by the imaginary distance procedure in which the coordinate z in the propagation direction is changed to $j\tau$ [15]. The effective index is evaluated by the growth in the field amplitude [16], as shown in (17) at the bottom of the next page. For evaluation of the effective index defined by $n_{\text{eff}} = \beta/k$, the reference index n_0 has to be a value close to the exact one. It should be noted, however, that the exact value is unknown in practice. In this paper, we adopt a new technique of iteratively renewing n_0 [17]. The effectiveness of this technique is shown in

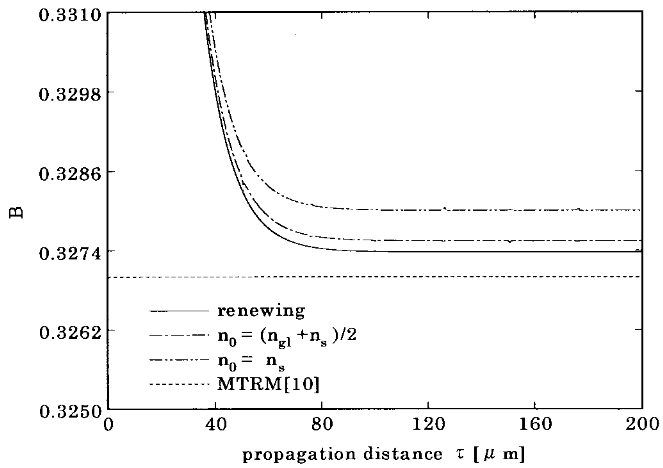


Fig. 4. Convergence behavior of the normalized propagation constant B as a function of propagation τ.

Fig. 4, in which the normalized propagation constant $B = (n_{\text{eff}}^2 - n_s^2)/(n_{gl}^2 - n_s^2)$ is presented as a function of τ. The data are for the quasi-TE mode with $t = 0.5$ μm. The transverse mesh size $\Delta (= \Delta x = \Delta y)$ and propagation step length $\Delta\tau$ are taken to be $\Delta = 0.025$ μm and $\Delta\tau = 0.05$ μm, respectively. As the input field, we choose a step function as

$$\phi(x, y, 0) = \begin{cases} 1, & \text{for } |x| \le 1.5\ \mu\text{m and } 0 \le y \le 1\ \mu\text{m} \\ 0, & \text{otherwise} \end{cases}$$

for the major component and zero for the minor component. When we fix n_0 to be n_s or $(n_{gl} + n_s)/2$, B converges to a different value. In contrast, renewing n_0 iteratively leads to monotone convergence to the same value regardless of an initial value of n_0 (it has been confirmed that B converges to the exact value in a two-dimensional waveguide [17]). The convergence value is close to a value obtained with the modal transverse resonance method (MTRM) as will be discussed in detail.

The convergence behavior of B for the quasi-TE mode as a function of transverse mesh size Δ is shown in Fig. 5, where t is chosen to be 0.5 μm. In this calculation, $\Delta\tau$ is fixed to be 0.05 μm regardless of Δ (although a larger $\Delta\tau$ is available when Δ is large). For comparison, the results obtained using the combination of other FD formulas [1], [12] are also shown. It is revealed that the use of (14)–(16) achieves faster convergence. Although not illustrated, a similar tendency is also observed in the quasi-TM mode. The results regarding the semivectorial (sv) and full-vectorial (fv) cases with the improved FD formulas are found to have almost the same convergence behavior.

Table I tabulates the B values obtained from the present technique in both the quasi-TE and quasi-TM modes. The mesh size Δ is taken to be 0.025 μm. For reference, the data for the semivectorial case are also presented. The B values are expressed with the deviations $(B - B_{\text{MTRM}}) \times 10^4$ from

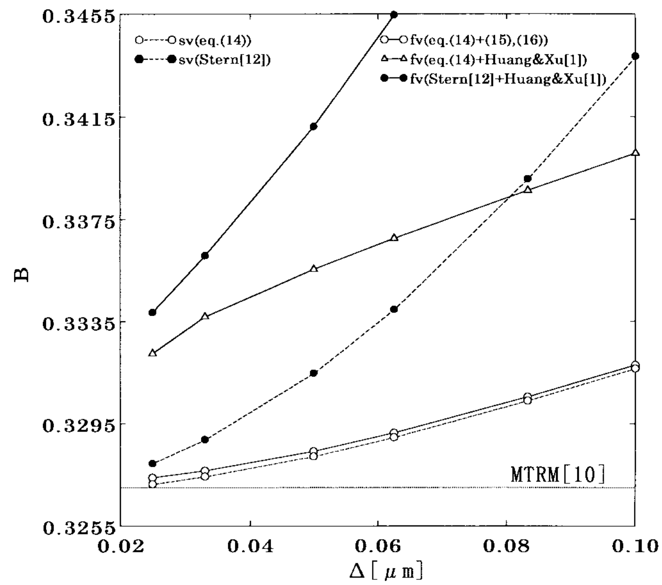


Fig. 5. Convergence behavior of the normalized propagation constant B as a function of transverse mesh size Δ.

TABLE I
NORMALIZED PROPAGATION CONSTANT B OBTAINED WITH MTRM AND DEVIATIONS IN SEMIVECTORIAL AND FULL-VECTORIAL CASES

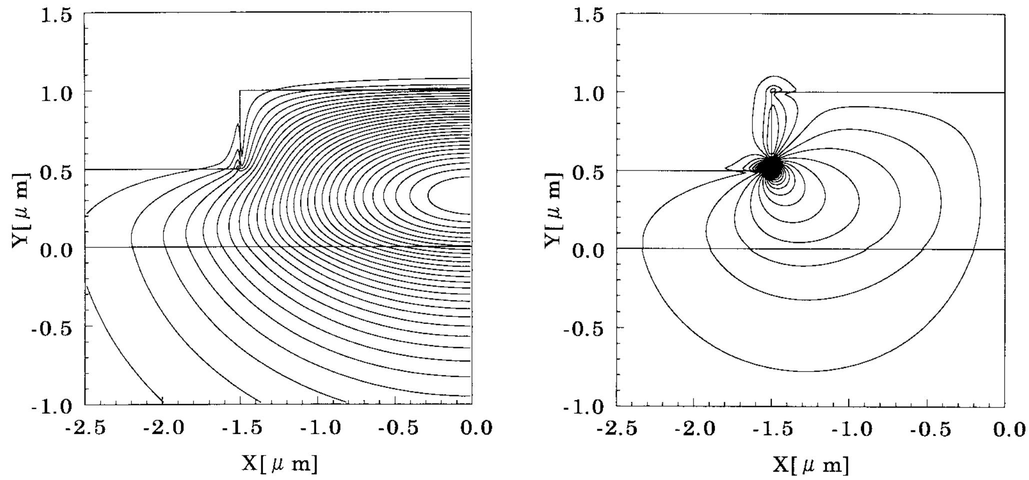
		quasi-TE mode			
t	MTRM[10]	sv	fv	sv_{EXTR}	fv_{EXTR}
0.1	0.3019	+3	+4	-1	0
0.3	0.3110	+2	+4	-2	+1
0.5	0.3270	+1	+4	-3	0
0.7	0.3510	+4	+5	+1	+1
0.9	0.3883	+6	+3	+1	0
		quasi-TM mode			
t	MTRM[10]	sv	fv	sv_{EXTR}	fv_{EXTR}
0.1	0.2674	+2	+2	0	0
0.3	0.2751	+1	+2	-1	0
0.5	0.2890	0	+1	-2	0
0.7	0.3107	0	+1	-2	-1
0.9	0.3455	+1	+1	-1	-1

the MTRM. The four-digit values of B_{MTRM}'s are believed to be exact [10], [11]. Table I also presents extrapolated values at $\Delta = 0$ and indicates that the difference between the semivectorial and full-vectorial results is slight. It should be noted, however, that the data on the full-vectorial case remarkably agree with B_{MTRM}'s. The deviation for fv_{EXTR} is only within ± 1. It can be said that accurate evaluation of the mixed derivatives greatly contributes to improvement of accuracy in terms of agreement with the MTRM.

Typical field distributions in the quasi-TE and quasi-TM modes are illustrated in Figs. 6 and 7, respectively. Singularities and discontinuities of the fields are clearly displayed.

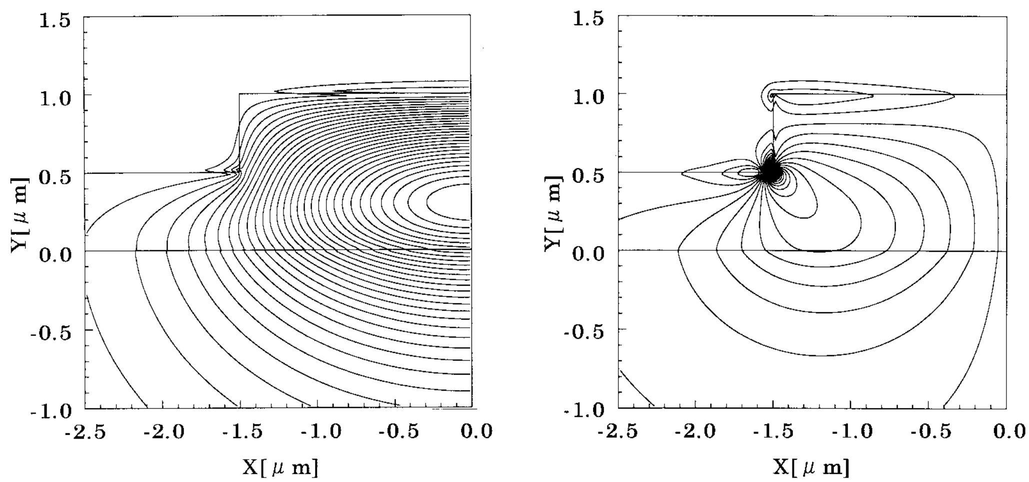
Comparison in deviations with other techniques is shown in Fig. 8. All the data are derived using an extrapolation

$$\beta(\tau) = n_0 k + \frac{\left[\ln\left\{\int \phi(x, y, \tau + \Delta\tau)\, dx\, dy\right\} - \ln\left\{\int \phi(x, y, \tau)\, dx\, dy\right\}\right]}{\Delta\tau} \tag{17}$$



(a) (b)

Fig. 6. Field distributions in the quasi-TE mode: (a) E_x and (b) E_y.



(a) (b)

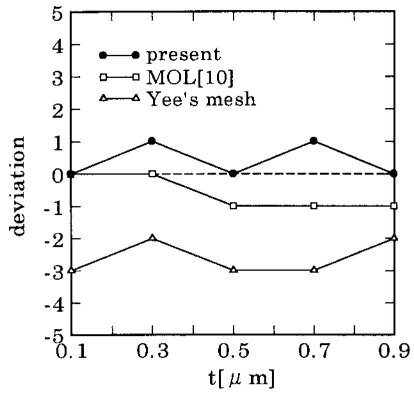
Fig. 7. Field distributions in the quasi-TM mode: (a) E_y and (b) E_x.

technique and expressed as a function of t. One of the data was obtained by Pregla using the method of lines (MOL) [10], [18]. Another data was obtained using the Yee's mesh VBPM [19], [20]. In general, all the results relatively agree with the data of the MTRM. Strictly speaking, however, the MOL achieves better results in the quasi-TE mode than the quasi-TM mode, while the Yee's mesh VBPM indicates opposite tendency. It is noteworthy that the present method is successful for both the quasi-TE and the quasi-TM mode.

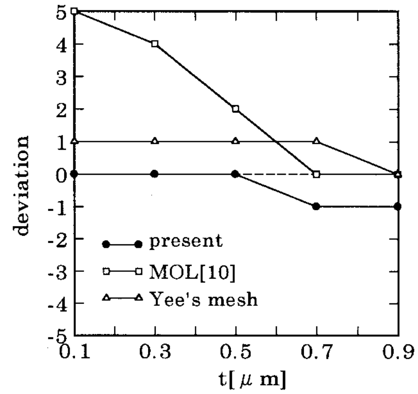
Fig. 9 shows another interesting comparison among three different discretization schemes: Stern type (present), Bierwirth type [21], and Yee type [20]. The rib waveguide configuration to be considered here is the one used in [21]. Note that in contrast to the Stern scheme, the discontinuity lines are just on mesh points in the Bierwirth scheme. Also note that in the Yee scheme, the components of $\mathbf{E}$ and $\mathbf{H}$ are interlaced within a unit cell. It is worth mentioning that the present scheme again shows the fastest convergence, although each scheme is second-order accurate. The reason why a Stern-type scheme shows faster convergence than a Bierwirth-type scheme is probably due to the fact that the Stern-type scheme avoids evaluation of the fields at the corners of the rib waveguide. One should note that quite recently, Hadley succeeded in deriving a high-accuracy formula in the Bierwirth type [22]. It seems, however, that the high-accuracy formula is effective except for corner points.

V. Conclusions

We have presented an improved vectorial finite-difference BPM based on the McKee–Mitchell scheme. The present scheme is more stable than the conventional Peaceman–Rachford scheme and achieves high computational efficiency in comparison with an iterative solver. The mixed derivatives in the coupled wave equations are evaluated taking into account discontinuities of refractive indexes. The present BPM ensures second-order accuracy, provided that the discontinuity lies midway between two mesh points. The propagation constants of a rib waveguide for a classical benchmark are evaluated using the imaginary distance procedure in both quasi-TE and quasi-TM modes. The



(a)



(b)

Fig. 8. Comparison in deviations from MTRM as a function of t: (a) quasi-TE mode and (b) quasi-TM mode.

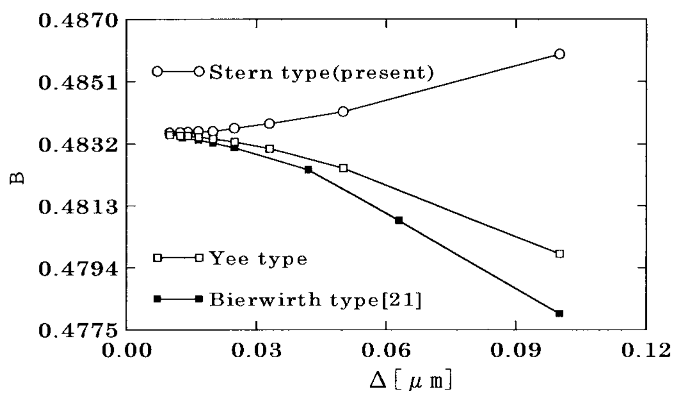


Fig. 9. Comparison in convergence behavior of the normalized propagation constant B among three discretization schemes.

obtained results remarkably agree with the values derived with the modal transverse resonance method.

APPENDIX

When a discontinuity lies between points $i-1$ and i, the FD formulas corresponding to (14)–(16), respectively, are derived as follows:

$$\frac{\partial^2 \phi_i}{\partial x^2} = \frac{2(\phi_{i-1} + b_2\phi_i + c_2\phi_{i+1})}{d\Delta x^2} + O(\Delta x^2) \qquad (18)$$

where $b_2 = -(3\theta'+1)/2 - m'\Delta x^2(\theta'+\Gamma')$, $c_2 = (\theta'+1)/2 + m'\Delta x^2\Gamma'$, and $d = 1+\theta'+m'\Delta x^2\Gamma'$, in which $\theta' = n_i^2/n_{i-1}^2$, $m' = k^2(n_i^2 - n_{i-1}^2)/8$, and $\Gamma' = \theta'/2 + 1/6$

$$\frac{\partial \phi_i}{\partial x} = \frac{-\phi_{i-1} - b_1\phi_i + c_1\phi_{i+1}}{d\Delta x} + O(\Delta x^2) \qquad (19)$$

where $b_1 = (1-\theta')/2 - m'\Delta x^2\theta'$ and $c_1 = (\theta'+1)/2$

$$\frac{\partial \tilde{\phi}_i}{\partial x} = \frac{-\theta'\tilde{\phi}_{i-1} - b_1\tilde{\phi}_i + c_1\tilde{\phi}_{i+1}}{d\Delta x} + O(\Delta x^2). \qquad (20)$$

The coefficient d can be approximated by $1+\theta'$ without significant effects.

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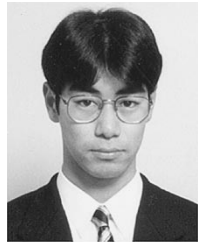

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