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Modified Finite-Difference Formula for the Analysis of Semivectorial Modes in Step-Index Optical Waveguides

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***Abstract*—The modified finite-difference formula is presented for the second derivative of a semivectorial field in a step-index optical waveguide. The present formula achieves a truncation error of $O(\Delta x^2)$ provided the discontinuity coincides with a mesh point or lies midway between two mesh points. Furthermore, the formula allows a general position of the interface, when used with the beam-propagation method (BPM). To demonstrate the effectiveness of the formula, asymmetric step-index waveguides are analyzed using the imaginary-distance BPM.**

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

I. Introduction

When a step-index optical waveguide is analyzed using a finite-difference method, care has to be taken at an interface between two different media [1]. Stern [2] developed the finite-difference formula for a semivectorial field in waveguides with refractive-index discontinuities. Subsequently, Kim and Ramaswamy [3] extended Stern's expression to a general position of the interface with respect to mesh points. Meanwhile, Vassallo [4] generalized Stern's expression and proposed the improved finite-difference formulas for scalar and semivectorial fields. The study similar to that of Vassallo was also made by Wijnands *et al.* [5]. It should be noted, however, that all the expressions presented so far have had a truncation error of $O(\Delta x)$ for semivectorial fields.

The purpose of this letter is to present an improved finite-difference formula for a semivectorial field, which ensures a truncation error of $O(\Delta x^2)$ provided the interface coincides with a mesh point or lies midway between two mesh points. When used with the beam-propagation method (BPM), the present formula allows a general position of the interface without the knowledge of the propagation constant. To demonstrate its higher accuracy than previous formulas, an asymmetric step-index slab waveguide and an embedded waveguide are examined. The accuracy of the mode profile and the propagation constant is evaluated using the imaginary-distance BPM [6]–[8].

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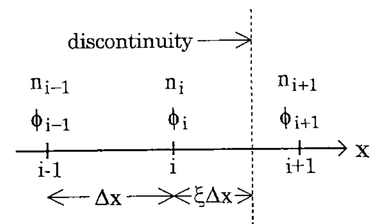

Fig. 1. Mesh points near a discontinuity.

II. Discussion

Following the procedure developed by Vassallo [4], we treat three consecutive mesh points with a discontinuity between points i and $i+1$, as shown in Fig. 1. The interface is at distance $\xi\Delta x$ (with $0 \le \xi < 1$) from point i. We derive the finite-difference approximation for the second derivative at point i.

We consider the one-dimensional Helmholtz equation expressed as

$$\frac{\partial^2\phi(x)}{\partial x^2} + [k^2n^2(x) - \beta^2]\phi(x) = 0 \quad (1)$$

where k is the free-space wavenumber, β is the propagation constant, and $n(x)$ is the index profile.

To obtain the finite-difference formula regarding $\partial^2\phi_i/\partial x^2$, we first express the fields ϕ_{i-1} and ϕ_{i+1} using Taylor's series expansion. ϕ_{i-1} is given as

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

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

$$\phi_{i+1} = \phi_R + (1-\xi)\Delta x\frac{\partial\phi_R}{\partial x} + (1-\xi)^2\frac{\Delta x^2}{2}\frac{\partial^2\phi_R}{\partial x^2} + (1-\xi)^3\frac{\Delta x^3}{6}\frac{\partial^3\phi_R}{\partial x^3} + O(\Delta x^4). \quad (3)$$

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

$$\phi_L = \phi_i + \xi\Delta x\frac{\partial\phi_i}{\partial x} + \xi^2\frac{\Delta x^2}{2}\frac{\partial^2\phi_i}{\partial x^2} + \xi^3\frac{\Delta x^3}{6}\frac{\partial^3\phi_i}{\partial x^3} + O(\Delta x^4). \quad (4)$$

Since the relation between ϕ_R and ϕ_L is given by

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

ϕ_{i+1} can be rewritten in the form

$$\begin{aligned}\phi_{i+1} = {}&[\theta + \theta m\Delta x^2]\phi_i\\ &+ \left[1 - \xi + \theta\xi + m\Delta x^2\left(\theta\xi + \frac{1-\xi}{3}\right)\right]\Delta x\frac{\partial\phi_i}{\partial x}\\ &+ [\theta\xi^2 + 2\xi(1-\xi) + \theta(1-\xi)^2]\frac{\Delta x^2}{2}\frac{\partial^2\phi_i}{\partial x^2}\\ &+ [\theta\xi^3 + 3\xi^2(1-\xi) + 3\theta\xi(1-\xi)^2\\ &+ (1-\xi)^3]\frac{\Delta x^3}{6}\frac{\partial^3\phi_i}{\partial x^3} + O(\Delta x^4)\end{aligned} \quad (5)$$

where

$$\theta = n_i^2/n_{i+1}^2 \quad \text{and} \quad m = \tfrac{1}{2}k^2(1-\xi)^2(n_i^2 - n_{i+1}^2).$$

The finite-difference formula for the second derivative can be obtained by substituting (2) into (5). Unfortunately, (5) is not simple. Therefore, Vassallo neglected the Δx^3 terms, and contented himself with a zeroth-order formula. However, in this formulation we retain the Δx^3 terms. Then, we establish the following finite-difference formula:

$$\frac{\partial^2\phi_i}{\partial x^2} = \frac{a\phi_{i-1} + b\phi_i + c\phi_{i+1}}{d\Delta x^2} + e\frac{\Delta x}{3}\frac{\partial^3\phi_i}{\partial x^3} + O(\Delta x^2) \quad (6)$$

where

$$\begin{aligned}a &= 1 + (\theta - 1)\xi + m\Delta x^2\Gamma\\ b &= -2 - (\theta-1)(1+\xi) - m\Delta x^2(\theta + \Gamma)\\ c &= 1\\ d &= 1 + \tfrac{1}{2}(\theta-1)(2\xi^2 - \xi + 1) + \tfrac{1}{2}m\Delta x^2\Gamma\\ e &= -(\theta-1)\xi(\xi-1)(2\xi-1)/d\end{aligned}$$

in which $\Gamma = \theta\xi + \frac{1}{3}(1-\xi)$. It is worth mentioning that the coefficient of $\partial^3\phi_i/\partial x^3$ vanishes when either $\xi = 0$ or $\xi = 0.5$. In other words, (6) achieves a truncation error of $O(\Delta x^2)$ provided the interface coincides with a mesh point or lies midway between two mesh points. Now we comment on the relation between (6) and previous formulas. After neglecting the $\partial^3\phi_i/\partial x^3$ term, we obtain Vassallo's expression [4] with $\Gamma = 0$. Furthermore, (6) reduces to Stern's expression [2] by making $m = 0$ and $\xi = 0.5$.

To investigate the properties of various formulas, we first analyze an asymmetric step-index slab waveguide. The refractive indices of the core, substrate and superstrate are chosen to be $n_{\rm core} = 3.512$, $n_{\rm sub} = 3.17$ and $n_{\rm sup} = 1.0$, respectively. The core width is taken to be $w = 0.5$ μm. The imaginary-distance BPM [6]–[8] is used to obtain the lowest eigenmode at a wavelength of $\lambda = 1.55$ μm.

Consideration is given to the accuracy of the field profile. The overlap integral between the numerical and exact solutions is evaluated. The correlation between them predicts the accuracy of the finite-difference formula. The results as a function

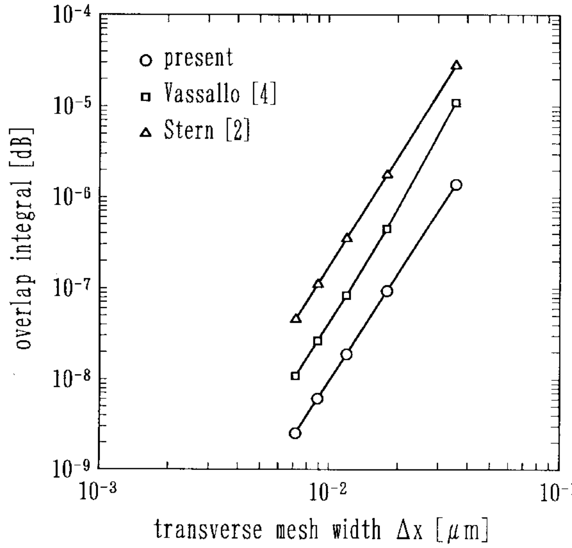

Fig. 2. Overlap integral between the numerical and exact fields in an asymmetric slab waveguide as a function of transverse mesh width.

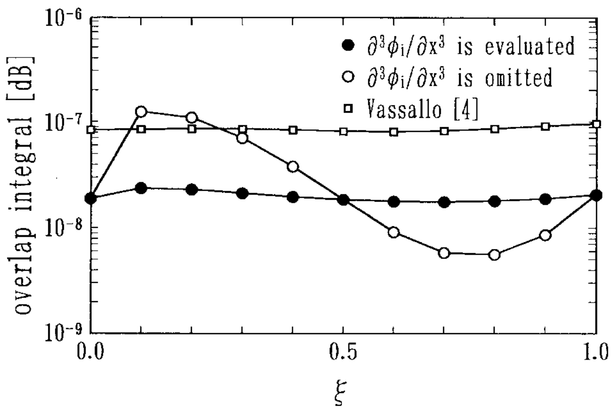

Fig. 3. Overlap integral between the numerical and exact fields in an asymmetric slab waveguide as a function of interface position.

of transverse mesh width are shown in Fig. 2. In this analysis, ξ is fixed to be 0.5. The propagation step length is taken to be $\Delta z = 0.1$ μm. The computational window dimension is fixed to be 6 μm. Calculations are made at a propagation distance of 50 μm. No significant additional computation time is observed for the present formula, and the memory requirement of the present formula is the same as that of Vassallo's one. It is clearly seen that the present formula leads to substantial improvement in accuracy over not only Stern's one but also Vassallo's one.

It is interesting to investigate the properties of (6) as a function of ξ, with the $\partial^3\phi_i/\partial x^3$ term being omitted. Fig. 3 shows the overlap integral as a function of ξ. In this calculation, Δx is chosen to be $w/42 \simeq 0.0119$ μm, and other numerical parameters are the same as those in Fig. 2. For comparison, the results obtained from Vassallo's expression are also presented. It is seen that the results obtained from (6) show oscillatory behavior as a function of ξ. As expected, the result exhibits the same value at $\xi = 0$ and 0.5, while achieving higher accuracy. In contrast, Vassallo's expression is insensitive to the change in ξ.

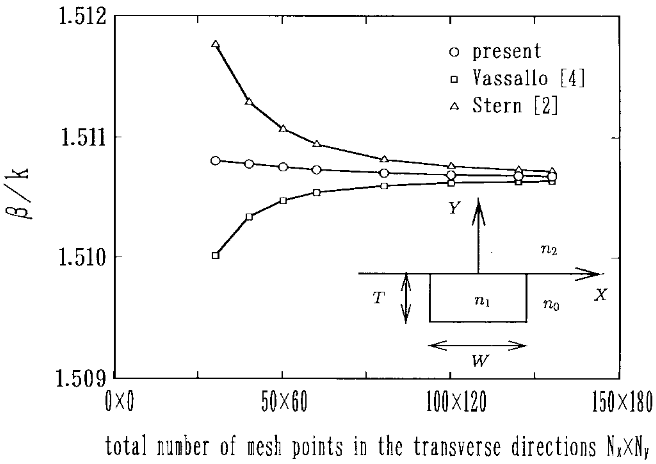

Fig. 4. Effective index of an embedded waveguide as a function of the total number of mesh points in the transverse directions.

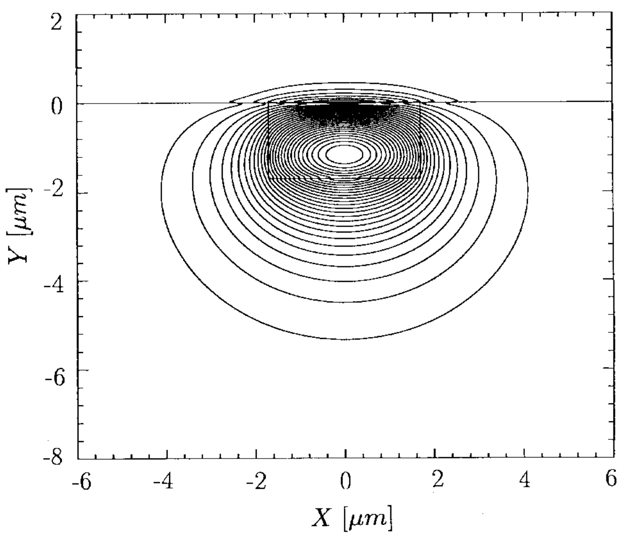

Fig. 5. Contour plots of the field.

To eliminate the dependence of ξ on accuracy in (6), we have to evaluate $\partial^3\phi_i/\partial x^3$. It should be noted that when (6) is used with the BPM, we can evaluate $\partial^3\phi_i/\partial x^3$, just as in the case of the generalized Douglas scheme [9]. The third derivative can be regarded as $\delta(\partial^2\phi_i/\partial x^2)$, where $\delta = (\phi_i - \phi_{i-1})/\Delta x + O(\Delta x)$. The second derivative is replaced using the Fresnel equation, so that the truncation error of (6) is reduced to $O(\Delta x^2)$. The result obtained from this technique is also presented in Fig. 3. It is found that the dependence of ξ on accuracy is almost eliminated. Alternatively, we can eliminate the second derivative using (1). In this case, the second term in the right-hand side of (6) becomes $[(k^2n_{i-1}^2 - \beta^2)\phi_{i-1} - (k^2n_i^2 - \beta^2)\phi_i]e/3$. Calculation shows that the results are almost the same as those obtained using the Fresnel equation. It should be noted, however, that the latter technique requires the knowledge of β.

Finally, we apply the present formula to the alternating-direction implicit method, and analyze a three-dimensional embedded waveguide shown in the inset of Fig. 4. The refractive indices are chosen to be $n_0 = 1.5$, $n_1 = 1.55$, and $n_2 = 1.0$, respectively. The aspect ratio of W/T is two. The quasi-TM mode at a wavelength of $\lambda = 1.55$ μm is considered. The computational window dimensions are fixed to be $L_x = 17$ μm and $L_y = 10.2$ μm. Since the exact mode profile cannot be obtained in a three-dimensional waveguide, we assess the accuracy using the convergence of β/k. Fig. 4 shows β/k as a function of the total number of mesh points, $N_x \times N_y$, in the transverse directions. The propagation step length is $\Delta z = 0.25$ μm. We can find faster convergence of the present formula. The contour plots of the field are illustrated in Fig. 5. The electric-field discontinuities across the horizontal interfaces are clearly visible.

III. Conclusion

The modified finite-difference formula which ensures a truncation error of $O(\Delta x^2)$ has been presented for the analysis of a semivectorial field in a step-index optical waveguide. The formula is derived by taking into account the higher order term, which is related to the interface conditions at a discontinuity. To assess the accuracy, the overlap integral in an asymmetric slab waveguide and the propagation constant of a three-dimensional embedded waveguide are evaluated by the imaginary-distance beam-propagation method. The present formula offers substantial improvement in the analysis of the semivectorial fields compared with the conventional ones.

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