New method for nonparaxial beam propagation

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A new method for solving the wave equation is presented that is nonparaxial and can be applied to wide-angle beam propagation. It shows very good stability characteristics in the sense that relatively larger step sizes can be taken. An implementation by use of the collocation method is presented in which only simple matrix diagonalization or inversion is needed. The method is hence faster and is also highly accurate. © 2004 Optical Society of America

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1. INTRODUCTION

Recently several schemes have been suggested for wide-angle and bidirectional beam propagation through guided-wave devices.1–13 In general, this nonparaxial propagation would involve solving directly the wave equation, which contains a second-order partial derivative with respect to z (the general direction of propagation) as against the first-order partial derivative in the paraxial wave equation. All the methods for nonparaxial beam propagation discussed in the literature approach this problem iteratively; a numerical effort equivalent to solving the paraxial equation several times is involved. The actual number of iterations depends on the desired accuracy and the obliquity of the beam. Many of these methods neglect the backward-propagating components and solve the one-way wave equation; but even methods that deal with bidirectional propagation employ special techniques either to suppress or to model evanescent modes, which are a source of instability in these methods.8–10 In all these methods, the square root of the propagation operator involved in the wave equation is approximated in various ways. One of the approximations used is based on the Padé approximants.1,11 We have recently shown that a direct numerical solution (DNS) of the scalar wave equation gives very good accuracy and is also numerically efficient.11 The method is nonparaxial and hence is applicable to wide-angle as well as to bidirectional propagation. We used the collocation method15–17 to formulate our equations. In this paper we present a new method of solving the nonparaxial wave equation that uses symmetrized splitting of the operators. Examples show that this method is more tolerant to larger step sizes than other methods, including the DNS.14

2. SPLIT-STEP NONPARAXIAL METHOD

For simplicity, we shall confine our discussions in this paper to two-dimensional wave propagation for which the scalar wave equation is given by

\[
\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial z^2} + k_0^2 n^2(x, z) \psi(x, z) = 0, \tag{1}
\]

where \( \psi(x, z) \) represents one of the Cartesian components of the electric field (generally referred to as the scalar field) and \( n^2(x, z) \) defines the refractive-index distribution of the medium. The time dependence of the field is assumed to be exp(i\omega t), and \( k_0 = \omega/c \) is the free-space wave number.

Equation (1) can be rewritten as

\[
\frac{\partial \Phi}{\partial z} = H(z) \Phi(z), \tag{2}
\]

where

\[
\Phi(z) = \begin{bmatrix} \psi \\ \frac{\partial \psi}{\partial z} \end{bmatrix}, \quad H(z) = \begin{bmatrix} 0 & 1 \\
-\nabla_0^2 - k_0^2 n^2 & 0 \end{bmatrix}. \tag{3}
\]

The operator \( H \) can be written as a sum of two operators, one representing the propagation through a uniform medium of index, say \( n_r \), the other representing the effect of the index variation of the guiding structure; thus

\[
H(z) = H_1 + H_2(z)
= \begin{bmatrix} 0 & 1 \\
-\nabla_0^2 - k_0^2 n_r^2 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\
k_0^2 (n_r^2 - n^2) & 0 \end{bmatrix}. \tag{4}
\]

A formal solution of Eq. (2), after use of the symmetrized splitting of summation of operators as in Eq. (4), can be written as

\[
\Phi(z + \Delta z) = P Q(z) \Phi(z) + O((\Delta z)^3), \tag{5}
\]

where

\[
P = \exp\left(\frac{1}{2} H_1 \Delta z\right), \quad Q(z) = \exp(H_2 \Delta z). \tag{6}
\]

The operator \( P \) represents propagation in the uniform medium \( n_r \) over a distance of \( \Delta z/2 \) and hence can be evaluated by using any method such as the collocation, finite-difference, or fast-Fourier-transform methods. The operator \( Q(z) \) can also be easily evaluated because of the specific form of the matrix, and it can be easily seen that
since
\[(H_2)^m = 0, \quad m \geq 2,\]
(8)
because of the special form of the matrix $H_2$. It may be noted that for lossless propagation the matrix $P$ would be Hermitian, while the matrix $Q$ always has a determinant value equal to unity.

The split-step nonparaxial (SSNP) method given above can be implemented with any of the numerical methods employed to solve the wave equation, e.g., the fast-Fourier-transform beam-propagation method (BPM), finite-difference (FD) BPM, or the collocation method. In this paper we discuss implementation by use of the collocation method; implementation by use of the FD-BPM will be discussed in a future paper.

### 3. IMPLEMENTATION IN THE COLLOCATION METHOD

We have implemented the SSNP formalism in the collocation method, in which the wave equation is converted to a matrix ordinary differential equation by using the representation of the field $\psi(x, z)$ as a linear combination of a set of orthogonal basis functions, $\phi_n(x)$:

$$\psi(x, z) = \sum_{n=1}^{N} c_n(x) \phi_n(x),$$
(9)

where $c_n(x)$ are the expansion coefficients, $n$ is the order of the basis functions, and $N$ is the number of basis functions used in the expansion. The choice of $\phi_n(x)$ depends on the boundary conditions and the symmetry of the guiding structure. The expansion coefficients $c_n(x)$ are unknown and represent the variation of the field with $z$. In the collocation method, we directly obtain the formal solution of Eq. (1) by requiring that the differential equation, Eq. (1), be satisfied exactly by the expansion, Eq. (9), at $N$ collocation points $x_j, j = 1, 2, ..., N$, which are chosen such that these are the zeros of $\phi_{N+1}(x)$. Thus, by using this condition, and with some algebraic manipulations, one converts the wave equation, Eq. (1), into a matrix ordinary differential equation:

$$d^2 \Psi/dz^2 + [S_0 + k_0^2 n_r^2 I + R(z)] \Psi(z) = 0,$$
(10)

with

$$\Psi(z) = \begin{bmatrix} \phi_1(x_1, z) \\ \phi_2(x_2, z) \\ \vdots \\ \phi_N(x_N, z) \end{bmatrix},$$
$$R(z) = k_0^2 \begin{bmatrix} \Delta n^2(x_1, z) & 0 & 0 & \cdots & 0 \\ 0 & \Delta n^2(x_2, z) & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \Delta n^2(x_N, z) \end{bmatrix},$$
(11)

where $\Delta n^2(x_m, z) = n^2(x_m, z) - n_r^2$; $m = 1, 2, ..., N$; and $S_0$ is a constant known matrix defined by the basis functions. We refer to Eq. (10) as the collocation equation. In deriving this equation from the wave equation, Eq. (1), no approximation has been made except that $N$ is finite and Eq. (10) is exactly equivalent to Eq. (1) as $N \to \infty$. Thus the accuracy of the collocation method improves indefinitely as $N$ increases. The collocation equation is a matrix ordinary differential equation and can be solved as an initial value problem by using any standard method, such as the Runge–Kutta method, as we have done in the DNS. In this paper we solve this equation by using the SSNP discussed in Section 2.

We have chosen here a set of sinusoidal functions as the basis functions and, following the procedure outlined in Section 2, we obtain the formal solution of Eq. (10) as in Eq. (5), with the operators $P$ and $Q$ and the field function $\Phi$ now being block matrices,

$$\Phi(z) = \begin{bmatrix} \Psi \\ d\Psi/dz \end{bmatrix},$$
$$P = \exp \left\{ \frac{\Delta z}{2} \begin{bmatrix} 0 & 1 \\ -(S_0 + k_0^2 n_r^2 I) & 0 \end{bmatrix} \right\},$$
$$Q(z) = \begin{bmatrix} I & 0 \\ -R(z) & I \end{bmatrix},$$
(12)

where $I$ and $0$ are the unit and the null matrices, respectively. The operator $P$ represents propagation in a uniform medium of index $n_r$ over a distance $\Delta z/2$ and can be easily obtained as a constant square matrix by using the basis functions and their properties. It has to be evaluated only once. Each propagation step thus requires 12 multiplications of an $N \times N$ square matrix with a column matrix except at the first and the last steps where eight more such multiplications are required. We would like to emphasize that using the sinusoidal basis functions in the collocation method here has an advantage, since no fast Fourier transform, matrix inversion, or matrix diagonalization need be done for propagation through a uniform medium, and all matrices involved are obtained analytically; the details are presented in Appendix A.

### 4. NUMERICAL RESULTS

We consider a number of examples to show the effectiveness of the method. In the first example, we consider the propagation of the fundamental mode through a tilted, graded-index waveguide, with index profile given by $n^2(x) = n_r^2 + 2n_2 \Delta n \text{sech}^2(2x/w)$, $n_r = 2.1455$, $\Delta n = 0.003$, $w = 5 \mu m$, and $\lambda = 1.3 \mu m$. The computation was done with 530 collocation points, and the width of the numerical window was $\sim 185 \mu m$. As a measure of accuracy, we computed an error (ERR), that includes the effects of both the dissipation in power as well as the loss of shape of the propagating mode:

$$\text{ERR} = 1 - \left( \int |\psi_{\text{exact}}|^2 dx \right) / \left( \int |\psi_{\text{inp}}|^2 dx \right),$$
(13)

where $\psi_{\text{inp}}$, $\psi_{\text{calc}}$, and $\psi_{\text{exact}}$ are the input, the propagated, and the exact fields, respectively.

The first result for a straight waveguide, which we have plotted in Fig. 1, shows the performance of the method with respect to the stability of the method for relatively larger values of $\Delta z$. The DNS based on the
Runge–Kutta solution of the collocation equation\textsuperscript{14} becomes unstable for $\Delta z > 0.1$ $\mu$m, whereas the SSNP method remains stable even for 1 $\mu$m. To the best of our knowledge, a step size equal to or larger than 1 $\mu$m for nonparaxial propagation has not been reported before. Even with such a large step, an accuracy better than 0.001 in propagation over a distance of 1000 $\mu$m is significantly better than the accuracies reported in the literature. In Fig. 2 we have plotted the error in propagation (ERR) as a function of the tilt angle. The figure shows that the SSNP method gives accuracy of the order of $10^{-4}$ even with a step size of 0.25 $\mu$m, which is much better than that obtained by Shibayama et al.\textsuperscript{5} To illustrate the point, let us consider the error for a tilt angle of 50°. The error in the best results reported by Shibayama et al.\textsuperscript{5} for the three-step generalized Douglas (GD) scheme is $\sim 0.04$ with $\Delta z = 0.05$ $\mu$m, whereas in our method the error is less than 0.001 with $\Delta z = 0.25$ $\mu$m. This would thus mean much faster and more accurate propagation. Of course, one gets better accuracy with the DNS, since the single-step error in the Runge–Kutta method (used in the DNS) is $O((\Delta z)^3)$ as against $O((\Delta z)^5)$ in the SSNP method, but then the computation effort is significantly reduced with the latter method.

We next consider propagation of the TE$_1$ mode in step-index waveguides. Figure 3 shows a plot of ERR as a function of the propagation steps for the step-index waveguide\textsuperscript{6} with $n_{clad} = 1.002$, $n_{core} = 1.000$, $\lambda = 1.0$ $\mu$m, and $w = 15.092$ $\mu$m. Even with a step size as large as 0.4 $\mu$m, the propagation is extremely stable and highly accurate, while DNS becomes unstable for this step size. Figure 4 shows performance with variation in tilt angle of the waveguide. We can see that the curves for the present method and DNS\textsuperscript{14} are very close, except for the SSNP method with step size 0.4 $\mu$m at 0°, where error is higher. However, the error value even with 0.4-$\mu$m step size is better than that at 50° reported by Yamauchi et al.\textsuperscript{6} The SSNP method gives better accuracy with twice the step size used by Yamauchi et al.\textsuperscript{6}; in fact, only 500 computation points are required as against 1800 by Yamauchi et al.\textsuperscript{6}

Figures 5 and 6 show performance of the method for the TE$_1$ mode in the benchmark waveguide\textsuperscript{19} with $n_{clad} = 3.3$, $n_{core} = 3.17$, $\lambda = 1.55$ $\mu$m, and $w = 8.8$ $\mu$m. As the refractive-index change from core to cladding is very large here, only small step sizes can be taken, yet the SSNP method is stable for a step size of 0.2 $\mu$m, as shown in Fig. 5. In fact, the performance at large tilt angles with 0.2-$\mu$m step size is quite close to that for the DNS,\textsuperscript{14} as shown in Fig. 6. We may note that oscillatory behavior in the error curves becomes more pronounced for the step-index waveguide with larger index jump at the core—
cladding interface (compare Figs. 3 and 5). This may be attributed to the fact that any discretization would approximate the index step by an interpolating curve between two successive sample points around the step. As expected this oscillation becomes larger as $D_z$ increases from 0.01 to 0.2 μm [although the log scale deceptively shows nearly equal oscillations].

The final example is that of propagation of the TE$_{10}$ mode in the benchmark waveguide$^{19}$ described above, and we have obtained the power remaining in the guide after propagation of 100 μm at a tilt angle of 20°. Table 1 compares the SSNP method with other methods. It is quite obvious from the table that with fewer points, the SSNP method shows higher accuracy. The method is also faster than the DNS,$^{14}$ taking only about half the time. It is also much easier to implement.

An important parameter to choose is the reference refractive index $n_r$. Although, in principle, its value can be arbitrarily chosen, the value in general affects the accuracy. However, as Fig. 7 shows, the accuracy with the new method is largely insensitive to the choice of $n_r$.

We would like to add that neither the SSNP method nor the DNS method is very sensitive to perturbations in the value of the initial field or its derivative. We have carried out preliminary investigations by adding and subtracting a small error ($10^{-3}$) alternately in the initial field and its derivative at successive sample points. The error in the overlap integral was $1.9 \times 10^{-2}$ as against $2.6 \times 10^{-5}$ for propagation of the TE$_1$ mode at 0° for 100 μm with a propagation step size of 0.1 μm, in the benchmark waveguide$^{19}$ where $n_{co} = 3.3$, $n_{clad} = 3.17$, $\lambda = 1.55$ μm, and $w = 8.8$ μm. Thus the propagation remains stable.

### Table 1. Comparison of Error–Power Loss in Propagation to 100 μm in the Benchmark$^a$ Step-Index Waveguide for TE$_{10}$ Modes with Different Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>$N_x$</th>
<th>$N_z$</th>
<th>Power in Waveguide at 20°</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSNP</td>
<td>1000</td>
<td>800</td>
<td>0.96</td>
</tr>
<tr>
<td>DNS$^a$</td>
<td>1000</td>
<td>800</td>
<td>0.90</td>
</tr>
<tr>
<td>AMIGO$^b$</td>
<td>1429</td>
<td>1311</td>
<td>0.95</td>
</tr>
<tr>
<td>FD2BPM$^c$</td>
<td>1000</td>
<td>2048</td>
<td>0.95</td>
</tr>
<tr>
<td>PTBPM$^c$</td>
<td>1000</td>
<td>256</td>
<td>0.55</td>
</tr>
<tr>
<td>LETI-FD</td>
<td>200</td>
<td>1024</td>
<td>0.15</td>
</tr>
</tbody>
</table>

$^a$Ref. 14  
$^b$Ref. 19.

### 5. CONCLUSIONS

We have presented a new method for solving the non-paraxial wave equation based on a symmetrized splitting of the operator. We have implemented this method with the collocation method. We have also included comparison with reported results of other methods. The method shows better stability with relatively larger step sizes being possible. The method involves only simple multiplication of matrices, and no numerical diagonalization or inversion of any matrix is needed. It is therefore much faster and easier to implement and is more efficient than other methods.

### APPENDIX A: EVALUATION OF exp(H$_1$$\Delta z$)

This amounts to a solution of the collocation Eq. (10) without the $\mathbf{R}(z)$ term, i.e., propagation in a medium of uniform refractive index $n_r$ over a distance $\Delta z$, that is, solution of the equation

$$ \frac{d^2 \Psi}{dz^2} + S\Psi(z) = 0, $$

(A1)
where \( S = S_0 + k_0^2 n_z^2 I \) is a constant matrix. Equation (A1) can also be written as
\[
\partial \Phi / \partial z = H_1 \Phi(z),
\]  
where \( \Phi(z) \) is defined in Eq. (12), and
\[
H_1 = \begin{bmatrix} 0 & I \\ -S & 0 \end{bmatrix}
\]
is a constant matrix and has to be evaluated just once. A formal solution of Eq. (A2) can be written as
\[
\Phi(z + \Delta z) = \exp(H_1 \Delta z) \Phi(z).
\]  
Equation (A3)

The evaluation of \( \exp(H_1 \Delta z) \) can be done by diagonalization of \( H_1 \); however, \( H_1 \) is a \( 2N \times 2N \) nonsymmetric matrix and its diagonalization may involve complex matrix algebra and hence, present some difficulties. We present here a much simpler and analytical method for evaluating \( \exp(H_1 \Delta z) \).

Since Eq. (A1) represents propagation in a uniform medium, the propagation can be obtained by an eigenvalue decomposition method. Thus the solution of Eq. (A1) over a single step can be written as
\[
\Psi(z + \Delta z) = \cos(\sqrt{S} \Delta z) \Psi(z) + \frac{1}{\sqrt{S}} \sin(\sqrt{S} \Delta z) \Psi'(z),
\]  
(A4)
\[
\Psi'(z + \Delta z) = -\sqrt{S} \sin(\sqrt{S} \Delta z) \Psi(z) + \cos(\sqrt{S} \Delta z) \Psi'(z).
\]  
(A5)

Using this solution in Eq. (A3) gives
\[
\exp(H_1 \Delta z) = \begin{bmatrix} \cos(\sqrt{S} \Delta z) & \frac{1}{\sqrt{S}} \sin(\sqrt{S} \Delta z) \\ -\sqrt{S} \sin(\sqrt{S} \Delta z) & \cos(\sqrt{S} \Delta z) \end{bmatrix}.
\]  
(A6)

To evaluate the functions of the matrices involved in Eq. (A6), we use the diagonalization procedure. Thus, let \( S = V \Lambda V^{-1} \) where \( V \) and \( \Lambda \) are the eigenvectors and eigenvalues of \( S \), respectively. Then, we have
\[
\sqrt{S} \Delta z = V(\sqrt{\Lambda} \Delta z) V^{-1}, \quad \sqrt{\Lambda} = \text{diag}().
\]  
(A7)

and
\[
\cos(\sqrt{S} \Delta z) = V \cos(\sqrt{\Lambda} \Delta z) V^{-1}, \quad \sin(\sqrt{S} \Delta z) = V \sin(\sqrt{\Lambda} \Delta z) V^{-1}.
\]  
(A8)

Thus
\[
\exp(H_1 \Delta z) = \begin{bmatrix} V & 0 \\ 0 & V \end{bmatrix} \begin{bmatrix} \cos(\sqrt{\Lambda} \Delta z) & \frac{1}{\sqrt{\Lambda}} \sin(\sqrt{\Lambda} \Delta z) \\ -\sqrt{\Lambda} \sin(\sqrt{\Lambda} \Delta z) & \cos(\sqrt{\Lambda} \Delta z) \end{bmatrix} \begin{bmatrix} V^{-1} & 0 \\ 0 & V^{-1} \end{bmatrix}.
\]  
(A9)

The operator \( P \) in Eq. (12) is thus given by Eq. (10) with \( \Delta z \) replaced by \( \Delta z/2 \).

In the case of sinusoidal basis functions in the collocation method,\(^6\) the form of \( S \) is such that the eigenvalue decomposition required as per Eq. (A7) is simply done analytically. In this case, we choose the basis functions as
\[
\phi_n(x) = \cos(v_n x) \quad \text{for } n = 1, 3, 5, \ldots N - 1,
\]
\[
= \sin(v_n x) \quad \text{for } n = 2, 4, 6, \ldots N,
\]  
(A11)

where \( v_n = n \pi / 2L \), with the computation window running from \(-L \) to \( L \). The collocation points are at
\[
x_j = \left( \frac{2j}{N + 1} - 1 \right) L, \quad j = 1, 2, 3, \ldots N.
\]  
(A12)

The matrix \( S \) in this case is then given by\(^6,7\)
\[
S = A \Lambda A^{-1} + k_0^2 n_z^2 I = A(G + k_0^2 n_z^2 I)A^{-1},
\]  
(A13)

where \( A \) is a constant square matrix with elements as \( A_{ij} = \phi_j(x_i) \) and the matrix \( G \) is given by
\[
G = \text{diag}(-v_1^2, -v_2^2, -v_3^2, \ldots -v_N^2).
\]  
(A14)

Thus we have
\[
V = A, \quad \Lambda_i = k_0^2 n_z^2 - v_i^2.
\]  
(A15)

Further, it can be shown that
\[
V^{-1} = A^{-1} = \left( \frac{2}{N + 1} \right) A^T.
\]  
(A16)

Thus no matrix eigenvalue equation need be solved. With these values of \( V \) and \( \Lambda \), one obtains the following from Eq. (A10):
\[
\exp(H_1 \Delta z) = \left( \frac{2}{N + 1} \right) \begin{bmatrix} A & 0 \\ 0 & A \end{bmatrix}
\times \begin{bmatrix} c_1 & 0 & \cdots & 0 & s_1 & 0 & \cdots & 0 \\ 0 & c_2 & \cdots & 0 & s_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & c_N & 0 & 0 & \cdots & s_N \\ \bar{s}_1 & 0 & \cdots & 0 & c_1 & 0 & \cdots & 0 \\ 0 & \bar{s}_2 & \cdots & 0 & 0 & c_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \bar{s}_N & 0 & 0 & \cdots & c_N \end{bmatrix}
\times \begin{bmatrix} A^T & 0 \\ 0 & A^T \end{bmatrix}.
\]  
(A17)

where
\[
c_i = \cos(\sqrt{\Lambda_i} \Delta z), \quad s_i = 1/\sqrt{\Lambda_i} \sin(\sqrt{\Lambda_i} \Delta z),
\]
\[
\bar{s}_i = -\sqrt{\Lambda_i} \sin(\sqrt{\Lambda_i} \Delta z).
\]  
In cases where \( \Lambda_i \) is imaginary [see Eq. (A15)], the quantities \( c_i, s_i, \) and \( \bar{s}_i \) remain real, and sine and cosine functions are evaluated through the corresponding hyperbolic functions.
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