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A New Finite-Difference Based Method for Wide-Angle Beam Propagation

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Abstract **-- A novel split-step finite difference method for wide-angle beam propagation is presented. The formulation allows solution of the second order scalar wave equation without having to make the slowly varying envelope and one-way propagation approximations. The method is highly accurate and numerically efficient requiring only simple matrix multiplication for propagation. The method can be used for bi-directional propagation as well.**

Index Terms -- **Beam Propagation, Wide angle method, Finite Difference Method, Split-step method.**

I. Introduction

Modeling of practical guided-wave devices requires solution of the wave equation in a structure that may have complex refractive index distribution and/or several branches. In most such structures, the paraxial approximation for beam propagation is not valid and may lead to large error in simulations. Thus, non-paraxial solutions are required. Several schemes have been suggested for wide-angle and bi-directional beam propagation through guided-wave devices [1]-[9]. All Most of the methods for non-paraxial beam propagation discussed in the literature approach this problem iteratively, in which a numerical effort equivalent to solving the paraxial equation several times is involved. Most of these the wide angle (unidirectional) methods neglect the backward propagating components and solve the one-way wave equation. 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]-[8]. Recently, we have proposed a new method [10] based on symmetrized splitting of the operator for non-paraxial propagation using the collocation method [11]. In this paper, we show that the split-step non-paraxial scheme can be implemented efficiently in the finite-difference based propagation method without resorting to the paraxial approximation.

II. Formulation

We consider, for simplicity, two-dimensional propagation; the scalar wave equation is then given by

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

We write this equation as

$$\frac{\partial \mathbf{\Phi}}{\partial z} = \mathbf{H}(z)\,\mathbf{\Phi}(z), \tag{2}$$

where

$$\mathbf{\Phi}(z) = \begin{bmatrix} \psi \\ \dfrac{\partial \psi}{\partial z} \end{bmatrix} \quad \text{and} \quad \mathbf{H}(z) = \begin{bmatrix} 0 & 1 \\ -\dfrac{\partial^2}{\partial x^2} - k_0^2 n^2 & 0 \end{bmatrix}. \tag{3}$$

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

$$\mathbf{H}(z) = \begin{bmatrix} 0 & 1 \\ -\dfrac{\partial^2}{\partial x^2} - k_0^2 n_r^2 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ k_0^2(n_r^2 - n^2) & 0 \end{bmatrix} \equiv \mathbf{H}_1 + \mathbf{H}_2(z)$$

A formal solution of Eq. (2) after symmetrized splitting of operators can be written as

$$\mathbf{\Phi}(z+\Delta z) = \mathbf{P}\,\mathbf{Q}(z)\,\mathbf{P}\,\mathbf{\Phi}(z) + O\big((\Delta z)^3\big) \tag{4}$$

where $\mathbf{P} = e^{\frac{1}{2}\mathbf{H}_1 \Delta z}$ and $\mathbf{Q}(z) = e^{\mathbf{H}_2 \Delta z}$ represent the propagation in uniform space and effect of the refractive index variation of the guiding structure, respectively. Thus, the new field at $z + \Delta z$ is simply the product $\mathbf{P}\mathbf{Q}(z)\mathbf{P}\mathbf{\Phi}(z)$. The concept of splitting of operators is independent of the scheme used for propagation. In the finite-difference implementation, we have a set of $\psi_j(z) \equiv \psi(x_j, z); \; j = 1, 2, \cdots, N$ specifying the field at different nodes x_j, at which the refractive index is known as $n_j^2(z) \equiv n^2(x_j, z)$. The evaluation of $\mathbf{Q}(z)$ is straightforward, by expanding of the exponential and noting that $[\mathbf{H}_2(z)]^m = 0$ for $m \geq 2$ due to the special form of $\mathbf{H}_2(z)$. Thus,

$$\mathbf{Q}(z) = \Delta z \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ -k_0^2\,\mathbf{R}(z) & \mathbf{I} \end{bmatrix}, \tag{5}$$

where $\mathbf{R}(z)$ is a diagonal matrix with $R_j(z) = n_j^2(z) - n_r^2$ as the diagonal elements. The evaluation of $\mathbf{P}$, on the other hand, amounts to solving the wave equation, Eq. (2), for a medium with a constant refractive index, n_r. Thus, we obtain [10]

$$\mathbf{P} = \begin{pmatrix} \cos(\sqrt{\mathbf{S}}\,\Delta z/2) & \sin(\sqrt{\mathbf{S}}\,\Delta z/2)\big/\sqrt{\mathbf{S}} \\ -\sqrt{\mathbf{S}}\,\sin(\sqrt{\mathbf{S}}\,\Delta z/2) & \cos(\sqrt{\mathbf{S}}\,\Delta z/2) \end{pmatrix} \tag{6}$$

where the operator $\mathbf{S}$ is an F-D representation of $\partial^2/\partial x^2 + k_0^2 n_r^2$. In general, $\partial^2/\partial x^2$ is represented by a 3-point central difference formula with a truncation error of Δx^2 as in the Crank-Nicholson (CN) scheme. However, this has been

found to be a limitation and a better approximation with a truncation error of Δx^4 has been used in the Generalized Douglas (GD) scheme [3],[4]. The improvements are limited to this level since these methods being implicit require a solution of the system of simultaneous equations at each propagation step, and to keep the process computationally efficient the system must remain tridiagonal to enable application of the Thomas algorithm. On the other hand, our method is explicit in nature; hence, there is no such requirement and the accuracy of the F-D representation of $\partial^2/\partial x^2$ can be increased to an arbitrary order using the expansion [12]:

$$\Delta x^2 \frac{\partial^2}{\partial x^2} = \left[2\sinh^{-1}\left(\frac{\delta_x}{2}\right)\right]^2 = \delta_x^2 - \frac{1}{12}\delta_x^4 + \frac{1}{90}\delta_x^6 \cdots \quad (7)$$

where $\delta_x^2\psi_p = \psi_{p+1} - 2\psi_p + \psi_{p-1}$, and the δ_x^2 operator can be represented by a tri-diagonal matrix. Use of the first term in the series given by Eq. 7, corresponds to the approximation made in the Crank-Nicholson (CN) scheme, and the first two terms to that in the Generalized Douglas (GD) scheme. As the number of terms in the series expansion is increased, the matrix becomes denser; however, the accuracy of the approximation for $\partial^2/\partial x^2$ increases. The increase in matrix density does not alter the computation speed or efficiency, as the number of matrix multiplications required for singe step propagation does not depend on the density of $\mathbf{S}$. Physically, increasing the number of terms in the series in Eq. 7, corresponds to an increase in the number of nodal points which are used in approximating $\partial^2/\partial x^2$, leading to a better and better representation of the derivative with respect to x, without having to adopt an iterative, multi-step procedure required in the conventional Padé analysis. It may be also b e noted that the evaluation of $\mathbf{P}$ has to be done only once. Thus, the increase in number of terms in the series expansion leads only to increase in the one time computation of $\mathbf{P}$ and does not noticeably increase the overall computation time.

III. Numerical Examples

We consider the example of the propagation of the fundamental mode through a tilted graded-index waveguide [3], for a propagation distance of $100\,\mu$m with a propagation step size of $0.05\,\mu$m. As a measure of accuracy, we computed the overlap integral and an error (ERR), which includes the effects of both the dissipation in power as well as the loss of shape of the propagating mode [10]. We have used 900 computation points for this calculation.

Figure 1 shows the variation of error (ERR) as higher order terms in the series of Eq.7 are considered. It can be clearly seen that with increase in the number of terms (order corresponds to the exponent of the last term at which the series is truncated), the error in propagation decreases substantially. This improvement in accuracy is not accompanied by an increase in computation time for propagation. This fact is
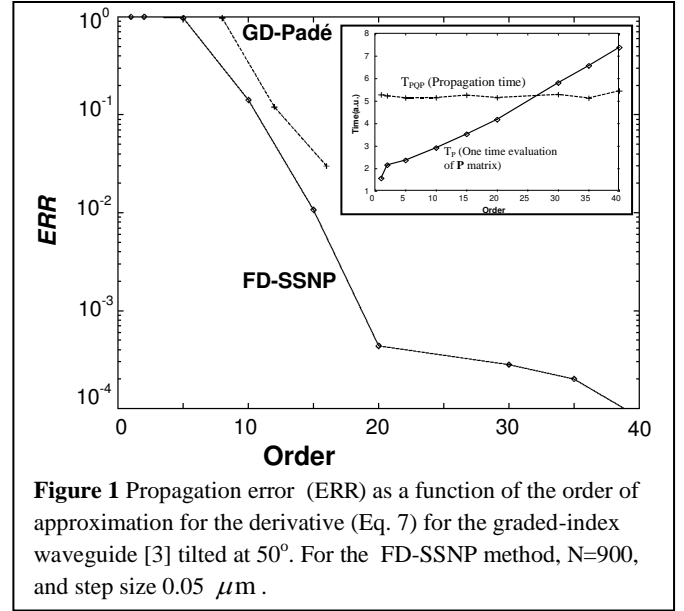

Figure 1 Propagation error (ERR) as a function of the order of approximation for the derivative (Eq. 7) for the graded-index waveguide [3] tilted at 50°. For the FD-SSNP method, N=900, and step size $0.05\,\mu$m.

illustrated by the figure shown in the inset, (see Fig.1) which shows separately the time, T_P, required for the one time computation of $\mathbf{P}$ and the time, T_{PQP}, required for the actual step-wise propagation (involving evaluation of $\mathbf{Q}$ as well as matrix multiplications as per Eq.4 at each step). The total time required for propagation would be $T_{total} = T_P + N_z\,T_{PQP}$, where N_z is the number of propagation steps. In the present case, N_z=2000. Ideally, T_{PQP} should remain a constant independent of the order. However, for our calculations we have used a multi-user MATLAB and the computation speed varies marginally with the number of user logged in at any given instant. This may have been the reason for small variations in T_{PQP}.

The order that we have used is up to 40. This may seem very high in comparison to the orders used in Padé based finite-difference schemes. One can understand this apparent difference in the following way. Our scheme is explicit while those based on Padé approximants are implicit. Generally, the order of an implicit scheme refers to the highest order in an explicit scheme with the same truncation error. However, in Padé approximant terminology, the zeroeth order refers to paraxial approximation which involves single use of the paraxial propagation operator, i.e., it is of order one in the explicit scheme. Thus, the third order Padé corresponds to 4th order in the paraxial propagation operator. Now, the paraxial operator, in the explicit form, corresponds the use of δ_x^2 for the CN scheme and δ_x^4 in the generalized GD scheme. Thus, the order in δ_x of a third-order (3-step) Padé approximants based method with the CN scheme would be 8 and with the GD scheme would be 16. Shibayama et al. [3] have used the GD scheme for 1, 2 and 3-order Padé approximants based method. Figure 1, which includes their results for the GD scheme shows that the order of error obtained in the GD scheme and the FD-SSNP are comparable for a given order.
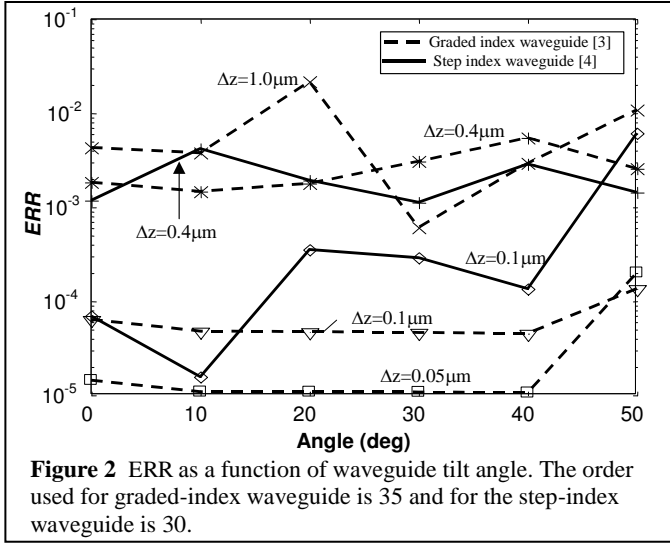
Figure 2 ERR as a function of waveguide tilt angle. The order used for graded-index waveguide is 35 and for the step-index waveguide is 30.

Table I ERR as a function of propagation distance. N=900, order=30, $n_r = \beta/k_o$ for the step index waveguide [4].

Step Size (μm)	ERR after propagation for number of steps			
	250	500	750	1000
0.10	2.54×10^{-4}	6.40×10^{-5}	1.44×10^{-4}	2.47×10^{-4}
0.25	4.63×10^{-4}	1.12×10^{-4}	2.62×10^{-4}	4.48×10^{-4}
0.40	4.34×10^{-3}	1.03×10^{-3}	2.50×10^{-3}	4.16×10^{-4}

has excellent efficiency in terms of increased accuracy, lower computation cost and easier implementation.

The advantage of our method is that the order can be increased without any significant increase in the computational effort and with substantial increase in accuracy.

Figure 2 shows variation of the error (ERR) as a function of the tilt angle of the waveguide. We have included in this figure the results for two cases: propagation of the fundamental mode in the graded-index waveguides [3] described above, and the propagation of the TE$_1$ mode of step-index waveguide described in [4]. The propagation distance in both cases is $100 \, \mu$m. We find that with only 900 computation points and step size $1 \, \mu$m, the error for all angles from 0 to 50 degrees is less than 0.03 which is the best value reported by Shibayama et al. [3] for the 3-step method with a small step size, $0.05 \, \mu$m. Similarly, the results for the step-index waveguide [4] show that the present method has much less error with several times larger step-sizes and only half the number of transverse grid points, 900. Note that the present method is non-iterative unlike the method of Yamauchi et al.[4] which is a 3-step iterative method. Table I shows the stability performance of the method with respect to propagation step size for a large propagation distance ($1000 \, \mu$m) for the untilted step index waveguide [4]. The propagation remains stable and the error is low even for a large step size such as $0.4 \, \mu$m. These comparisons show the superiority of the method in terms of computational accuracy and efficiency.

IV. Conclusions
A finite difference solution of the second order wave equation implemented in the split step format has been presented for the first time. The formulation is non-iterative and allows arbitrary increase in accuracy in determining the transverse derivatives, without any significant increase in computation. The method is an explicit transfer matrix method involving only simple matrix multiplication for propagation, and is stable with larger step sizes than reported in other existing methods. The method

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