Multistep method for wide-angle beam propagation

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A new beam-propagation method is presented whereby the Padé approximant wide-angle propagation operator is factored into a series of simpler Padé (1, 1) operators, thus leading naturally to a multistep method whose component steps are each solvable by using readily available paraxiallike solution techniques. The resulting method allows accurate approximations to true Helmholtz propagation while incurring only a modest numerical penalty. In addition, the tridiagonal form of the component steps allows the straightforward use of the previously reported transparent boundary condition.

The beam-propagation method has proven to be an extremely important tool in the simulation of guidedwave optics since its inception. Although initially limited to the study of paraxial beams, methods have recently been reported¹⁻⁴ that include approximate treatments of wide-angle propagation. Such extensions are invaluable not only for the simulation of propagation at large angles to the axis but also because they allow accurate propagation through regions whose refractive index may differ greatly from the input reference index.

However, all the methods currently available for wide-angle propagation suffer from serious drawbacks. Those based on eigenfunction expansions³ require recalculation of the eigenfunctions whenever there is a change in waveguide structure. This is numerically expensive because of the large number of eigenfunctions that must be included and also requires relatively complicated coding. Another method based on an expansion of the field in terms of a set of so-called Lanczos vectors² has been found to exhibit convergence problems.⁵ Several authors^{1,4,6} have employed various Padé approximations of the Helmholtz operator. In one case⁶ this approach leads to difference equations that are only first order in the propagation step size. Otherwise, the lowerorder Padé approaches¹ are numerically attractive, but their range of validity is still somewhat limited.

In an attempt to broaden this range, a recent method⁴ utilized a sequence of higher-order Padé approximant propagation operators to provide an arbitrarily close approximation to true Helmholtz propagation. Unfortunately, this increase in accuracy was obtained only at the expense of a corresponding increase in matrix bandwidth as the order of approximation was increased. Thus, complicated generalizations of the simple Thomas tridiagonal algorithm to treat matrix equations of bandwidth 2n + 1 for a Padé (n,n) scheme were required. Although the n = 2 case is not particularly difficult, algorithms for n > 2 involve significantly greater complexity and run times and were therefore not tested.

In this Letter, a simple finite-difference beampropagation method is presented whereby the higher-order Padé approximant operators derived previously⁴ are expressed as factors of Padé (1,1)operators, thus resulting in a simplified multistep algorithm. Because each component step is tridiagonal, wide-angle propagation may now be performed by using well-known, efficient solution algorithms commonly employed for paraxial propagation. (A similar factorization has recently been employed to perform high-order paraxial propagation.⁷) This capability should in turn allow the modeling of more complex photonic structures and systems than was previously possible, without undue numerical penalty. Furthermore, the fact that each component step is tridiagonal also allows a straightforward usage of the transparent boundary-condition algorithm previously reported for paraxial propagation.⁸

A description of the present simplified method begins with the scalar propagation equation obtained using a Padé (n,n) approximation of the true Helmholtz operator,⁴

$$\frac{\partial H}{\partial z} = \frac{iN}{D}H,\tag{1}$$

where N and D are polynomials of degree n in the operator P, defined as

$$P \equiv k_0^2 \left[\frac{\epsilon(\overline{x})}{\epsilon_0} - \overline{n}^2 \right] + \nabla_{\perp}^2, \qquad (2)$$

and z refers to the distance along the axis of propagation. In Eq. (2), k_0 is the vacuum wave vector, $\epsilon(x)$ is the dielectric function of the medium, and \overline{n} is the reference index. If Eq. (1) is discretized using standard centered differencing, we obtain

$$D(H^{m+1} - H^m) = \frac{i\Delta z}{2}N(H^m + H^{m+1}), \qquad (3)$$

where the superscript indicates position along the z axis. Equation (3) may be conveniently recast in the form

$$H^{m+1} = \frac{\sum_{i=0}^{n} \xi_{i} P^{i}}{\sum_{i=0}^{n} \xi_{i}^{*} P^{i}} H^{m},$$
(4)

where $\xi_0 = P^0 = 1$ and the other ξ 's are easily determined from the coefficients of the polynomials N and D.⁴

Since a polynomial of degree n can always be factored in terms of its n roots, we may rewrite Eq. (4) as

$$H^{m+1} = \frac{(1+a_1P)(1+a_2P)\dots(1+a_nP)}{(1+a_1^*P)(1+a_2^*P)\dots(1+a_n^*P)}H^m.$$
 (5)

Simple relationships exist between the two parameter sets defined by Eqs. (4) and (5). For example, for n = 2 we have

$$a_1 + a_2 = \xi_1,$$

 $a_1 a_2 = \xi_2,$ (6)

and for n = 3 we have

$$a_{1} + a_{2} + a_{3} = \xi_{1},$$

$$a_{1}a_{2} + a_{2}a_{3} + a_{1}a_{3} = \xi_{2},$$

$$a_{1}a_{2}a_{3} = \xi_{3}.$$
(7)

In general, determination of the a's requires the one-time solution of an nth-order complex algebraic equation.

It is apparent from the form of Eq. (5) that an nthorder Padé propagator may be decomposed into an n-step algorithm for which the *i*th partial step takes the form

$$H^{m+\frac{i}{n}} = \frac{1+a_i P}{1+a_i^* P} H^{m+\frac{i-1}{n}}.$$
 (8)

Each such partial step is unitary and tridiagonal (block tridiagonal for propagation in three dimensions). These two important properties imply that the resulting algorithm is fast and unconditionally stable. The run time for an *n*th-order propagator is obviously *n* times the paraxial run time. Because the latter is usually short, the resulting algorithm is capable of providing extremely accurate wide-angle propagation with only a modest numerical penalty.

The tridiagonal form of the constituent steps also affords another advantage, allowing the straightforward use of the transparent boundary-condition algorithm previously developed for paraxial propagation.⁸ This algorithm has been shown to simplify greatly the modeling of problems in which radiation loss at the boundaries is encountered. Although currently in use for paraxial propagation,⁹ previous attempts to extend it to higher-order methods had been unsuccessful. By using the present multistep method, its use is identical to that in paraxial propagation, except that the field ratio⁸ should only be updated after a complete propagation step.

The formalism described above applies to both two- and three-dimensional propagation. However, its application to three-dimensional problems still awaits efficient methods for the solution of the component step described by Eq. (8), because the well-known split-step method¹ is not second-order accurate when a is not purely imaginary. Consequently, we demonstrate the accuracy and utility of the above approach using only two-dimensional

test cases. The first such test case involves the propagation of an initial Gaussian beam through a uniform medium at an angle of 45° with respect to the z axis. The vacuum wavelength for this calculation was 1.06 μ m, the medium was given an index of refraction of unity, the reference index was also set to unity, and the initial Gaussian intensity profile had a width of 2.828 μ m at the 1/e points. The beam was propagated with a 0.01- μ m step size on a field of width 50 μ m that contained 1280 mesh points in order to minimize discretization error. The propagation was performed by using both twostep (n = 2) and three-step (n = 3) methods and was subsequently compared with a known analytic solution for true Helmholtz propagation computed by numerical evaluation of a complex Fourier integral.

The resulting intensity profiles computed by using the two-step method and the analytic solution are shown in Fig. 1, along with the paraxial result to provide additional perspective. The two-step results are highly accurate and appear to be identical (as they should be) to results for this same test case reported previously⁴ that used a Padé (2, 2) operator and a pentadiagonal solution algorithm. Corresponding results for the three-step method are shown in Fig. 2. These results are clearly more accurate than those obtained using the two-step method, reproducing the analytic results to within 1%. More importantly, however, these latter results were obtained with virtually no increase in code complexity and only 50% more run time than the two-step method. Indeed, further increases in accuracy (higher-order methods) will require still smaller fractional increases in run time, thus aptly illustrating the real power of this approach. By comparison, the propagation of a beam using a Padé (3, 3) operator and a single step would require the use of more complicated and time-consuming band matrix inversion routines.

The second test case involves the computation of the effective mode index of a simple ridge waveguide by using beam propagation and, more specifically,



Fig. 1. Intensity profiles resulting from the propagation of an initial Gaussian beam having a 45° phase tilt a distance of 10 μ m through a uniform medium. Results for the two-step method are compared with the exact analytic results. Paraxial results are included for additional perspective.



Fig. 2. Intensity profiles resulting from the propagation of an initial Gaussian beam having a 45° phase tilt a distance of 10 μ m through a uniform medium. Results for the three-step method are compared with the exact analytic results. An increase in accuracy compared with the results shown in Fig. 1 is clearly indicated.



Fig. 3. Error in the calculated mode index of a simple ridge waveguide is plotted versus the reference index error (reference index minus the correct mode index) for several propagation schemes. Parameters for the calculation are given in the text.

its dependence on the input reference index. Because true Helmholtz propagation does not involve a reference index, insensitivity of the calculated mode index to this input index serves as a convenient measure of propagation accuracy.⁴ For this test, light of wavelength 1.064 μ m was propagated along a 2.0- μ m-wide waveguide of indices 3.34179 (outside) and 3.34865 (inside) until a steady-state fundamental mode profile was obtained. By using this profile as

input, the mode index was then determined from the change in phase between adjacent propagation steps together with the assumed reference index. As expected, an input reference index of 3.34562 resulted in a calculated mode index of the same value, regardless of the propagator used. However, as the reference index was increased from this value, an error was observed in the calculated mode index that varied significantly with the propagation method, as is shown in Fig. 3. This figure clearly shows a decreasing sensitivity of the calculated mode index to errors in the reference index for the higher-order methods as required. For the three-step method [labeled Padé (3, 3)], a reference index error equivalent to propagation through air with a reference index appropriate to GaAs was still found to result in a mode index error of less than 10^{-3} .

In conclusion, this Letter describes the simplification of the Padé approximant approach to wideangle beam propagation to a multistep method whose component steps are each tridiagonal in form. This simplification allows the use of well-developed, efficient paraxial solution techniques to accomplish accurate wide-angle propagation and thus make possible the modeling of wide-angle photonic devices such as microlenses. This simplified form also allows the use of the transparent boundary condition to remove radiation scattered to the problem boundaries. Although present usage of this multistep approach is restricted to two-dimensional propagation, application to three dimensions will follow automatically once an efficient method for solution of the component-step block tridiagonal equations is discovered.

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