# Wide-angle beam propagation using Padé approximant operators

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A new beam-propagation method is presented whereby the exact scalar Helmholtz propagation operator is replaced by any one of a sequence of higher-order $(n, n)$ Padé approximant operators. The resulting differential equation may then be discretized to obtain (in two dimensions) a matrix equation of bandwidth $2n + 1$ that is solvable by using standard implicit solution techniques. The final algorithm allows (for $n = 2$) accurate propagation at angles of greater than 55 deg from the propagation axis as well as propagation through materials with widely differing indices of refraction.

The beam-propagation method is at present the most widely used tool employed in the study of guided-wave optics, largely owing to its numerical speed and simplicity. These attractive properties result chiefly from the use of the paraxial (Fresnel) approximation, which in turn severely limits the formalism in the following two respects. First, beams containing appreciable Fourier components at angles of more than a few degrees from the propagation axis will experience substantial phase errors; thus the method cannot treat wide-angle propagation. Second, beams propagating through regions with indices of refraction that differ by more than a few percent from the input reference index will also suffer serious phase distortion.

Attempts to generalize the formalism so as to overcome these limitations have been few indeed[1-4] owing to the severe mathematical difficulties[2] that typically accompany only modest advances in generality. So-called wide-angle wave equations have been studied previously in connection with the propagation of acoustic waves.[5] In the arena of guided-wave optics, methods tried include a Padé approximant scheme[1,2] (a special case of the present, more general, formalism), an approach based on the method of lines,[3] and another utilizing iterative Lanczos reduction.[4] The method of lines is essentially an eigenfunction expansion technique that often requires considerable numerical effort for waveguides of nonconstant cross section. Propagation by Lanczos reduction is a new technique whose validity for true wide-angle propagation is still under investigation.[6] In this Letter I describe the application of the Padé approximant formalism to optical beam propagation. This approach offers substantial improvements in both wide-angle propagation and index variation tolerance while incurring (in the two-dimensional case) only a modest numerical penalty. The formalism is generalizable to arbitrarily high order, with a concomitant increase in numerical complexity.

We begin by considering the scalar Helmholtz equation obtained by using the slowly varying envelope formalism:

$$\frac{\partial H}{\partial z} - \frac{i}{2k}\frac{\partial^2 H}{\partial z^2} = \frac{iP}{2k}H, \tag{1}$$

where $k = k_0\bar{n}$ with $k_0$ the free-space propagation constant and $\bar{n}$ the (input) reference refractive index and where the operator $P$ is defined by

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

We may formally rewrite Eq. (1) in the form

$$\frac{\partial H}{\partial z} = \frac{\dfrac{iP}{2k}}{1 - \dfrac{i}{2k}\dfrac{\partial}{\partial z}}H. \tag{3}$$

Although of little use in its present form, Eq. (3) suggests the recurrence relation

$$\left.\frac{\partial}{\partial z}\right|_n = \frac{\dfrac{iP}{2k}}{1 - \dfrac{i}{2k}\left.\dfrac{\partial}{\partial z}\right|_{n-1}}. \tag{4}$$

If Eq. (4) is now used to replace the $z$ derivative in the denominator of Eq. (3) with an expression containing only the operator $P$, then a useful propagator of the form

$$\frac{\partial H}{\partial z} = \frac{iN}{D}H \tag{5}$$

results, where $N$ and $D$ are polynomials in $P$. If Eq. (5) is compared with a formal solution of Eq. (1) written in the well-known form

$$\frac{\partial H}{\partial z} = i\left(\sqrt{P + k^2} - k\right)H, \tag{6}$$

then it becomes clear that Eq. (5) contains in effect an $(n, d)$ Padé approximant[7] for the exact Helmholtz operator in Eq. (6), where $n$ and $d$ are the highest degrees of $P$ in the polynomials $N$ and $D$, respectively.

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**Table 1. Most Useful Low-Order Padé Approximants for the Helmholtz Operator in Terms of the Operator $P$ Defined in Eq. (2)**

| Order | Expression |
| --- | --- |
| (1, 0) | $\dfrac{P}{2k}$ |
| (1, 1)[a] | $\dfrac{\dfrac{P}{2k}}{1+\dfrac{P}{4k^2}}$ |
| (2, 2) | $\dfrac{\dfrac{P}{2k}+\dfrac{P^2}{4k^3}}{1+\dfrac{3P}{4k^2}+\dfrac{P^2}{16k^4}}$ |
| (3, 3) | $\dfrac{\dfrac{P}{2k}+\dfrac{P^2}{2k^3}+\dfrac{3P^3}{32k^5}}{1+\dfrac{5P}{4k^2}+\dfrac{3P^2}{8k^4}+\dfrac{P^3}{64k^6}}$ |

[a] See Refs. 1 and 2.

The most useful low-order Padé approximant operators that result from the application of Eq. (3) are shown in Table 1.

An assessment of the accuracy of the various Padé approximant operators for wide-angle propagation may be made for the case of a single plane-wave component by comparing the predicted phase factor from Eq. (5) with the exact value obtained from Eq. (6). For this comparison we set $\overline{n}^2 = \epsilon/\epsilon_0$ so that $P \rightarrow \nabla_\perp{}^2 = -k^2 \sin^2\theta$ for propagation at an angle $\theta$ with respect to the $z$ axis. Figure 1 shows the phase error obtained with a variety of propagators relative to the exact value of $-2ik \sin^2(\theta/2)$. As is clearly seen in the figure, the paraxial propagator leads to sizable errors even for angles of less than 20 deg. By contrast, the (1, 1) Padé approximant operator[1,2] is highly accurate to ~30 deg. This operator should be the recommended replacement for the paraxial operator, since it offers a substantial improvement in accuracy with virtually no numerical penalty. Curves for the next two higher Padé approximants demonstrate increased accuracy at large angles, although now at the expense of some increase in numerical complexity. The utility of the present approach may be more fully appreciated by noting that the curve for the (3, 3) case is mostly obscured by another curve, labeled Expan (15th order). This latter curve was computed by following the more conventional approach of expanding the square-root expression in Eq. (6) in powers of $P$ up to order 15. It is remarkable that operationally equivalent accuracy is obtained with only a third-order Padé approximation. However, this finding is consistent with the properties of Padé approximants, which typically behave much better for large arguments than do the corresponding power series.[7] Similarly, the (2, 2) Padé approximation is operationally equivalent to an expansion of order 7–8. Operationally equivalent means that the errors are similar for angles large enough to incur a significant error but possibly different for smaller angles where the errors from both approaches are small.

In a similar manner we may assess the ability of the various propagators to propagate a beam accurately through a region that has an index of refraction considerably different from the reference index. For this test, we set $\nabla_\perp{}^2 \rightarrow 0$ so that $P = k_0{}^2(\epsilon/\epsilon_0 - \overline{n}^2) \equiv -k^2(\Delta\epsilon/\overline{n}^2)$. Using Eq. (6) as the standard, we once again plot relative errors for each propagation method in Fig. 2. As before, the various Padé approximant operators afford dramatic improvements. The extreme case of a beam whose reference index is that of pure GaAs impinging upon an air interface corresponds to a relative dielectric constant variation of $-0.918$, marked by the vertical line in the figure. Even for this case the (3, 3) Padé is quite accurate and the (2, 2) Padé is tolerable, provided that discretization errors are minimized.

Finite-difference equations may be derived from Eq. (5) by clearing the denominator and centering with respect to $z$ in the usual way:

$$D(H^{n+1} - H^n) = \frac{i\Delta z}{2} N(H^n + H^{n+1}). \tag{7}$$

In Eq. (7), the superscripts designate the $z$ position. The use of centered spatial differencing results in the following form for the operator $P$ for the two-dimensional case:

$$PH\big|_i = \frac{1}{(\Delta x)^2}(\nu_i H_i + H_{i+1} + H_{i-1}), \tag{8}$$

where

$$\nu_i \equiv k_0{}^2(\Delta x)^2\left(\frac{\epsilon_i}{\epsilon_0} - \overline{n}^2\right) - 2. \tag{9}$$

Higher powers of $P$ are constructed by repeated applications of Eq. (8). It is apparent from the form of the above equations that difference equations constructed by using an $(m, m)$ Padé approximation require the inversion of a matrix of bandwidth $2m + 1$. It can also be easily shown that these difference equations are unitary and thus preserve the sum of the absolute value squared of the solution vector elements at each step. It should be pointed out,

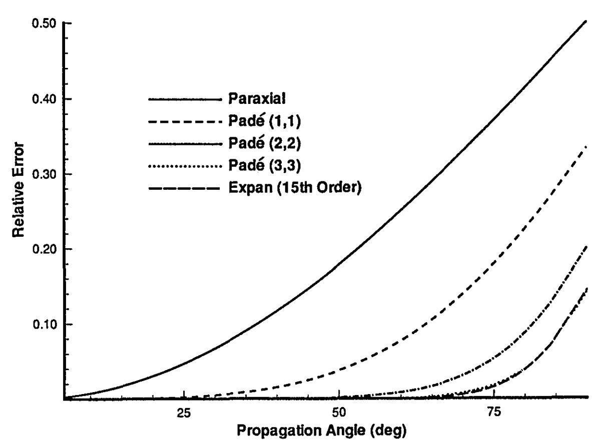


Fig. 1. Phase error incurred by the use of the operators shown for propagation of a plane wave at various angles with respect to the $z$ axis. The curve labeled Padé (3, 3) is mostly obscured by that corresponding to the operator obtained by expanding the square root in Eq. (6) to 15th order in $P$.

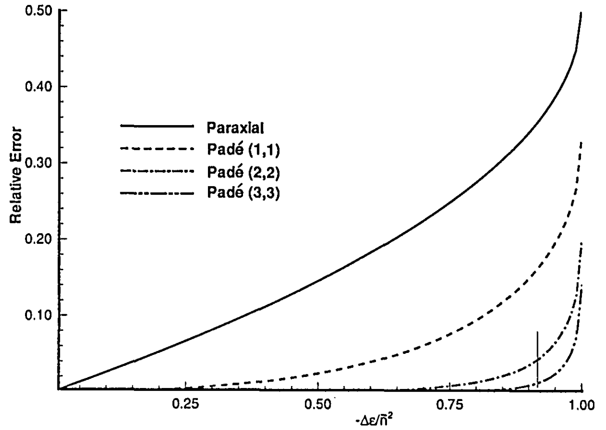


Fig. 2. Phase error incurred by the use of the operators shown for propagation of a plane wave along the $z$ axis through media of differing dielectric constants. In each case the reference index is 3.5 (corresponding to a dielectric constant of 12.25).

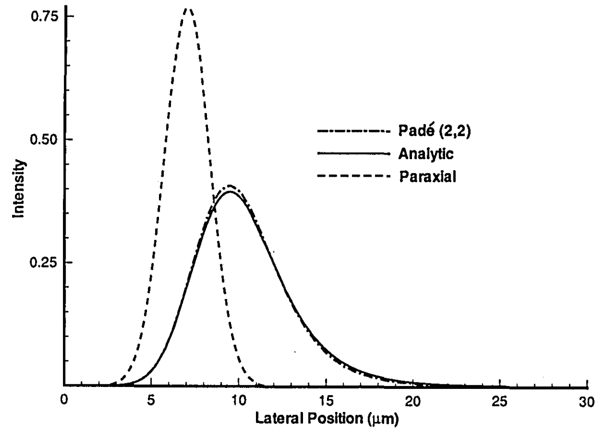


Fig. 3. Intensity profiles resulting from the propagation of an initial Gaussian beam with a 45-deg phase tilt a distance of 10 $\mu$m through a uniform medium. The beam was initially centered at zero, and the reference index employed was unity.

however, that for wide-angle propagation this latter quantity no longer has the interpretation of total beam energy. A proper treatment of energy conservation is a somewhat lengthy endeavor and is not dealt with here.

Dirichlet or Neumann boundary conditions for the above difference equations may be easily derived through the introduction of fictitious mesh points beyond the boundary, together with the application of either odd or even symmetry. More complicated boundary conditions such as the transparent boundary condition[8,9] previously developed for paraxial propagation are considerably more difficult to implement and are still under investigation.

Strictly speaking, extension of this formalism to three-dimensional problems requires the inversion of block $(2m + 1)$ diagonal matrices, a numerically intensive task. However, for a large category of interesting problems that are expected to be paraxial in one of the two transverse dimensions, the commonly employed split-step procedure[2] may be used, which thus greatly reduces the numerical effort.

Finally, a demonstration of the accuracy and utility of this technique follows from a comparison of wide-angle beam propagation between three different methods. This comparison was performed by first propagating an initial Gaussian beam having a 45-deg phase tilt through a uniform medium by using both paraxial and (2, 2) Padé wide-angle formalisms. The vacuum wavelength for this calculation was 1.06 $\mu$m, the medium was given an index of refraction of unity, and the initial Gaussian intensity profile had a width of 2.828 $\mu$m at the $1/e$ points. The beam was propagated with a 0.01-$\mu$m step size on a field of width 50 $\mu$m that contained 1280 mesh points in order to minimize the discretization error. The Padé propagation was performed by using an efficient pentadiagonal solution algorithm that is a simple generalization of the familiar Thomas tridiagonal algorithm. Intensity profiles obtained after a propagation distance of 10 $\mu$m with both methods were then compared with a known analytic solution for true Helmholtz propagation computed by numerical evaluation of a complex Fourier integral.

The resulting intensity profiles computed with the three methods just described are shown in Fig. 3. As is clearly seen, the paraxial calculation preserves the Gaussian shape, propagates at an incorrect angle, and underestimates the envelope spreading by almost a factor of 2. In contrast, the wide-angle calculation agrees with the analytic result to within $\sim 3\%$, accurately reproducing the correct non-Gaussian shape.

In conclusion, this Letter describes the application of the Padé approximant approach to wide-angle beam propagation. Although propagation at angles approaching 90 deg would require the solution of a matrix of moderate bandwidth, accurate propagation at angles of as much as 30 deg can be accomplished with a tridiagonal matrix, and accurate propagation at angles of greater than 55 deg can be accomplished with an easily solved pentadiagonal matrix. In addition, these schemes allow accurate propagation through media with a wide variety of refractive indices, thus decreasing the need for an accurate initial guess for the modal propagation constant.

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