Konrad-Zuse-Zentrum
für Informationstechnik Berlin

Takustraße 7
D-14195 Berlin-Dahlem
Germany

DAVID YEVICK[1], TILMANN FRIESE[2], FRANK SCHMIDT

A Comparison of Transparent Boundary Conditions for the Fresnel Equation

[1]Department of Physics, University of Waterloo Waterloo, Ontario N2L 3G1, Canada
[2]Department of Physics, University of Waterloo Waterloo, Ontario N2L 3G1, Canada

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Abstract: We establish the relationship between the transparent boundary condition (BPP) of Baskakov and Popov [Wave Motion **14** (1991) 121-128] and Pakpadakis et. al. [J. Acoust. Soc. Am. **92** (1992) 2030-2038] and a second boundary condition (SDY) introduced by Schmidt and Deuflhard [Comp. Math. Appl. **29** (1995) 53-76] and Schmidt and Yevick [J. Compu. Phys. **134** (1997) 96-107], that is explicitly tailored to the form of the underlying numerical propagation scheme. Our analysis demonstrates that if the domain is first discretized in the propagation direction, the SDY expression can be obtained by applying the exact sequence of steps used to derive the BPP procedure. The BPP method is thus an approximate realization of the computationally far simpler and unconditionally stable SDY boundary condition.

Keywords: Fresnel equation, transparent boundary conditions

Contents

1 Introduction

We consider the optical analog of the quantum-mechanical Schrödinger equation, namely the paraxial Fresnel equation

$$\partial_z v = \frac{i}{2\,k_0 n_0}\Big(\partial_x^2 + k_0^2(n^2 - n_0^2)\Big)v \tag{1}$$

for a waveguide with a longitudinal axis along the z-direction. For a forward-propagating electric field E and an $e^{-i\omega t}$ time-dependence, $v = e^{-ik_0 n_0 z}E$ is the slowly-varying component of the electric field. Here $k_0 = 2\pi/\lambda_0$ where λ_0 and n_0 are the vacuum wavelength and a suitably defined reference refractive index, respectively.

The goal of numerical boundary conditions is to supply a procedure such that the function v calculated in the internal domain of the computational window $\{x|x_- < x < x_+\}$ is the same as if computed on the infinite physical domain. For simplicity, since the derivation of these conditions is the same for x_- and x_+, we examine only a right boundary point $x_+ = 0$ below and further set $n = n_0$ in the exterior domain $\{x|x \leq x_- \cup x \geq x_+\}$, where v therefore satisfies

$$\partial_z v = \frac{i}{2\,k_0 n_0}\,\partial_x^2 v \tag{2}$$

Nonlocal (transparent) boundary conditions transform the outgoing property of waves in the external domain into a relation between the boundary value of the field at a given longitudinal position and the boundary values at all preceding propagation steps. Two methods for generating such conditions have been previously proposed. The first, introduced by Baskakov, Popov and Papadakis (BPP) is derived by Fourier transforming the paraxial or wide-angle equation with respect to the longitudinal, propagation variable.[1, 8] The outgoing wave condition then maps at each boundary point to a simple algebraic relation between the longitudinal derivative of each Fourier component of the field and the field value. Inverse Fourier transforming this relation yields the boundary field values $v(x_\pm, z)$ at a given longitudinal distance as an integral over all previous z-values of $\partial_x\, v(x_\pm, z)$ along the boundary. The integral must however subsequently be approximated by a discrete sum over the computed field values; to our knowledge no prior analysis exists of the errors incurred in this step. Recently, an exact, unconditionally stable version of the BPP formalism has been presented; however, the derivation and numerical implementation of the required formulas are quite involved.[9, 11]

More recently, a second, easily programmed non-local boundary condition was proposed by Schmidt and Deuflhard and later extended by Schmidt and Yevick (SDY).[12, 14] Unlike the standard BPP method, which is stable only if certain numerical procedures for approximating the integral over prior field values are employed,[10, 11], the SDY condition has been proved to be unconditionally stable.[12] Further, the SDY procedure fully incorporates the discrete nature of the propagation method.

A heuristic but useful derivation of the SDY procedure may be obtained by introducing the displacement or shift operator

$$s = e^{\Delta z \frac{\partial}{\partial z}} \tag{3}$$

with the property that $sE_{i+1} = E_i$ where Δz is the longitudinal step size, E_i denotes $E(x_b, z_i)$ and z_i is the longitudinal position at the end of i propagation steps.[13] Specializing to the Crank-Nicholson method

$$2ik_0 n_0 \frac{E_{i+1} - E_i}{\Delta z} = \frac{\partial^2}{\partial x^2}\left(\frac{E_{i+1} + E_i}{2}\right) \tag{4}$$

we find immediately that

$$\frac{\partial^2 E_{i+1}}{\partial x^2} = \lambda^2 \frac{1-s}{1+s} E_{i+1} \tag{5}$$

in which $\lambda = 4ik_0 n_0/\Delta z$. Defining the square root such that $\mathrm{Re}\sqrt{i\left(\frac{1-s}{1+s}\right)} \geq 0$ for $s \in \mathbf{C}$, and $\lambda = \sqrt{\lambda^2}$ with $\mathrm{Re}\,\lambda \geq 0$ the condition that all Fourier components of the propagating field be outgoing or exponentially decreasing at the right boundary is

$$\frac{\partial E_{i+1}}{\partial x} = \lambda \sqrt{\frac{1-s}{1+s}} E_{i+1} \tag{6}$$

The square-root expression $\sqrt{\frac{1-s}{1+s}}$ is then expanded as a Taylor series in s after which the relationship $s^m E_{j+1} = E_{j+1-m}$ yields the required boundary condition for $\frac{\partial E_{i+1}}{\partial x}$ in terms of the present and past boundary values $E_{i+1},\ E_i,\ E_{i-1}\ldots E_1$.

In the next section we establish the relationship between the BPP and SDY approaches through a new derivation of a slightly modified SDY procedure. This derivation repeats the exact sequence of operations as required to obtain the BPP method.

2 Basakov-Popov-Papadakis (BPP) Formulation

To derive the BPP nonlocal boundary condition, we first Fourier transform the paraxial equation with respect to the longitudinal, z coordinate. The Fourier coefficients

$$c(x,k) = \int_{-\infty}^{\infty} v(x,z)\, e^{-ikz}\, \mathrm{d}z \tag{7}$$

satisfy

$$\partial_x^2\, c(x,k) = 2\, k_0 n_0 k\, c(x,k) \tag{8}$$

The requirement that the Fourier components of v at the rightmost boundary point x_+ all correspond to outward propagating or decaying waves as $x \to \infty$ yields the boundary condition

$$\sqrt{2\,k_0 n_0 k}\,c(x_+,k) + \partial_x\,c(x_+,k) = 0. \tag{9}$$

After inverse Fourier transforming we obtain

$$\begin{aligned} v(x_+,z) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} c(0,k)\,e^{ikz}\,\mathrm{d}k \\ &= -\frac{1}{2\pi}\sqrt{\frac{i}{2\,k_0 n_0}}\int_{-\infty}^{\infty}\frac{1}{\sqrt{ik}}\,\partial_x\,c(x_+,k)\,e^{ikz}\,\mathrm{d}k \end{aligned} \tag{10}$$

Substituting

$$\frac{1}{\sqrt{ik}} = \frac{1}{\sqrt{\pi}}\int_0^{\infty}\zeta^{-\frac{1}{2}}\,e^{-ik\zeta}\,\mathrm{d}\zeta$$

leads to the desired Neumann-to-Dirichlet boundary condition

$$v(x_+,z) = -(1+i)\frac{1}{\sqrt{4\pi k_0 n_0}}\int_0^{\infty}\zeta^{-\frac{1}{2}}\,\partial_x\,v(x_+,z-\zeta)\,\mathrm{d}\zeta \tag{11}$$

While Eq.(11) expresses the electric field at a given boundary point in terms of the history of its transverse derivatives at the boundary, the expression is in the form of a continuous integral while numerical propagation procedures determine the electric field only at a discrete set of grid points. Accordingly the integral must be approximated by an expression of the form

$$v(x_+,z) = -(1+i)\frac{1}{\sqrt{4\pi k_0 n_0}}\sum_{j=0}^{\infty}\alpha_j\,\partial_x\,v(x_+,z-j\Delta z) \tag{12}$$

In this paper, three standard choices for the parameter α will be analyzed.[7] The first of these corresponds to associating the value of v at $z_0 + j\Delta z$ with the integral

$$\int_{z_0+j\Delta z}^{z_0+(j+1)\Delta z}\frac{1}{\sqrt{k}}dk \tag{13}$$

in the forward direction to yield (Rectangular rule 1)

$$\alpha_j = 2\sqrt{\Delta z}\left((j+1)^{\frac{1}{2}} - j^{\frac{1}{2}}\right), \quad \alpha_0 = 2\sqrt{\Delta z}. \tag{14}$$

If we instead employ an integral in the reverse direction, we obtain (Rectangular rule 2)

$$\alpha_j = 2\sqrt{\Delta z}\left(j^{\frac{1}{2}} - (j-1)^{\frac{1}{2}}\right), \quad \alpha_0 = 0 \tag{15}$$

which we will later demonstrate is best suited to an implicit numerical propagation method. The BPP coefficients that will similarly be found to be best adapted to the Crank-Nicholson procedure are derived by applying a trapezoidal integration rule to the interval between $z+(j-1)\Delta z$ and $z+(j+1)\Delta z$. This yields (Trapezoidal rule)

$$\alpha_j = \frac{4}{3}\sqrt{\Delta z}\left((j+1)^{\frac{3}{2}} - 2j^{\frac{3}{2}} + (j-1)^{\frac{3}{2}}\right), \quad \alpha_0 = \frac{4}{3}\sqrt{\Delta z} \tag{16}$$

Unlike the SDY method below, the stability of the above procedure is only guaranteed for certain ranges of parameter values which necessarily depend on the integration method.[10, 11]

3 Schmidt-Deuflhard-Yevick (SDY) Formulation

We now proceed to establish the connection between the BPP and SDY formalisms. In particular, we present a new derivation for (a slightly modified version of) the SDY formalism that parallels the above discussion of the BPP method, while incorporating the discrete nature of the propagation algorithm from the beginning. This requires that we express the electric field as a Fourier series over the set of discrete longitudinal points $z_0 + j\Delta z$ rather than as a Fourier integral over z, i.e. we write

$$c_k(x) = \frac{1}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} v(x,z)\, e^{-2\pi i k z/T}\, \mathrm{d}z \tag{17}$$

The size of the interval T over which the Fourier series is taken is here arbitrary, however, we will apply our final results in the $T \to \infty$ limit (identical results can be derived for the $z > 0$ half-space). Next, we must write an equation that specializes to the Crank-Nicholson formulation. To do this, we insert Eq.(17) into Eq.(4). This yields for the Fourier coefficients $v_k(x)$,

$$\begin{aligned}\partial_x^2\, c_k(x) &= \frac{4\,k_0 n_0}{i\Delta z}\,\frac{e^{2\pi i k\Delta z/T} - 1}{e^{2\pi i k\Delta z/T} + 1}\, c_k(x) \\ &= \frac{4\,k_0 n_0}{\Delta z}\,\tan\left(\frac{\pi k \Delta z}{T}\right) c_k(x)\end{aligned} \tag{18}$$

The general solution for $c_k(x)$ is

$$c_k(x) = A_k\, e^{\sqrt{\frac{4\,k_0 n_0}{\Delta z}\tan\left(\frac{\pi k\Delta z}{T}\right)}\,x} + B_k\, e^{-\sqrt{\frac{4\,k_0 n_0}{\Delta z}\tan\left(\frac{\pi k\Delta z}{T}\right)}\,x} \tag{19}$$

Thus, in analogy with Eq.(9), to insure that the field in the right external region be either decaying or outward-propagating (the case of non-zero reflection at the boundary is described in Appendix A) we must impose $A_k = 0$ so that

$$\sqrt{\frac{4\,k_0 n_0}{\Delta z}\,\tan\left(\frac{\pi k\Delta z}{T}\right)}\, c_k(x_+) + \partial_x\, c_k(x_+) = 0 \tag{20}$$

We convert the above property of the Fourier coefficients to a boundary condition on the electric field by inverse discrete Fourier transforming as follows

$$\begin{aligned} v(x_+, z) &= \sum_{k=-\infty}^{\infty} c_k(x_+)\, e^{2\pi i k z/T} \\ &= -\sqrt{\frac{i\Delta z}{4\, k_0 n_0}} \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{i \tan\left(\frac{\pi k \Delta z}{T}\right)}}\, \partial_x\, c_k(x_+)\, e^{2\pi i k z/T} \end{aligned} \tag{21}$$

To evaluate this expression, we expand in powers of $e^{-2\pi i k \Delta z/T}$ according to

$$\frac{1}{\sqrt{i \tan\left(\frac{\pi k \Delta z}{T}\right)}} = \sum_{j=0}^{\infty} \beta_j\, e^{-2\pi i j k \Delta z/T} \tag{22}$$

After subsequently summing over the index k, we obtain the discrete boundary condition

$$v(x_+, z) = -(1+i)\sqrt{\frac{\Delta z}{8\, k_0 n_0}} \sum_{j=0}^{\infty} \beta_j\, \partial_x\, v(x_+, z - j\Delta z) \tag{23}$$

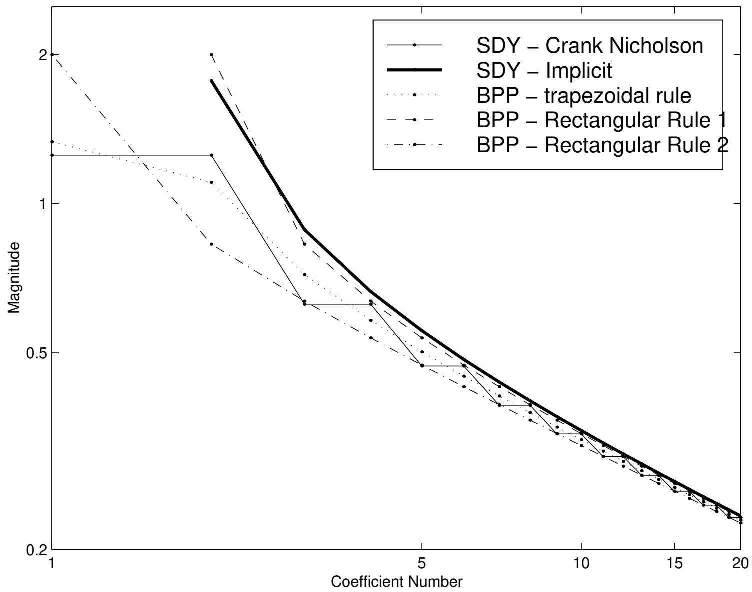
where

$$\beta_j = \left(1, 1, \frac{1}{2}, \frac{1}{2}, \frac{1\cdot 3}{2\cdot 4}, \frac{1\cdot 3}{2\cdot 4}, \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}, \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}, \ldots\right) \tag{24}$$

This is the exact analog of the BPP result, Eq.(11), except that the coefficients are now precisely matched to the Crank-Nicholson formalism (coefficients for other numerical propagation procedures can of course be derived in an exactly analogous fashion). Note that the β_j are the absolute values of the coefficients that result from the Taylor series expansion of Eq.(6) and are in fact those obtained by solving for v in terms of $\partial_z v$ in Eq.(6) prior to expanding in powers of s. In a similar fashion, Eq.(11) can be reformulated to express $\partial_z v$ in terms of v; however, the resulting integral formulas are in this case far more cumbersome (cf. Appendix B).

Thus while a common derivation can be presented for both the SDY and BPP methods, the SDY method is intrinsically more accurate since it fully incorporates the structure of the underlying discrete propagation method and has additionally been proven to be unconditionally stable.[12] Finally, observe that the above analysis strictly applies only in the limit of zero transverse grid point spacing. To generate a exact version of the SDY procedure for finite Δx requires the introduction of an additional shift operator that relates two adjacent transverse electric field values. An exact formulation has also been presented for the BPP method, however both the derivation and the analytic formulas for the coefficients are highly complex.[10, 11]

Figure 1: The coefficients for the BPP backward rectangular integration formula, (dashed), the BPP forward integration formula (dashed-dotted) the BPP trapezoidal integration formula (dotted), the modified SDY Crank-Nicholson method (solid line), and the modified SDY implicit method (thick solid line).



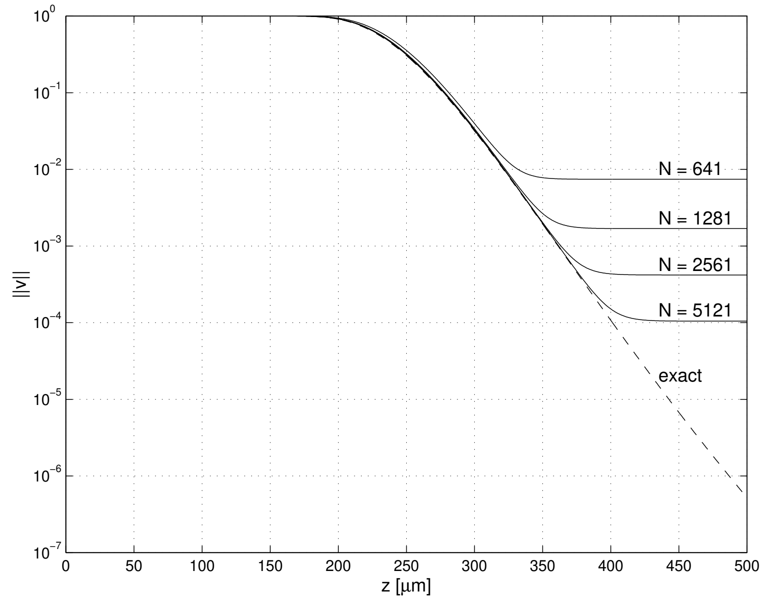
4 Numerical Verification

In the preceding discussion, we developed a slightly modified version of the SDY method that corresponds to an exact realization of the BPP formalism. To illustrate the practical importance of our results, we perform a direct comparison of the exact, SDY and approximate, BPP coefficients followed by a representative calculation with the modified technique. Accordingly, we first determine the inherent accuracy of the standard BPP formalism. In Fig. 1, we display the normalized coefficients, resulting from Eq.(14) (dashed), Eq.(15) (dashed-dotted) and Eq.(16) (dotted) together with the corresponding coefficients for the full discrete formulation for the Crank-Nicholson (solid line), and implicit (thick solid line) propagation methods, given by the Taylor series coefficients of $\frac{\sqrt{\pi}}{2}\left(\frac{1+s}{1-s}\right)^{1/2}$, and $\frac{\sqrt{\pi}}{2}(1-s)^{-1/2}$, cf. Eq.(23). Clearly, the BPP trapezoidal rule coefficients are closest to the exact Crank-Nicholson coefficients while applying the rectangular rule 2 (backward integration formula) for the BPP integral instead leads to an acceptable approximation to the exact implicit method coefficients. In each case, however, the BPP values display a noticeable error, especially at small j.

Finally, we verify the modified SDY procedure, Eq.(23) by considering the reflection of a Gaussian beam described by

$$E(x,0) = e^{-x^2/100} e^{-k_0 n_0 \sin(\pi/9)x} \tag{25}$$

Figure 2: The power remaining in the computational window for a Gaussian beam impinging on the computational window boundary for the modified SDY method as a function of propagation distance and number of transverse grid points.



from the computational window boundary as a function of the number of transverse grid points. In the calculation, the computational window width is 150μm, $n = n_0 = 1$, the longitudinal step size $\Delta z = 0.4\mu$m and the vacuum light wavelength $\lambda = 1.55\mu$m. Examining Fig. 2, which displays the power remaining in the computational window as a function of propagation distance and number of transverse grid points, N, we observe that the reflection induced by the transparent boundary condition decreases as the square of the grid point spacing. This behavior, which is entirely analogous to that Fig.(5) of Ref.[13], arises from the second-order nature of the finite-element method applied to implement the continuous derivative appearing in the modified SDY boundary condition. In applying transparent boundary condition to the Crank-Nicholson method, Eq.(4), we have written e.g. for the right-hand boundary

$$\frac{\partial^2 v}{\partial x^2}(x_+, z) \approx \frac{2}{(\Delta z)^2}\left(v(x_+ - \Delta x, z) - v(x_+, z) + \Delta x \frac{\partial v}{\partial x}(x_+, z)\right) \tag{26}$$

and

$$\frac{\partial^2 v}{\partial x^2}(x_+ - \Delta x, z) \approx \frac{1}{4(\Delta z)^2}\left(v(x_+ - 3 * \Delta x, z) - v(x_+ - \Delta x, z) + 2\Delta x \frac{\partial v}{\partial x}(x_+, z)\right) \tag{27}$$

The partial derivatives appearing on the right-hand side of the above equations are then replaced by values computed by Eq.(23) or Eq.(12) and the derivative $\frac{\partial v}{\partial x}(x_+, z)$ is regarded as a separate, fictitious degree of freedom. While such a formulation is non-Hermitian, the imaginary part of the (three) spurious eigenvalues associated with the Crank-Nicholson propagation matrix vanish in the limit of zero grid point spacing. An alternative procedure is to replace $\frac{\partial v}{\partial x}(x_+, z)$ in Eq.(23) or Eq.(12) by $v(x_+ + \Delta x, z) - v(x_+, z)$ and then to consider $v(x_+ + \Delta x, z)$ as the additional degree of freedom.

Conclusions

While the BPP formalism has previously been the preferred method for implementing transparent boundary conditions in two-dimensional paraxial propagation problems, we have demonstrated in this paper that the unconditionally stable SDY procedure has the same theoretical justification as the BPP method yet is intrinsically more accurate and simpler to implement. Our theoretical development has also established the intrinsic error of the BPP formulation and has provided a correspondence between different methods of approximating the continuous BPP result and discrete numerical propagation schemes. In the context of two companion papers which extend the SDY formalism to wide-angle propagation algorithms,[15, 16, 19] the results of this article clearly establish the practical and theoretical importance of future generalizations of the SDY procedure.

Appendix A - Continuous Version of SDY method

The BPP formalism can be easily modified to yield a Dirichlet to Neumann boundary condition that is the analog of the standard SDY formula, Eq.(6). In this case we obtain in place of Eq.(11)

$$\partial_z v(x_+, z) = \\ (1-i)\sqrt{\frac{n_0 k_0}{\pi i}}\left(\frac{1}{2}\int_0^z (z')^{-3/2} v(x_+, z-z')dz' - \lim_{z'\to 0}\sqrt{z'}v(x_+, z-z')\right) \tag{28}$$

Presumably because of the numerical complications associated with removing the divergence in the integral expression, this result has to our knowledge not appeared previously in the literature.

Appendix B - Incorporation of Boundary Reflection

If the refractive index in the region external to the boundary is inhomogeneous, each Fourier component c_k will be partially reflected with an effective reflection coefficient R_k at the computational window boundary. Eq.(20) then becomes

$$\frac{1-R_k}{1+R_k}\sqrt{\frac{4\,k_0 n_0}{\Delta z}\,\tan\left(\frac{\pi k \Delta z}{T}\right)}\,c_k(x_+) + \partial_x\, c_k(x_+) = 0 \tag{29}$$

Expanding $(1-R_k)/(1+R_k)$, viewed as a function of the discrete argument k, as the Fourier series

$$\frac{1-R_k}{1+R_k} = \sum_{j=0}^{\infty} \xi_j e^{-i2\pi jk\Delta z/T} \tag{30}$$

we obtain after inverse Fourier transforming

$$\partial_z v(0,z) = -(1-i)\sqrt{\frac{2k_0 n_0}{\Delta z}} \sum_{j=0}^{\infty} \left(\sum_{l=0}^{j} \alpha_{j-l}\xi_l \right) v(0, z - j\Delta z) \tag{31}$$

in place of Eq.(12). Obviously the major difficulty in applying Eq.(31) is the limited number of reflection coefficients for which the inner sum has a simple analytic form.[17, 18]

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