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Transparent Boundary Conditions for a Wide-Angle Approximation of the One-Way Helmholtz Equation

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We present nonlocal discrete transparent boundary conditions for a fourth-order wide-angle approximation of the two-dimensional Helmholtz equation. The boundary conditions are exact in the sense that they supply the same discrete solution on a bounded interior domain as would be obtained by considering the problem on the entire unbounded domain with zero boundary conditions at infinity. The proposed algorithm results in an unconditionally stable propagation method. Numerical examples from optics illustrate the efficiency of our approach. © 2000 Academic Press

Key Words: Helmholtz equation; wide-angle approximation; transparent boundary conditions; finite element method.

1. INTRODUCTION

Many time-harmonic scattering and wave propagation problems in electromagnetics, optics, and acoustics can be modeled by the scalar Helmholtz equation. If the problem under investigation has a dominant scattering aspect, e.g., the scattering of a beam from an arbitrary-shaped particle, the full Helmholtz equation must generally be solved as a boundary value problem on an unbounded domain. This requires scattering-theory approaches such as boundary element methods [1], infinite element methods [6], or methods for solving the interior problem subject to Dirichlet-to-Neumann radiation boundary conditions [10].

However if a dominant wave-guiding mechanism is present, the Helmholtz equation is typically approximated either by the paraxial wave equation or by wide-angle equations. Such one-way approximations reformulate the original boundary value problem as an initial boundary value problem. Such a transformation, when applicable, replaces the second partial derivative operator with respect to the propagation direction in the Helmholtz equation with a first derivative. As a result, propagation algorithms can be applied that require far less memory than the numerical realization of the full scattering problem.

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In approximating the Helmholtz equation by a paraxial or wide-angle equation, we must address two issues:

(i) The relationship between the Helmholtz operator and various wide-angle operators.

(ii) The construction of boundary conditions that suppress artificial reflections at the boundary of the computational domain.

Since the first topic has been the subject of detailed investigation [8], we will here consider the wide-angle operator as given regardless of its approximation properties and concentrate on the second of the above issues.

Initial attempts to provide transparent boundary conditions for the lowest order wide-angle equation resulting from the [1, 1]-Padé approximation of the (pseudo-differential) square-root Helmholtz operator were provided by Papadakis [13], Yevick and Thomson [18], and Arnold and Ehrhardt [2]. In the last of these references derivations of both the well-posedness of the wide-angle equation based on the [1, 1]-Padé approximation is proved and the computational form of the discrete transparent boundary conditions is given. Unfortunately, the authors' presentation is rather complex as a result of their use of the direct and inverse Laplace transforms with respect to the propagation coordinate. Similar considerations apply to transparent boundary conditions for time domain simulations of wave propagation problems as outlined in [7].

The main goal of the present paper is to extend our previous derivation of transparent boundary conditions for the paraxial (Schrödinger) equation [14] in a straightforward manner to wide-angle operators that contain a fourth-order derivative with respect to the spatial (transverse) variable. Our approach requires Laplace transforms only in the transverse direction and, in contrast to the above-mentioned methods, does not require an inverse Laplace transformation. Our derivation is further simplified through the introduction of a shift operator along the propagation direction as described in Ref. [16]. To our knowledge, no other exact transparent boundary condition has been derived for a fourth-order wide-angle method. Additionally, to discretize the fourth-order transverse derivative, cubic C^1-elements are required while our paraxial analysis is instead based on continuous linear finite elements [14]. The cubic C^1-element formulation is of interest, however, even for the solution of second-order equations because of the far greater accuracy attainable with cubic elements. The fourth-order problem thus provides insight into generalizations of the paraxial algorithm that are required to attain greater accuracy or to solve more general higher order wide-angle problems.

Another procedure for implementing wide-angle approximations involves recasting wide-angle representations of the Helmholtz operator, that can be of arbitrarily high transverse order, as products or sums of expressions involving only second-order transverse derivatives [4]. A generalization of Ref. [14] applicable to such operator-splitting techniques is examined in a companion paper [15], which considers arbitrary rational Padé approximations for the square-root Helmholtz operator. Finally, it should be noted that numerous alternative approaches exist to the solution of the interior problem. Some examples of these are the Engquist–Majda-type local approximation based on Padé approximants [5], the factorized boundary conditions of Higdon [9], and the perfectly matched layers of Bérenger [3]. However, in contrast to our procedure, these methods do not involve an implicit determination of the corresponding exterior solution and cannot be adjusted according to the structure of the underlying propagation algorithm.

2. PRELIMINARY CONSIDERATIONS

In accordance with the discussion of the previous section, we consider the one-way Helmholtz equation

$$u' = i\sqrt{P}\,u, \qquad u(0) = u_0,$$

where u' denotes the derivative of u with respect to z, and the operator P is given by

$$P = \frac{\partial^2}{\partial x^2} + f(x).$$

Setting $v = \exp(-\mathrm{i}\sqrt{\mu}\,z)u$ yields the initial value problem

$$v' = \mathrm{i}(\sqrt{P} - \sqrt{\mu})v = \mathrm{i}\sqrt{\mu}\left(\sqrt{1 + \frac{P-\mu}{\mu}} - 1\right)v, \quad v(0) = v_0 = u_0,$$

for the function v. To obtain the wide-angle equation of interest in this paper, the square-root expression is replaced by its [2, 0]-Padé approximant, which corresponds to the quadratic Taylor polynomial

$$\sqrt{1+\zeta} - 1 \approx \frac{1}{2}\zeta - \frac{1}{8}\zeta^2.$$

The starting point of our investigations is thus formed by the initial value problem

$$v' = \frac{\mathrm{i}\sqrt{\mu}}{2}\left[\left(\frac{P-\mu}{\mu}\right) - \frac{1}{4}\left(\frac{P-\mu}{\mu}\right)^2\right]v, \quad v(0) = v_0. \tag{1}$$

We assume that the function f is real, bounded, and positive, and that the parameter μ, to be characterized later, is real and positive.

The principal goal of this paper is to solve (1) numerically on a computational domain $\{(x, z) \in \mathbb{R}^2 : x_- < x < x_+,\ z \geq 0\}$ such that the boundary condition

$$\lim_{x\to\pm\infty} v(x, z) = 0, \quad \forall z \geq 0 \tag{2}$$

at infinity is fulfilled subject to the additional assumptions:

(i) The function f is equal to the constant value μ in the two external domains $x \leq x_-$ and $x \geq x_+$.

(ii) The initial value v_0 is supported in $\Omega = (x_-, x_+)$.

As a result of the above two conditions, the Laplace transforms of v possess a simple algebraic structure that we will exploit in Section 3.2 to facilitate the derivation of our subsequent boundary condition. For notational simplicity, we specialize to the case $f = \mu$. The more general condition $f = \text{const},\ f \neq \mu$, is considered in the context of an analysis of higher order Padé approximations in [15]. In a similar manner, we have imposed condition ii) to simplify our calculations. While condition ii) may in fact be relaxed for some initial fields with noncompact support, additional inhomogeneous parts in the final results (14) and (15) for the nonlocal boundary conditions are generated, as can be seen from the analysis of

[11]. This reference presents a transparent boundary condition based on the [1, 0]-Padé-type approximation to the propagation operator that is valid for initial fields with non-compact support and even for media with a linear dependence on the transverse coordinate. However, the derivation that is followed first applies a Laplace transform in the propagation direction after which the resulting differential equation is solved directly. As a result, an inverse Laplace transform is required to obtain the desired boundary condition in contrast to the method employed in this paper. In order to guarantee the desired decay of the solution towards infinity, appropriate boundary conditions must be imposed on the function v at the finite boundary points $x_\pm$. We remark that our derivation of these conditions is not restricted to the case of condition i) and can be extended to arbitrary values of the parameter μ.

2.1. *Implicit Midpoint Discretization*

As the first step towards deriving our transparent boundary conditions, we assume that problem (1) has been discretized with respect to z through the implicit midpoint rule

$$\left(1-\frac{\delta}{4}A\right)v_{k+1}(x)=\left(1+\frac{\delta}{4}A\right)v_k(x),\quad k=0,1,\ldots, \tag{3}$$

where the operator A is given by

$$A=\left(\frac{P-\mu}{\mu}\right)-\frac{1}{4}\left(\frac{P-\mu}{\mu}\right)^2.$$

The parameter $\delta=\mathrm{i}\sqrt{\mu}\,\Delta z$ is proportional to the step size Δz in the propagation direction. Denoting for brevity $\partial_x=\partial/\partial x$, from the assumptions of the previous paragraph, the corresponding recursion (3) in the exterior domain ($x\le x_-$ and $x\ge x_+$) is

$$\left[1-\frac{\delta}{4}\left(\frac{1}{\mu}\partial_x^2-\frac{1}{4\mu^2}\partial_x^4\right)\right]v_{k+1}(x)=\left[1+\frac{\delta}{4}\left(\frac{1}{\mu}\partial_x^2-\frac{1}{4\mu^2}\partial_x^4\right)\right]v_k(x), \tag{4}$$

with initial data $v_0=0$. To apply a finite element method in the interior domain $\Omega=(x_-,x_+)$, we reformulate (3) as a variational problem; that is, we determine $v_{k+1}\in H^2(\Omega)$ such that the relation

$$(w,v_{k+1})-\frac{\delta}{4}[a(w,v_{k+1})+b(w,v_{k+1})]=(w,v_k)+\frac{\delta}{4}[a(w,v_k)+b(w,v_k)], \tag{5}$$

in which

$$\begin{aligned}a(w,v)&=\frac{1}{\mu}(w,gv)-\frac{1}{\mu}(\partial_x w,\partial_x v)-\frac{1}{4\mu^2}\left(\partial_x^2 w+gw,\partial_x^2 v+gv\right),\\ b(w,v)&=-\frac{1}{4\mu^2}\left[w\left(\partial_x^3 v-4\mu\partial_x v\right)\Big|_{x_-}^{x_+}-\partial_x w\,\partial_x^2 v\Big|_{x_-}^{x_+}\right],\end{aligned}$$

and $g=f-\mu$, is fulfilled for all $w\in H^2(\Omega)$. The expression $(\cdot,\cdot)$ represents the standard scalar product in the space $L^2(\Omega)$, while the space $H^2(\Omega)$ consists of all twice differentiable functions in the weak sense. Since we assumed $f=\mu$ in the exterior domain, boundary terms containing g are absent.

In the following section we will transform the boundary condition (2) at infinity to conditions on the values of the quantities $\partial_x^3 v_j - 4\mu\partial_x v_j$ and $\partial_x^2 v_j$ at the finite boundary points $x_\pm$. These conditions guarantee that the solution properly decays in the exterior domain $x \leq x_-$ and $x \geq x_+$ despite the fact that we solve (1) only within the interior domain $\Omega = (x_-, x_+)$. To keep the presentation of our method compact, we will represent the values of the derivatives $\partial_x v_j$, $\partial_x^2 v_j$, and $\partial_x^3 v_j$ at the boundary points $x_\pm$ by $\dot{v}_j(x_\pm)$, $\ddot{v}_j(x_\pm)$, and $\dddot{v}_j(x_\pm)$.

3. WIDE-ANGLE BOUNDARY CONDITIONS

3.1. *Initial Propagation Step*

We now derive our wide-angle boundary condition, *specializing* to the solution at the right boundary point x_+; the derivation for the left boundary point is entirely analogous. For notational simplicity, we further set $x_+ = 0$.

To motivate our recursive technique, we first consider the initial propagation step. For this step, it is only necessary to solve a homogeneous, linear ordinary differential equation with constant coefficients. Since an explicit solution to this problem is available, we can study the influence of the free constants on the asymptotic solution that supplies the desired boundary condition for the step. The function $v_1(x)$ in the right exterior domain $x \geq x_+ = 0$ satisfies the homogeneous fourth-order ordinary differential equation

$$\left[1 - \frac{\delta}{4}\left(\frac{1}{\mu}\partial_x^2 - \frac{1}{4\mu^2}\partial_x^4\right)\right] v_1(x) = 0,$$

which has as its general solution

$$v_1(x) = A_1 \exp(\alpha_1 x) + A_2 \exp(\alpha_2 x) + A_3 \exp(-\alpha_2 x) + A_4 \exp(-\alpha_1 x), \tag{6}$$

with

$$\alpha_1 = \sqrt{2\mu}\sqrt{1 + \sqrt{1 - \frac{4}{\delta}}} \qquad \text{and} \qquad \alpha_2 = \sqrt{2\mu}\sqrt{1 - \sqrt{1 - \frac{4}{\delta}}}. \tag{7}$$

In the remaining part of this paper we will assume that the square-root function is defined in such a way that the relation $\Re\sqrt{\zeta} \geq 0$ holds for all $\zeta \in \mathbb{C}$. This assumption implies that the relations $\Re\alpha_1 \geq 0$ and $\Re\alpha_2 \geq 0$ are valid. The exterior solution therefore only decays if the values of $v_1(0)$, $\dot{v}_1(0)$, $\ddot{v}_1(0)$, and $\dddot{v}_1(0)$ are such that the coefficients A_1 and A_2 in the general solution (6) vanish. The relationship between the A_j in (6) and the boundary values of v_1 is given through the linear system of equations

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ \alpha_1 & \alpha_2 & -\alpha_2 & -\alpha_1 \\ \alpha_1^2 & \alpha_2^2 & \alpha_2^2 & \alpha_1^2 \\ \alpha_1^3 & \alpha_2^3 & -\alpha_2^3 & -\alpha_1^3 \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{bmatrix} = \begin{bmatrix} v_1(0) \\ \dot{v}_1(0) \\ \ddot{v}_1(0) \\ \dddot{v}_1(0) \end{bmatrix}.$$

By multiplying this linear system with the matrix

$$\begin{bmatrix} \alpha_1\alpha_2 & \alpha_1+\alpha_2 & 1 & 0 \\ -\alpha_1\alpha_2(\alpha_1+\alpha_2) & -(4\mu+\alpha_1\alpha_2) & 0 & 1 \end{bmatrix}$$

we find, after applying the Vieta root theorem $\alpha_1^2+\alpha_2^2=4\mu$,

$$\gamma\begin{bmatrix} \alpha_1 & \alpha_2 \\ -\alpha_1\alpha_2 & -\alpha_1\alpha_2 \end{bmatrix}\begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} \alpha_1\alpha_2 v_1(0) + (\alpha_1+\alpha_2)\dot{v}_1(0) + \ddot{v}_1(0) \\ -\alpha_1\alpha_2(\alpha_1+\alpha_2)v_1(0) - (4\mu+\alpha_1\alpha_2)\dot{v}_1(0) + \dddot{v}_1(0) \end{bmatrix}, \tag{8}$$

where $\gamma = 2(\alpha_1+\alpha_2)$. Accordingly, imposing the boundary conditions

$$\begin{aligned} \dddot{v}_1(0) - 4\mu\,\dot{v}_1(0) &= \alpha_1\alpha_2(\alpha_1+\alpha_2)\,v_1(0) + \alpha_1\alpha_2\,\dot{v}_1(0) \\ -\ddot{v}_1(0) &= \alpha_1\alpha_2\,v_1(0) + (\alpha_1+\alpha_2)\,\dot{v}_1(0) \end{aligned} \tag{9}$$

generates a homogeneous linear system from which A_1 and A_2 can be determined. Since the relations $\alpha_1 \neq 0$, $\alpha_2 \neq 0$, and $\alpha_1 \neq \pm\alpha_2$ are valid for all $\delta \in \mathrm{i}[0,\infty)$, the determinant $-4\alpha_1\alpha_2(\alpha_1+\alpha_2)^2(\alpha_1-\alpha_2)$ of the coefficient matrix in system (8) is always non-zero. Accordingly, for our special choice of boundary conditions (9), (8) implies $A_1 = A_2 = 0$. The boundary conditions (9) for the function v_1 therefore ensure that the solution in the right exterior domain has only decaying components. In the following section the above treatment will be extended to the function v_{k+1} for $k \geq 0$, corresponding to subsequent propagation steps.

3.2. *Subsequent Propagation Steps*

To derive the full transparent wide-angle boundary condition associated with (1) in a compact form we introduce, as in Ref. [14], the Laplace transforms

$$V_j(p) = \int_0^\infty \exp(-px)v_j(x)\,dx$$

of the functions v_j. The recurrence relation (4) in the exterior domain then becomes

$$\left[1-\frac{\delta}{4}\left(\frac{p^2}{\mu}-\frac{1}{4}\frac{p^4}{\mu^2}\right)\right]V_{k+1}(p) - \frac{\delta}{4}b_{k+1}(p) = \left[1+\frac{\delta}{4}\left(\frac{p^2}{\mu}-\frac{1}{4}\frac{p^4}{\mu^2}\right)\right]V_k(p) + \frac{\delta}{4}b_k(p), \tag{10}$$

with the boundary terms

$$b_j(p) = \left(\frac{1}{4}\frac{p^3}{\mu^2}-\frac{p}{\mu}\right)v_j(0) + \left(\frac{1}{4}\frac{p^2}{\mu^2}-\frac{1}{\mu}\right)\dot{v}_j(0) + \frac{1}{4}\frac{p}{\mu^2}\ddot{v}_j(0) + \frac{1}{4}\frac{1}{\mu^2}\dddot{v}_j(0).$$

From relation (10) we readily see by induction and decomposition into partial fractions that the Laplace transform of the function v_{k+1} in the right exterior domain for arbitrary boundary values $v_{k+1}(0)$, $\dot{v}_{k+1}(0)$, $\ddot{v}_{k+1}(0)$, and $\dddot{v}_{k+1}(0)$ possesses the form

$$V_{k+1}(p) = \sum_{j=1}^{k+1}\left[\frac{A_1^{(j\,k+1)}}{(p-\alpha_1)^j} + \frac{A_2^{(j\,k+1)}}{(p-\alpha_2)^j} + \frac{A_3^{(j\,k+1)}}{(p+\alpha_2)^j} + \frac{A_4^{(j\,k+1)}}{(p+\alpha_1)^j}\right],$$

where the zeros α_1, α_2 are given by (7). If we further introduce the shift operator s by

$$V_k = sV_{k+1},$$

we obtain from (10) the alternative representation

$$\underbrace{\left[(1-s) - \frac{\delta}{4}\left(\frac{p^2}{\mu} - \frac{1}{4}\frac{p^4}{\mu^2}\right)(1+s)\right]}_{a(p)} V_{k+1}(p) = \frac{\delta}{4}(b_k(p) + b_{k+1}(p)). \tag{11}$$

The above expression is the starting point for the subsequent derivation of our transparent boundary condition.

At the beginning of the section we introduced p as the variable dual to the spatial coordinate x in accordance with the standard integral definition of the Laplace transform. An alternative point of view, however, is to consider p as a differential operator which can be defined in an algebraic way. This algebraic counterpart to the Laplace transformation, introduced by Mikusiński [12], does not offer a practical advantage in the current context—as long as we consider the transverse direction—and is therefore not employed in this paper. On the other hand, introducing a *discrete* shift operator s implements Mikusiński's approach in the propagation direction, which provides several important advantages. In particular, the standard procedure for obtaining boundary conditions from *discrete* evolution equations such as (10) is to apply a Z-transformation, which is the discrete counterpart of the Laplace transformation, to perform algebraic operations on the resulting equations, and finally to transform back to the original domain. Through the introduction of the operator, s, however, we are able to manipulate the partial differential equation directly without applying forward and reverse Laplace transforms. The basic fact from the algebraic operator theory is that power series in s are well-defined operators and they are always convergent.

We next reformulate the boundary condition (2) at infinity for the right exterior domain as the condition that the Laplace transform V_{k+1} of the function v_{k+1} is regular in the entire right p half-plane. That is, if the polynomial a on the left hand side of Eq. (11) approaches zero, our choice of boundary conditions must ensure that the right hand side of (11) likewise vanishes.

The zeros of the polynomial a that may correspond to poles of V_{k+1} in the right half-plane are

$$p_1 = \sqrt{2\mu}\sqrt{1 + \sqrt{1 - \frac{4}{\delta}\frac{1-s}{1+s}}} \qquad \text{and} \qquad p_2 = \sqrt{2\mu}\sqrt{1 - \sqrt{1 - \frac{4}{\delta}\frac{1-s}{1+s}}}.$$

Hence we have to ensure that the two relations

$$b_k(p_{1,2}) + b_{k+1}(p_{1,2}) = 0$$

are valid. Since initially $v_0 = 0$ in the exterior domain we can assume by induction that $b_k(p_{1,2}) = 0$. We thus arrive at the conditions $b_{k+1}(p_{1,2}) = 0$, which are explicitly

$$\begin{bmatrix} \frac{1}{4}\frac{p_1^3}{\mu^2} - \frac{p_1}{\mu} & \frac{1}{4}\frac{p_1^2}{\mu^2} - \frac{1}{\mu} & \frac{1}{4}\frac{p_1}{\mu^2} & \frac{1}{4}\frac{1}{\mu^2} \\ \frac{1}{4}\frac{p_2^3}{\mu^2} - \frac{p_2}{\mu} & \frac{1}{4}\frac{p_2^2}{\mu^2} - \frac{1}{\mu} & \frac{1}{4}\frac{p_2}{\mu^2} & \frac{1}{4}\frac{1}{\mu^2} \end{bmatrix} \begin{bmatrix} v_{k+1}(0) \\ \dot{v}_{k+1}(0) \\ \ddot{v}_{k+1}(0) \\ \dddot{v}_{k+1}(0) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Applying the Vieta root theorem $p_1^2 + p_2^2 = 4\mu$ leads to the following equivalent form of the above equations:

$$\frac{1}{4\mu^2}\begin{bmatrix} p_1 & 1 \\ p_2 & 1 \end{bmatrix}\begin{bmatrix} p_1 p_2 & p_1 + p_2 & 1 & 0 \\ -p_1 p_2(p_1 + p_2) & -(4\mu + p_1 p_2) & 0 & 1 \end{bmatrix}\begin{bmatrix} v_{k+1}(0) \\ \dot{v}_{k+1}(0) \\ \ddot{v}_{k+1}(0) \\ \dddot{v}_{k+1}(0) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

This relationship finally yields the transparent boundary conditions

$$\begin{aligned} \dddot{v}_{k+1}(0) - 4\mu\dot{v}_{k+1}(0) &= p_1 p_2(p_1 + p_2)v_{k+1}(0) + p_1 p_2\dot{v}_{k+1}(0) \\ -\ddot{v}_{k+1}(0) &= p_1 p_2 v_{k+1}(0) + (p_1 + p_2)\dot{v}_{k+1}(0) \end{aligned} \tag{12}$$

for the function v_{k+1} at the right boundary point.

To conclude the construction of the boundary conditions, we expand the operators $p_1 p_2$, $p_1 + p_2$, and $p_1 p_2(p_1 + p_2)$ in their Taylor series according to

$$p_1 p_2 = \sum_{j=0}^{\infty} \beta_j s^j, \qquad p_1 + p_2 = \sum_{j=0}^{\infty} \gamma_j s^j, \qquad \text{and} \qquad p_1 p_2(p_1 + p_2) = \sum_{j=0}^{\infty} \delta_j s^j. \tag{13}$$

Since $s^j v_{k+1} = v_{k+1-j}$, the right hand side of (12) can now be evaluated in a practical fashion. The convergence of the above series is shown in Ref. [12, pp. 149]. Applying the identities

$$p_1 p_2 = \alpha_1\alpha_2\sqrt{\frac{1-s}{1+s}} \qquad \text{and} \qquad (p_1 + p_2)^2 = 4\mu + 2p_1 p_2$$

gives for the Taylor coefficients in (13)

$$\begin{aligned} &\beta_0 = \alpha_1\alpha_2 & &\beta_j = \begin{cases} -\beta_{j-1}, & j \text{ odd} \\ -\frac{j-1}{j}\beta_{j-1}, & j \text{ even} \end{cases} \\ &\gamma_0 = \alpha_1 + \alpha_2 & &\gamma_j = \frac{1}{\gamma_0}\left(\beta_j - \frac{1}{2}\sum_{i=1}^{j-1}\gamma_{j-i}\,\gamma_i\right), \quad j \ge 1 \\ &\delta_0 = \alpha_1\alpha_2(\alpha_1 + \alpha_2) & &\delta_j = \sum_{i=0}^{j}\beta_{j-i}\,\gamma_i, \end{aligned}$$

where α_1 and α_2 are taken from (7). Since v_0 is assumed to vanish for the exterior domain, we finally obtain for the transparent boundary conditions at the right boundary point x_+

$$\begin{aligned} \dddot{v}_{k+1}(x_+) - 4\mu\dot{v}_{k+1}(x_+) &= \sum_{j=0}^{k}\delta_j v_{k+1-j}(x_+) + \sum_{j=0}^{k}\beta_j\dot{v}_{k+1-j}(x_+), \\ -\ddot{v}_{k+1}(x_+) &= \sum_{j=0}^{k}\beta_j v_{k+1-j}(x_+) + \sum_{j=0}^{k}\gamma_j\dot{v}_{k+1-j}(x_+). \end{aligned} \tag{14}$$

Here we have applied a translation $x \mapsto x + x_+$ in order to generalize (12) to arbitrary positions of the right computational window boundary. Note that for $k = 0$, (14) coincides with the previously determined boundary conditions (9) for the function v_1.

In a similar fashion, we can obtain the corresponding boundary conditions

$$
\begin{aligned}
-\dddot{v}_{k+1}(x_-) + 4\mu\,\dot{v}_{k+1}(x_-) &= \sum_{j=0}^{k} \delta_j\, v_{k+1-j}(x_-) - \sum_{j=0}^{k} \beta_j\, \dot{v}_{k+1-j}(x_-),\\
\ddot{v}_{k+1}(x_-) &= -\sum_{j=0}^{k} \beta_j\, v_{k+1-j}(x_-) + \sum_{j=0}^{k} \gamma_j\, \dot{v}_{k+1-j}(x_-),
\end{aligned}
\tag{15}
$$

for the left boundary point x_-. The equations (14) and (15) guarantee that the function v_{k+1} in the exterior domain $x \le x_-$ and $x \ge x_+$ satisfies the boundary condition (2) at infinity and therefore allow the proper solution of problem (1) within the finite subdomain Ω.

4. FINITE ELEMENT DISCRETIZATION AND STABILITY PROPERTIES

4.1. *Cubic Finite Elements*

We now implement our transparent boundary conditions for the approximate solution of (1) within the framework of a cubic finite element scheme [17] and further investigate the stability properties of the resulting method. Such a discretization in the interior domain Ω on a set of grid points $x_- = x_1 < x_2 < \cdots < x_{n-1} < x_n = x_+$ leads from the weak formulation (5) to the algebraic system

$$
\left(\mathbf{M} - \frac{\delta}{4}\mathbf{A}\right)\mathbf{v}_{k+1} - \frac{\delta}{4}\mathbf{b}_{k+1} = \left(\mathbf{M} + \frac{\delta}{4}\mathbf{A}\right)\mathbf{v}_k + \frac{\delta}{4}\mathbf{b}_k.
$$

Here the sparse, real, and symmetric system matrix $\mathbf{A}$ and mass matrix $\mathbf{M}$ are

$$
\mathbf{A}_{l\,m} = a(\phi_l, \phi_m) \qquad \text{and} \qquad \mathbf{M}_{l\,m} = (\phi_l, \phi_m), \quad l, m = 1, \ldots, 2n,
$$

in which ϕ_l, ϕ_m denote the basis functions formed by cubic finite elements. The vectors $\mathbf{v}_j$ contain the degrees of freedom associated with the cubic finite elements such that

$$
\mathbf{v}_j = \begin{bmatrix} v_j(x_1) \\ \dot{v}_j(x_1) \\ \vdots \\ v_j(x_n) \\ \dot{v}_j(x_n) \end{bmatrix},
$$

while the vectors $\mathbf{b}_j$ consist of the boundary terms and are consequently

$$
\mathbf{b}_j = -\frac{1}{4\mu^2} \begin{bmatrix} -\dddot{v}_j(x_1) + 4\mu\,\dot{v}_j(x_1) \\ \ddot{v}_j(x_1) \\ \mathbf{0} \\ \dddot{v}_j(x_n) - 4\mu\,\dot{v}_j(x_n) \\ -\ddot{v}_j(x_n) \end{bmatrix}.
$$

In this formulation, our boundary conditions (14) and (15) for both v_k and v_{k+1} generate the following algebraic system after a slight rearrangement of the boundary contributions:

$$\left(\mathbf{M} - \frac{\delta}{4}(\mathbf{A} + \mathbf{B})\right)\mathbf{v}_{k+1} = \left(\mathbf{M} + \frac{\delta}{4}\mathbf{A}\right)\mathbf{v}_k + \frac{\delta}{4}\mathbf{r}_k.$$

Here the matrix $\mathbf{B}$ is

$$\mathbf{B} = -\frac{1}{4\mu^2}\begin{bmatrix} \delta_0 & -\beta_0 & \mathbf{0} & 0 & 0 \\ -\beta_0 & \gamma_0 & \mathbf{0} & 0 & 0 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ 0 & 0 & \mathbf{0} & \delta_0 & \beta_0 \\ 0 & 0 & \mathbf{0} & \beta_0 & \gamma_0 \end{bmatrix},$$

while the vector $\mathbf{r}_k$ is given by

$$\mathbf{r}_k = -\frac{1}{4\mu^2}\sum_{j=1}^{k}\begin{bmatrix} (\delta_j + \delta_{j-1})v_{k+1-j}(x_1) - (\beta_j + \beta_{j-1})\dot{v}_{k+1-j}(x_1) \\ -(\beta_j + \beta_{j-1})v_{k+1-j}(x_1) + (\gamma_j + \gamma_{j-1})\dot{v}_{k+1-j}(x_1) \\ \mathbf{0} \\ (\delta_j + \delta_{j-1})v_{k+1-j}(x_n) + (\beta_j + \beta_{j-1})\dot{v}_{k+1-j}(x_n) \\ (\beta_j + \beta_{j-1})v_{k+1-j}(x_n) + (\gamma_j + \gamma_{j-1})\dot{v}_{k+1-j}(x_n) \end{bmatrix}.$$

The coefficients β_j, γ_j, and δ_j are defined through the recurrence relations of the preceding section.

4.2. *Numerical Stability*

Last, we demonstrate that our propagation method is unconditionally stable. Our arguments are in principle only valid in exact arithmetic. However, since we are simply solving a sequence of boundary value problems in the interior domain, our method is expected to remain stable for floating-point arithmetic as well. This expectation is consistent with the results of the numerical examples to be displayed in the following section.

The starting point for the stability analysis is obtained by multiplying the exterior problem (4) with each of the exterior solutions v_k and v_{k+1} and subsequently integrating by parts. We then have

$$(w, v_{k+1})_\pm - \frac{\delta}{4}\Big[a(w, v_{k+1})_\pm + b(w, v_{k+1})_\pm\Big] = (w, v_k)_\pm + \frac{\delta}{4}\Big[a(w, v_k)_\pm + b(w, v_k)_\pm\Big],$$

with $w \in \{v_k, v_{k+1}\}$ and

$$a(w, v)_\pm = -\frac{1}{\mu}(\partial_x w, \partial_x v)_\pm - \frac{1}{4\mu^2}\left(\partial_x^2 w, \partial_x^2 v\right)_\pm,$$
$$b(w, v)_\pm = \pm\frac{1}{4\mu^2}[w(x_\pm)(\dddot{v}(x_\pm) - 4\mu\, \dot{v}(x_\pm)) - \dot{w}(x_\pm)\ddot{v}(x_\pm)],$$

where the notation $(\cdot, \cdot)_\pm$ represents the L^2 scalar product in the right and left exterior domain. In the derivation of the above equations we explicitly use the equivalence between our transparent boundary conditions (14) and (15) and the boundary condition (2) at infinity.

If we add the equations above to the weak formulation (5) of the interior problem we arrive at the identities

$$(w, v_{k+1})_{\mathbb{R}} - \frac{\delta}{4} a(w, v_{k+1})_{\mathbb{R}} = (w, v_k)_{\mathbb{R}} + \frac{\delta}{4} a(w, v_k)_{\mathbb{R}},$$

in which

$$(w, v)_{\mathbb{R}} = (w, v)_- + (w, v) + (w, v)_+ \qquad \text{and}$$
$$a(w, v)_{\mathbb{R}} = a(w, v)_- + a(w, v) + a(w, v)_+,$$

since the boundary terms at $x_\pm$ cancel. By combining the equation for v_{k+1} with the complex conjugate equation for v_k and comparing the real parts of the right and left hand sides we obtain

$$(v_{k+1}, v_{k+1})_{\mathbb{R}} = (v_k, v_k)_{\mathbb{R}},$$

so that the L^2-norm calculated over the whole x-axis is conserved. As our arguments are equally valid if a finite element approximation is used to solve the problem in the interior domain, we have established that our method is unconditionally stable for both the continuous and the discrete case.

5. NUMERICAL EXAMPLES

Finally we demonstrate the performance of our proposed technique with the aid of two standard optical examples. In an optics context, the function f in the operator P of (1) corresponds to

$$f(x) = k_0^2 n^2(x).$$

Here, k_0 is the vacuum wave number of light, while $n(x)$ is the refractive index. We assume that the refractive index in the exterior domain is identically equal to n_0 so that the parameter

$$\mu = k_0^2 n_0^2.$$

Our initial conditions are of the form

$$v_0(x) = \frac{1}{\sqrt{a\sqrt{\pi/2}}} \exp(-(x/a)^2) \exp(-\mathrm{i}\sqrt{\mu}\, x \sin\varphi),$$

with $\varphi = \pi/6$.

5.1. *Homogeneous Medium*

We first evolve a Gaussian beam of width $a = 10\ \mu$m for a vacuum light wavelength of 1.55 μm in a constant refractive index medium with $n(x) = n_0 = 1$. The interior domain is $\Omega = (-75, 75)\ \mu$m, the propagation step size is $\Delta z = 0.4\ \mu$m, and the propagation length is 400 μm. Our computation for 1281 equally spaced grid points in Ω leads to Fig. 1, which displays the absolute value $|v|$ of the function v. The contour lines in Fig. 1 correspond to amplitudes separated by an order of magnitude from 10^{-1} to 10^{-8}. The residual reflection present in the figure, as shown extensively in [14], is associated with the fact that our

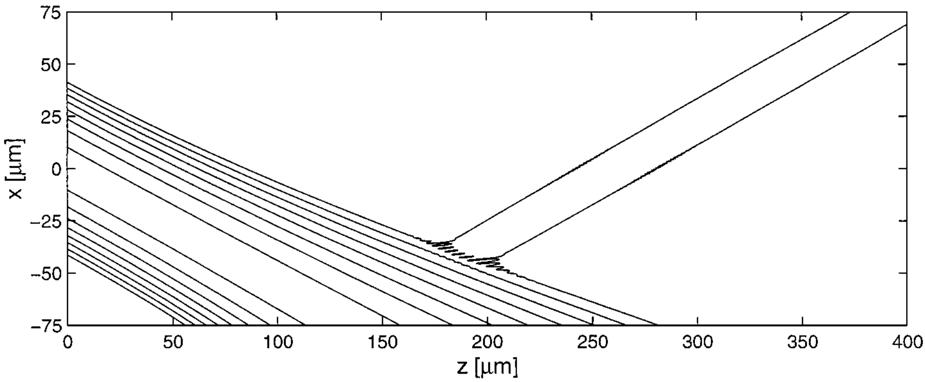

FIG. 1. Contour plot of the magnitude of the function v for a Gaussian beam propagating in a homogeneous medium for 1281 grid points.

transparent boundary conditions assume a continuous interior problem. Accordingly, the reflections must tend to zero as the number of grid points in the interior domain is increased. Instead, repeating our computation for 2561 grid points yields the results of Fig. 2, indicating that the boundary reflection is greatly reduced.

To study the sensitivity of the interior solution with respect to the width of the computational domain, we repeated the simulation of Fig. 1 with computational domains of different widths and compared the results. Thus in Fig. 3 the solution of Fig. 1, which was obtained on the domain $\Omega = (-75, 75)\ \mu$m, is compared both with a simulation on $\Omega = (-150, 150)\ \mu$m and with a simulation on $\Omega = (-300, 300)\ \mu$m, where both the spacing between transverse grid points and the propagation step length are fixed. (The solutions on the larger domains are projected after the simulation onto the smaller domain.) In the figure v_{large} refers to either of the $\Omega = (-150, 150)\ \mu$m or $\Omega = (-300, 300)\ \mu$m calculations while v_{small} is computed with $\Omega = (-75, 75)\ \mu$m and $||\cdot||$ is the discrete L^2-norm $(\mathbf{v}^H \mathbf{M} \mathbf{v})^{1/2}$. As expected, the error is nearly independent of the computational domain width. The largest absolute error, which occurs at the point where the maximum of the Gaussian coincides with the boundary, is on the order of the transverse discretization error. Indeed, this discretization error, which governs the rate of convergence, can be obtained from a graph of the L^2-norm of the discrete interior solution as a function of propagation distance

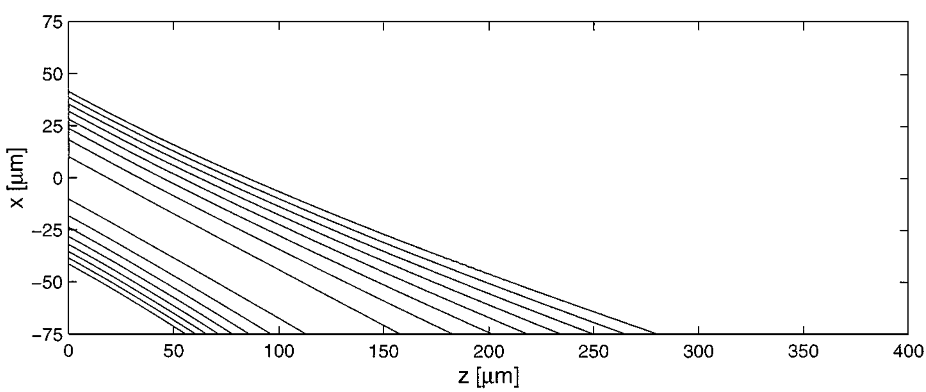

FIG. 2. As in Fig. 1, but for 2561 grid points.

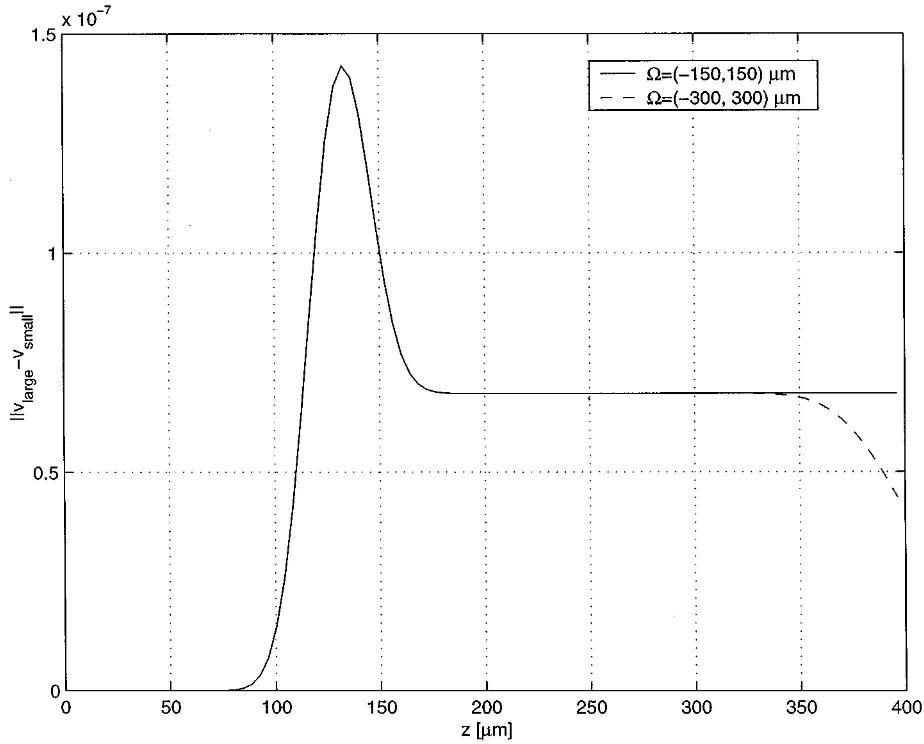

FIG. 3. The deviation of the field v computed on the domain, $\Omega = (-75, 75)\ \mu$m, of Fig. 1, from solutions computed on larger domains using the same spacings and boundary conditions. The error is nearly independent of the width of the computational domain, as evidenced by the nearly identical error curves.

for differing numbers of interior grid points, as in Fig. 4, which graphs the results of calculations performed with 641, 1281, 2561, and 5121 grid points in the interior domain. The magnitude of the reflections vanishes as $\mathcal{O}(\Delta x^4)$ as a consequence of the cubic finite element discretization of the interior problem. Observe that the discretization error for 1281 points is about 10^{-7}, which is nearly identical to that obtained in the previous figure.

5.2. *Refraction in a Layered Medium*

In Fig. 5, we display the reflection and refraction of the Gaussian beam at an interface between two homogeneous materials with different refractive indexes. Here, the vacuum light wavelength is 0.51 μm, the parameter a in v_0 is 1 μm, the computational domain is $\{(x, z) \in \mathbb{R}^2 : |x| < 8,\ 0 \leq z \leq 20\}$, the step size is $\Delta z = 0.0125$, and the mesh width is $\Delta x = 1/128$. The refractive index distribution is given by

$$n(x) = \begin{cases} 1, & |x| < 4 \\ 1.5, & \text{otherwise}. \end{cases}$$

The contour lines in Fig. 5 correspond to $|v| = 0.1, \ldots, 0.8$ while the dotted lines indicate the positions of the material interfaces. We remark that we obtain the same result if we set the boundary points $x_\pm$ equal to the location of the discontinuities in the material parameters and keep all other parameters fixed (so that in particular n_0 remains equal to the refractive index in the exterior domain).

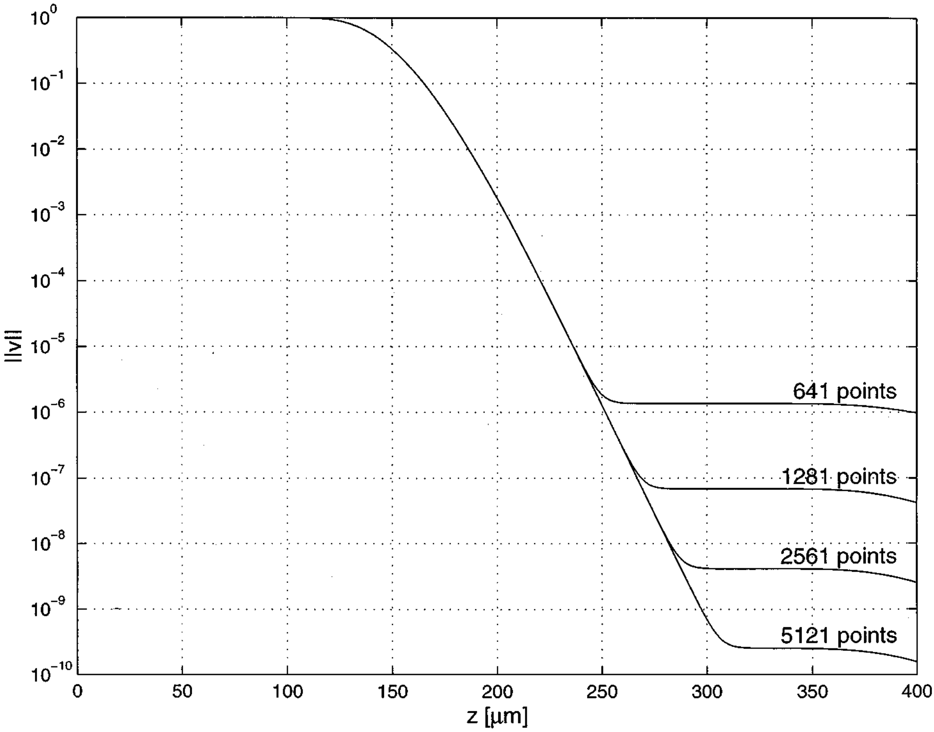

FIG. 4. The L^2-norm in the interior domain for 641, 1281, 2561, and 5121 transverse grid points.

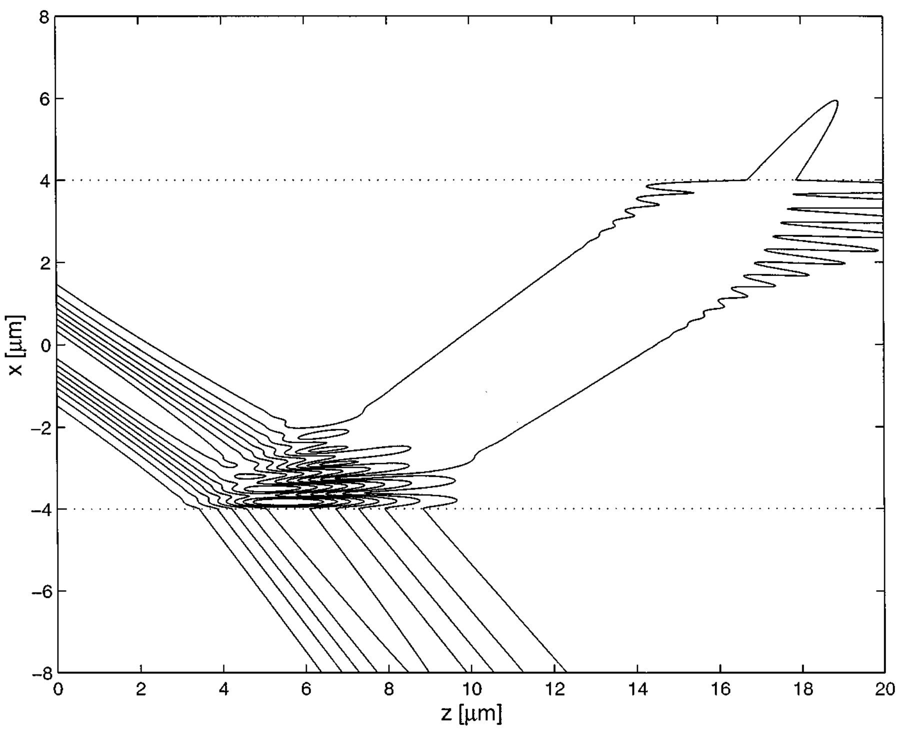

FIG. 5. Contour plot of the magnitude of the solution in a horizontally stratified medium.

6. CONCLUSIONS

We have applied Mikusiński's operational calculus to derive transparent boundary conditions for the wide-angle approximation (1) of the one-way Helmholtz equation. The resulting numerical method, which we have implemented with cubic finite elements, is unconditionally stable. The accuracy of the formalism has further been established through an analysis of the reflection of a Gaussian beam from the computational window boundary as a function of the grid point spacing. Although not considered here, wide-angle propagation methods based on the [2, 1]- or [2, 2]-Padé approximations to the square-root operator could in principle be analyzed with a straightforward but algebraically more complex extension of our procedure.

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