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Dirichlet-to-Neumann Maps for Unbounded Wave Guides

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Dirichlet-to-Neumann (DtN) boundary conditions for unbounded wave guides in two and three dimensions are derived and analyzed, defining problems that are suitable for finite element analysis. In the most general cases considered wave numbers may vary in arbitrary cross sections. The full DtN operator, in the form of an infinite series, is exact. Nonunique solutions may occur when this operator is truncated. Simple criteria for the number of terms in the truncated operator that guarantee unique solutions are presented. A simple modification of the truncated operator leads to uniqueness for any number of terms. Numerical results validate the performance of DtN formulations for wave guides and confirm the criteria for uniqueness. © 1998 Academic Press

1. INTRODUCTION

Problems in unbounded spatial domains are encountered frequently in various fields of application, such as acoustics, aerodynamics, electromagnetics, geophysics, and meteorology. Such problems pose a unique challenge to computation, since the unbounded region is in appropriate for direct discretization. A variety of numerical methods for exterior problems is reviewed in [16].

One commonly used method is to specify boundary conditions on an *artificial boundary*. For a linear scalar problem, this procedure may be summarized as follows:

(a) Introduce an artificial boundary $\mathcal{B}$, which partitions the original unbounded domain into two nonoverlapping regions: a bounded computational domain Ω and its unbounded complement D.

(b) By analyzing the problem in D, obtain a relation on $\mathcal{B}$ (exact or approximate) involving the unknown solution and its derivatives.

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(c) Use this relation as a boundary condition on $\mathcal{B}$, to obtain a well-posed problem in Ω.

(d) Solve the problem in Ω by computation, e.g., with the finite element method.

The relation obtained in step (b) and used as a boundary condition in step (c) is called an *artificial boundary condition* (ABC), or, in the context of wave problems, a *non-reflecting boundary condition*. The latter name comes from the fact that such a boundary condition is aimed at eliminating spurious reflection of waves from $\mathcal{B}$, which is otherwise present [15].

A standard ABC which is often imposed on $\mathcal{B}$ is simply the condition at infinity. However, in this case Ω must be quite large, or else the ABC gives rise to spurious reflections and pollutes the numerical solution [15]. On the other hand, a large computational domain is inefficient, leading to a large number of degrees of freedom. Therefore, the trend in recent work is to use a more accurate ABC on $\mathcal{B}$, which enables the use of a smaller computational domain. During the last two decades, many improved ABCs for various problems in unbounded domains were proposed (see reference in [15, 16]).

Most of the ABCs that have been proposed are local and approximate. A smaller number of *exact* nonlocal ABCs have been devised for various problems in unbounded domains. We mention the ABCs of Gustafsson *et al.* [11, 28], Hagstrom *et al.* [6, 29, 30 31, 32, 33], Ting and Miksis [52], Givoli and Cohen [18], Grote and Keller [25, 27], and Tsynkov *et al.* [50, 53, 54].

For general linear elliptic problems, Keller and Givoli [19, 37] devised an exact ABC on an artificial boundary of a simple shape (e.g., a circle or a sphere), called the Dirichlet-to-Neumann (DtN) boundary condition. Givoli, Keller, and others proposed combining DtN boundary conditions with finite element methods as a general approach to solve linear elliptic problems in unbounded domains [14, 16, 19, 20, 23, 37, 47]. In [17], the method was extended to treat the hyperbolic linear wave equation.

The DtN method has been shown to possess good computational properties and to be very effective in practice. It has been further analyzed and improved by Harari and Hughes [34, 35], Grote and Keller [26], and Malhotra and Pinsky [43]. The relation between the DtN method and the mode-matching method has been established by Astley [1]. Other schemes that use DtN-related ideas for various problems and configurations, can also be found in [3, 7, 10, 12, 13, 24, 39, 42, 44, 45, 55].

Similar to problems in exterior domains, unbounded acoustic wave guides [40, 49], or ducts, require special treatment for computation. For example, a parallel plate wave guide is handled by a sequence of localized radiation conditions in [38], and by integral equations in [41].

In the following, we derive DtN boundary conditions for unbounded wave guides. Boundary-value problems for unbounded acoustic wave guides in two and three dimensions, and their cross-sectional eigenfunctions are presented in Section 2. DtN formulations for computing such problems with finite elements are presented in Section 3. Analysis of these formulations shows the boundary conditions to be exact and presents simple criteria for selecting the number of terms to guarantee unique solutions. Local approximations provide a basis for modified boundary conditions that are unique for any number of terms. Numerical results that validate the performance of the finite elements with DtN boundary conditions in two and three dimensions and confirm the analytical results are presented in Section 4. Conclusions are drawn in Section 5.

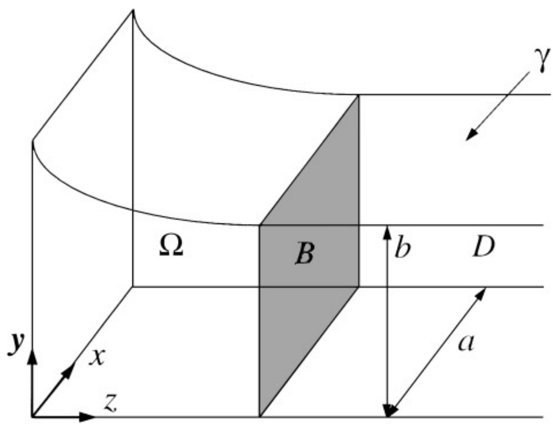

FIG. 1. An unbounded wave guide with rectangular cross section.

2. BOUNDARY-VALUE PROBLEMS FOR WAVE GUIDES

Let $\mathcal{R} \subset \mathbb{R}^d$ be a d-dimensional, semi-infinite, wave guide or duct. The region $\mathcal{R}$ may be partitioned into a bounded domain Ω and a unbounded cylinder $D = \mathcal{R}\backslash\Omega$ of uniform cross section C. The cylinder D is aligned so that its axis and, consequently, the wave guide walls are parallel to the z-axis of a Cartesian coordinate system (see Fig. 1 for an example with a rectangular cross section). In two dimensions the wave guide is a semi-infinite strip of constant width b (Fig. 2). The interface between the two regions Ω and D is the planar surface $\mathcal{B}$, normal to the z-axis and located at $z = z_0$. Thus $D = \{\mathbf{x} \mid \mathbf{x} \in \mathcal{R}, z > z_0\}$. The surface of the cylinder is denoted γ (Fig. 1). In two dimensions we position the coordinate system so that the walls γ are at $y = 0$ and $y = b$ (Fig. 2). Consequently, the cross section C is the interval $0 < y < b$ and the interface $\mathcal{B}$ is the straight segment $0 < y < b$ at $z = z_0$.

In the region $\mathcal{R}$ we wish to solve the Helmholtz equation

$$\Delta u + k^2 u + f = 0 \tag{1}$$

related to time-harmonic acoustic waves, subject to boundary conditions on the boundary

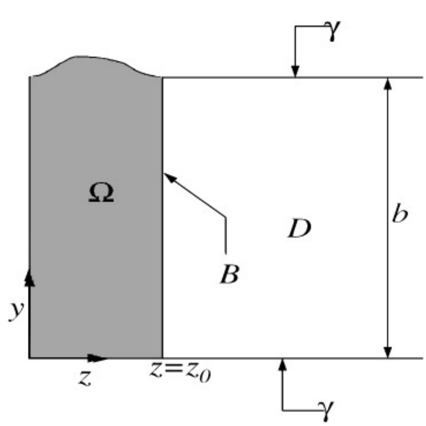

FIG. 2. An unbounded wave guide in two dimensions.

of $\mathcal{R}$ and the radiation condition that u is bounded and does not contain incoming waves as $z \to \infty$. (For a rigorous treatment of radiation conditions for wave guides see [46].) Here $u : \overline{\mathcal{R}} \to \mathbb{C}$ is the spatial component of the acoustic pressure; Δ is the Laplace operator; $k \in \mathbb{C}$ is the wave number, Im$k \geq 0$; and $f : \mathcal{R} \to \mathbb{C}$ is a prescribed source distribution. The artificial boundary is located so that $f = 0$ in D.

The boundary-value problem in the *bounded* region $\Omega = \mathcal{R} \backslash D$ may be solved by domain-based computation. For this purpose, boundary conditions must be specified on the artificial interface $\mathcal{B}$. In the following we derive such boundary conditions by the DtN method. Three cases of wall conditions on γ are considered,

$$\frac{\partial u}{\partial \nu} = 0 \qquad \text{Case 1} \tag{2}$$

$$u = 0 \qquad \text{Case 2} \tag{3}$$

$$\frac{\partial u}{\partial \nu} + \eta u = 0 \qquad \text{Case 3,} \tag{4}$$

where $\frac{\partial u}{\partial \nu}$ is the normal derivative. The coefficient η is related to impedance. Subsequent derivations and analyses are performed for Case 3, when wall conditions on γ need to be specified, with Cases 1 (Neumann) and 2 (Dirichlet) taken as limits for $\eta = 0$ and $\eta \to \infty$, respectively.

2.1. *Cross-sectional Eigenfunctions in a Cylinder*

Based on separation of variables for the Helmholtz equation, any solution in D satisfying the radiation condition may be modally decomposed

$$u = \sum_{n=0}^{\infty} A_n Y_n \exp(i\mu_n(z - z_0)), \tag{5}$$

where

$$A_n = \int_{\mathcal{B}} Y_n u \, dC. \tag{6}$$

The modes are ordered with *descending* values of the separation constants μ_n^2.

The separation constants, or cross-sectional eigenvalues μ_n^2 and orthogonal eigenfunctions $Y_n(y)$ and $Y_n(x, y)$ in two and three dimensions, respectively, are solutions of the cross-sectional eigenvalue problem

$$\Delta Y_n + \left(k^2 - \mu_n^2\right) Y_n = 0, \qquad \text{in } C \tag{7}$$

$$\frac{\partial Y_n}{\partial \nu} + \eta Y_n = 0, \qquad \text{on } \partial C, \tag{8}$$

where ∂C is the boundary of C. There may be a finite number of propagating modes, for which $\mu_n^2 > 0$ (the first mode, $n = 0$, is always propagating, except in the case of Dirichlet wall conditions, $\eta = 0$, in which it is trivial); there may be a single cutoff mode, for which $\mu_n^2 = 0$; and there is an infinite number of evanescent modes, for which $\mu_n^2 < 0$. In the most general case considered, the wave number may vary in the cross section of the wave guide, namely, $k = k(y)$ and $k = k(x, y)$ in two and three dimensions, respectively. The cross-sectional eigenvalue problem is then solved numerically for a finite number of eigenpairs.

2.2. *Constant Wave Number in a Rectangular Cross Section*

In the special case of a constant wave number in a wave guide with rectangular cross section $0 < x < a$ and $0 < y < b$, the cross-sectional eigenvalue problem is solved analytically

$$Y_{00} = \frac{2\eta e^{-\eta x} e^{-\eta y}}{\sqrt{(1 - e^{-2\eta a})(1 - e^{-2\eta b})}}, \qquad \mu_{00} = \sqrt{k^2 + 2\eta^2} \tag{9}$$

and for $m \geq 1$ and $n \geq 1$

$$Y_{m0} = \sqrt{\left(\frac{2}{a}\right) \Big/ \left(1 + \left(\frac{\eta a}{m\pi}\right)^2\right)} \sqrt{\frac{2\eta}{1 - e^{-2\eta b}}} \left(\cos\left(\frac{m\pi x}{a}\right) - \frac{\eta a}{m\pi} \sin\left(\frac{m\pi x}{a}\right)\right) e^{-\eta y}$$
$$\mu_{m0} = \sqrt{k^2 - \left(\frac{m\pi}{a}\right)^2 + \eta^2} \tag{10}$$

$$Y_{0n} = \sqrt{\frac{2\eta}{1 - e^{-2\eta a}}} \sqrt{\left(\frac{2}{b}\right) \Big/ \left(1 + \left(\frac{\eta b}{n\pi}\right)^2\right)} e^{-\eta x} \left(\cos\left(\frac{n\pi y}{b}\right) - \frac{\eta b}{n\pi} \sin\left(\frac{n\pi y}{b}\right)\right)$$
$$\mu_{0n} = \sqrt{k^2 + \eta^2 - \left(\frac{n\pi}{b}\right)^2} \tag{11}$$

$$Y_{mn} = \frac{2}{\sqrt{ab}} \Big/ \sqrt{\left(1 + \left(\frac{\eta a}{m\pi}\right)^2\right)\left(1 + \left(\frac{\eta b}{n\pi}\right)^2\right)} \left(\cos\left(\frac{m\pi x}{a}\right) - \frac{\eta a}{m\pi} \sin\left(\frac{m\pi x}{a}\right)\right)$$
$$\times \left(\cos\left(\frac{n\pi y}{b}\right) - \frac{\eta b}{n\pi} \sin\left(\frac{n\pi y}{b}\right)\right), \qquad \mu_{mn} = \sqrt{k^2 - \left(\frac{m\pi}{a}\right)^2 - \left(\frac{n\pi}{b}\right)^2}. \tag{12}$$

These eigenfunctions are orthonormal

$$\int_0^a \int_0^b Y_{kl} Y_{mn} \, dx \, dy = \delta_{km} \delta_{ln}. \tag{13}$$

In the limits of Neumann and Dirichlet wall conditions, respectively, the eigenfunctions are

$$\lim_{\eta \to 0} Y_{00} = \frac{1}{\sqrt{ab}}, \qquad \lim_{\eta \to \infty} Y_{00} = 0 \tag{14}$$

and for $m \geq 1$ and $n \geq 1$

$$\lim_{\eta \to 0} Y_{m0} = \sqrt{\frac{2}{ab}} \cos \frac{m\pi x}{a}, \qquad \lim_{\eta \to \infty} Y_{m0} = 0 \tag{15}$$

$$\lim_{\eta \to 0} Y_{0n} = \sqrt{\frac{2}{ab}} \cos \frac{n\pi y}{b}, \qquad \lim_{\eta \to \infty} Y_{0n} = 0 \tag{16}$$

$$\lim_{\eta \to 0} Y_{mn} = \frac{2}{\sqrt{ab}} \cos \frac{m\pi x}{a} \cos \frac{n\pi y}{b}, \qquad \lim_{\eta \to \infty} Y_{mn} = \frac{2}{\sqrt{ab}} \sin \frac{m\pi x}{a} \sin \frac{n\pi y}{b}. \tag{17}$$

This double index notation is converted to the single index notation of (5) by simply ordering the modes with descending values of μ_n^2, starting with $\mu_0 = \mu_{00}$ (or $\mu_0 = \mu_{11}$ for Dirichlet wall conditions).

2.3. *Constant Wave Number in a Strip*

In the special case of a constant wave number in a strip of constant width $0 < y < b$, the cross-sectional eigenvalue problem is solved analytically

$$Y_0 = \sqrt{\frac{2\eta}{1 - e^{-2\eta b}}} e^{-\eta y}, \qquad \mu_0 = \sqrt{k^2 + \eta^2} \tag{18}$$

and for $n \geq 1$

$$\begin{aligned} Y_n &= \sqrt{\left(\frac{2}{b}\right) \Big/ \left(1 + \left(\frac{\eta b}{n\pi}\right)^2\right)} \left(\cos\left(\frac{n\pi y}{b}\right) - \frac{\eta b}{n\pi} \sin\left(\frac{n\pi y}{b}\right)\right), \\ \mu_n &= \sqrt{k^2 - \left(\frac{n\pi}{b}\right)^2}. \end{aligned} \tag{19}$$

These eigenfunctions are orthonormal

$$\int_0^b Y_m Y_n \, dy = \delta_{mn}. \tag{20}$$

In the limits of Neumann and Dirichlet wall conditions, respectively, the eigenfunctions are

$$\lim_{\eta \to 0} Y_0 = \frac{1}{\sqrt{b}}, \qquad \lim_{\eta \to \infty} Y_0 = 0 \tag{21}$$

and for $n \geq 1$

$$\lim_{\eta \to 0} Y_n = \sqrt{\frac{2}{b}} \cos \frac{n\pi y}{b}, \qquad \lim_{\eta \to \infty} Y_n = -\sqrt{\frac{2}{b}} \sin \frac{n\pi y}{b}. \tag{22}$$

3. DtN FORMULATIONS

The DtN boundary condition is

$$\frac{\partial u}{\partial z} = -Mu \qquad \text{on } \mathcal{B}. \tag{23}$$

The two-dimensional map is obtained from the normal derivative of the modal representation (5) on the interface $\mathcal{B}$

$$Mu(y, z_0) = -i \sum_{n=0}^{\infty} \mu_n \int_0^b Y_n(y) Y_n(y') u(y', z_0) \, dy', \qquad 0 < y < b. \tag{24}$$

(In Case 2, Dirichlet wall conditions, the first term is trivial.) The three-dimensional map is also obtained from the normal derivative of the modal representation (5) on the interface $\mathcal{B}$

$$Mu(x, y, z_0) = -i \sum_{n=0}^{\infty} \mu_n \int_C Y_n(x, y) Y_n(x', y') u(x', y', z_0) \, dx' \, dy', \qquad (x, y) \in C. \tag{25}$$

(Note that in Case 2, Dirichlet wall conditions, trivial terms are *excluded* from the DtN map. Thus, e.g., for Dirichlet wall conditions in a rectangular cross section with a constant wave number, the first and largest eigenvalue is $\mu_0^2 = k^2 - (\pi/a)^2 - (\pi/b)^2$, which is μ_{11}^2 in the double-index notation.)

3.1. *Uniqueness*

To analyze the uniqueness of solutions to the DtN formulation we define the following functions:

- u_1 is the solution of the original problem with the unbounded wave guide in $\mathcal{R}$.
- u_2 is composed of two parts as

$$u_2 = \begin{cases} u_2^{\text{int}}, & \mathbf{x} \in \Omega \\ u_2^{\text{ext}}, & \mathbf{x} \in D, \end{cases}$$

where u_2^{int} is the solution of the DtN problem in Ω and u_2^{ext} is the solution of the problem in D with $u_2^{\text{ext}} = u_2^{\text{int}}$ on $\mathcal{B}$.

- $e := u_1 - u_2$ satisfies the homogeneous Helmholtz equation in $\Omega \cup D$ with homogeneous boundary data, and satisfies the radiation condition. Likewise for the complex conjugate $\bar{e}$.

LEMMA. *Let u be a solution of the homogeneous Helmholtz equation ($k^2 > 0$) in D. If*

$$\lim_{z\to\infty} \int_C |u|^2 \, dC = 0 \tag{26}$$

then $u \equiv 0$ in D.

Proof. This is by a theorem due to Rellich [56, p. 56].

THEOREM. $u_2^{\text{int}} = u_1|_\Omega$ *and hence the* DtN *solution is unique, whenever the original solution is unique.*

Note. A cutoff mode of the original solution may vary by an arbitrary multiplicative constant.

Proof. The first part of the proof is to establish the continuity of u_2 on $\mathcal{B}$, namely

$$u_2^{\text{ext}} = u_2^{\text{int}} \tag{27}$$

$$\begin{aligned} \frac{\partial u_2^{\text{ext}}}{\partial z} &= -M u_2^{\text{ext}} \\ &= -M u_2^{\text{int}} \\ &= \frac{\partial u_2^{\text{int}}}{\partial z}, \end{aligned} \tag{28}$$

where the first line follows from the definition of u_2^{ext}, the second line is the definition of the DtN map, M, the third line follows from the first and the last line from the definition of u_2^{int}. These continuity properties are inherited by e.

Showing that $\lim_{z\to\infty} \int_C |e|^2 \, dC = 0$ completes the proof. By the Lemma, this implies that $e \equiv 0$ in D. By the continuity of e and its normal derivative on $\mathcal{B}$, the DtN map is enforcing homogeneous Dirichlet *and* Neumann boundary conditions on the artificial boundary $\mathcal{B}$. This over-specification of boundary data precludes non-trivial solutions in Ω.

Recall the modal representation of solutions in D, Eq. (5). To complete the proof we show that $\lim_{z\to\infty} \int_C |e|^2 \, dC = 0$ for each type of mode separately.

For the evanescent modes this is straightforward: $|e|^2 \to 0$ as $z \to \infty$ since $\mu_n^2 < 0$ and hence $\lim_{z\to\infty} \int_C |e|^2\, dC = 0$.

For the cutoff mode $\mu_n^2 = 0$, so that e is independent of z in D. Thus, the DtN boundary condition for this case, a homogeneous Neumann boundary condition, is exact, and $u_2 = u_1$ if u_1 is unique.

For propagating modes we consider the variational form of the homogeneous problem (homogeneous equation with homogeneous boundary data) in Ω, which may be written as

$$a(e, e) = 0, \tag{29}$$

where

$$a(w, u) = (\nabla w, \nabla u) - (w, k^2 u) + (w, Mu)_{\mathcal{B}} \tag{30}$$

since e is an admissible weighting function. Directing our attention to the imaginary part yields

$$\begin{aligned} 0 &= -\operatorname{Im} a(e, e) \\ &= \int_{\mathcal{B}} -\operatorname{Im}\{\bar{e} M e\}\, dC \\ &= \frac{1}{2i} \int_{\mathcal{B}} \left(\bar{e}\frac{\partial e}{\partial z} - e\frac{\partial \bar{e}}{\partial z} \right) dC. \end{aligned} \tag{31}$$

This is a statement of zero energy flux through the artificial boundary. By continuity of e and its normal derivative on the artificial boundary, this expression may be related to quantities in the “tail” D

$$\begin{aligned} 0 &= \int_{\mathcal{B}} \left(\bar{e}\frac{\partial e}{\partial z} - e\frac{\partial \bar{e}}{\partial z} \right) dC \\ &= \int_D (\bar{e}\Delta e - e\Delta \bar{e})\, d\Omega - \lim_{z\to\infty} \int_C \left(\bar{e}\frac{\partial e}{\partial z} - e\frac{\partial \bar{e}}{\partial z} \right) dC \\ &= -\lim_{z\to\infty} \int_C \left(\bar{e}\frac{\partial e}{\partial z} - e\frac{\partial \bar{e}}{\partial z} \right) dC. \end{aligned} \tag{32}$$

The second line is obtained by integration by parts and the last follows from the fact that e satisfies the homogeneous Helmholtz equation in D.

Each propagating mode is outgoing and hence satisfies the radiation condition, written in integral form

$$\begin{aligned} 0 &= \lim_{z\to\infty} \int_C \left| \frac{\partial e}{\partial z} - i\mu_n e \right| dC \\ &= \lim_{z\to\infty} \int_C \left(\left| \frac{\partial e}{\partial z} \right|^2 + \mu_n^2 |e|^2 + i\mu_n \left(\bar{e}\frac{\partial e}{\partial z} - e\frac{\partial \bar{e}}{\partial z} \right) \right) dC \\ &= \lim_{z\to\infty} \int_C \left(\left| \frac{\partial e}{\partial z} \right|^2 + \mu_n^2 |e|^2 \right) dC, \end{aligned} \tag{33}$$

where the third line follows from (32). For propagating modes $\mu_n^2 > 0$ so that

$$\lim_{z\to\infty} \int_C |e|^2\, dC = 0 \tag{34}$$

which completes the proof.

3.2. *Truncated DtN Maps*

Let M^N be the DtN map *truncated* after N terms. In two dimensions

$$M^N u(y, z_0) = -i \sum_{n=0}^{N-1} \mu_n \int_0^b Y_n(y) Y_n(y') u(y', z_0)\, dy', \qquad 0 < y < b. \tag{35}$$

Recall that the modes are ordered with descending eigenvalues μ_n^2. (In Case 2, Dirichlet wall conditions, the first term is trivial so that M^N contains $N - 1$ non-trivial terms.) In three dimensions

$$M^N u(x, y, z_0) = -i \sum_{n=0}^{N-1} \mu_n \int_C Y_n(x, y) Y_n(x', y') u(x', y', z_0)\, dx'\, dy', \qquad (x, y) \in C. \tag{36}$$

(In Case 2, Dirichlet wall conditions, trivial terms are *excluded* from the truncated map, in contrast to the treatment in two dimensions. Thus, e.g., for Dirichlet wall conditions in a rectangular cross section with a constant wave number, the first and largest eigenvalue is $\mu_0^2 = k^2 - (\pi/a)^2 - (\pi/b)^2$, which is μ_{11}^2 in the double-index notation.)

Let v be the difference between two solutions of the problem in Ω with the DtN map replaced by M^N. v is a solution of the homogeneous problem. Thus, we have a statement of zero energy flux through the artificial boundary as before, this time in terms of the truncated map

$$\int_{\mathcal{B}} \operatorname{Im}\{\bar{v} M^N v\}\, dx\, dy = 0. \tag{37}$$

Again we employ modal decomposition

$$v = \sum_{n=0}^{\infty} A_n Y_n \qquad \text{on } \mathcal{B}, \tag{38}$$

where

$$A_n = \int_{\mathcal{B}} Y_n v\, dC. \tag{39}$$

Consider the one-term approximation $(N = 1)$ in three dimensions

$$\begin{aligned} M^1 v(x, y, z_0) &= -i\mu_0 \int_C Y_0(x, y) Y_0(x', y') v(x', y', z_0)\, dx'\, dy' \\ &= -i\mu_0 Y_0(x, y) \int_C Y_0(x', y') \sum_{n=0}^{\infty} A_n Y_n(x', y')\, dx'\, dy' \\ &= -i\mu_0 A_0 Y_0(x, y) \end{aligned} \tag{40}$$

by the orthonormality of the eigenfunctions Y_n. The condition of zero energy flux is

$$\begin{aligned} 0 &= \int_C \operatorname{Im}\{\bar{v}(x, y, z_0) M^1 v(x, y, z_0)\}\, dx\, dy \\ &= \operatorname{Im}\left\{ \int_C \sum_{n=0}^{\infty} \bar{A}_n Y_n(x, y)(-i\mu_0 A_0 Y_0)\, dx\, dy \right\} \\ &= -\operatorname{Im}\{i\mu_0\} |A_0|^2. \end{aligned} \tag{41}$$

Similarly, for the N-term approximation, we obtain the condition

$$\sum_{n=0}^{N-1} \mathrm{Im}\{i\mu_n\}|A_n|^2 = 0. \tag{42}$$

The same procedure is used to derive an identical condition for the two-dimensional case. As previously stated, there may be a finite number of propagating modes, for which $\mu_n \in \mathbb{R}^+$; there may be a single cutoff mode, for which $\mu_n = 0$; and there is an infinite number of evanescent modes, for which $-i\mu_n \in \mathbb{R}^+$. The modes are ordered with descending eigenvalues μ_n^2. Thus, the lowest modes are propagating modes, if any exist, followed by the cutoff mode, if it exists, and then the evanescent modes.

If there are no more than N propagating modes, then condition (42) implies $A_n = 0$ for those modes. The truncated DtN condition is a homogeneous Neumann condition on higher modes. This is exact for the cutoff mode, if it exists. There are no non-trivial solutions associated with the evanescent modes. Thus, in this case the homogeneous problem has only trivial solutions, and uniqueness of the original solution is not impaired.

If, however, there are more than N propagating modes, then condition (42) implies $A_n = 0$ only for $n = 0, \ldots, N-1$. Non-trivial contributions to higher propagating modes of the homogeneous problem may exist, allowing non-unique solutions to occur.

Thus, the criterion for uniqueness is quite simple, select N so that $\mu_N^2 \leq 0$, i.e., all propagating modes of the homogeneous problem are annihilated.

For constant wave numbers in a rectangular cross section, sufficient conditions for the truncated DtN map in terms of a double sum with indices $m = 0, \ldots, M-1$ and $n = 0, \ldots, N-1$ are

$$M \geq ka/\pi \qquad \text{and} \qquad N \geq kb/\pi. \tag{43}$$

This criterion is not sharp in the sense that it may include non-propagating modes in the truncated operator. However, this criterion cannot be improved if fixed limits are employed on both indices m and n. In Case 2, Dirichlet boundary conditions, fewer terms may be taken

$$M \geq ka/\pi - 1 \qquad \text{and} \qquad N \geq kb/\pi - 1. \tag{44}$$

For constant wave numbers in a strip we require

$$N \geq kb/\pi. \tag{45}$$

For variable wave numbers the eigenvalues μ_n^2 are found numerically. For uniqueness, the number of terms in the DtN map must be no less than the total number of positive eigenvalues (which is finite). For this reason a Sturm sequence check [2, p. 943] should be employed to verify that all positive eigenvalues are found. For a variable wave number $k = k(y)$ in a strip, the number of terms in the DtN operator sufficient to guarantee uniqueness may be conservatively estimated by

$$N \geq \max_{0 \leq y \leq b} k(y)b/\pi \tag{46}$$

according to [8, p. 411].

3.3. *Local DtN Boundary Conditions*

The truncated DtN map (in terms of a single sum, ordered with descending values of μ_n^2) is exact for functions that consist of only the first N modes. We now derive local boundary conditions that inherit this property. Consider a function that consists of the first N modes. (For Dirichlet boundary conditions trivial terms are excluded from the three-dimensional treatment, e.g., $\mu_0 = \mu_{11}$ in the double-index notation, and in two dimensions the first mode, $n = 0$, is trivial so that all appearances of Y_0 must be dropped from the following presentation.) On the artificial boundary

$$u = \sum_{n=0}^{N-1} A_n Y_n. \tag{47}$$

The eigenfunctions Y_n satisfy Eq. (7) and hence, for *constant* wave numbers

$$\Delta^l Y_n = \left(\mu_n^2 - k^2\right)^l Y_n, \tag{48}$$

where

$$\Delta^l Y_n = \underbrace{\Delta(\ldots\Delta(\Delta Y_n)\ldots)}_{l \text{ times}} \tag{49}$$

is the lth power of the Laplacian in C. Thus we may write

$$\Delta^l u = \sum_{n=0}^{N-1} \left(\mu_n^2 - k^2\right)^l A_n Y_n \qquad \text{on } \mathcal{B}. \tag{50}$$

The truncated DtN condition is

$$\frac{\partial u}{\partial z} = i \sum_{n=0}^{N-1} \mu_n A_n Y_n \qquad \text{on } \mathcal{B}. \tag{51}$$

Comparing Eqs. (50) and (51) suggests expressing the coefficients as linear combinations

$$\mu_n = \sum_{l=0}^{N-1} \beta_l \left(\mu_n^2 - k^2\right)^l, \qquad n = 0, \ldots, N-1, \tag{52}$$

where β_l are obtained by solving this $N \times N$ linear system. (For Dirichlet boundary conditions in two dimensions, the first mode, and hence the first equation in (52), is trivial. An upper limit of $N - 2$ on the sum is employed in this case.) Substitution into (51) yields the *local* expression, valid for constant wave numbers

$$\frac{\partial u}{\partial z} = i \sum_{n=0}^{N-1} \beta_n \Delta^n u \qquad \text{on } \mathcal{B} \tag{53}$$

(again, with an upper limit of $N - 2$ for Dirichlet boundary conditions in two dimensions).

The one-term local approximation is

$$\frac{\partial u}{\partial z} = i \mu_0 u \qquad \text{on } \mathcal{B} \tag{54}$$

and for the case of Dirichlet boundary conditions in two dimensions

$$\frac{\partial u}{\partial z} = i\mu_1 u \qquad \text{on } \mathcal{B}. \tag{55}$$

These one-term expressions are also valid for the more general case of wave numbers that vary within the cross section. An alternative approach [21] may be used to derive higher-order local boundary conditions for varying wave numbers.

As previously noted, uniqueness of the solution corresponds to enforcing zero energy flux through the artificial boundary, as in the first line of (41). Similarly, the difference between two solutions to the DtN problem with a one-term local approximation, v, must satisfy

$$\begin{aligned} 0 &= \int_{\mathcal{B}} \operatorname{Im}\{\bar{v} i\mu_0 v\}\, dC \\ &= \operatorname{Im}\{i\mu_0\} \int_{\mathcal{B}} |v|^2\, dC. \end{aligned} \tag{56}$$

If the first mode is propagating, i.e., $\mu_n^2 > 0$, then condition (56) implies that $v = 0$ on $\mathcal{B}$. In addition, v satisfies the DtN boundary condition on $\mathcal{B}$. Thus v satisfies homogeneous Dirichlet *and* Neumann boundary conditions on the artificial boundary. This over-specification of boundary data precludes non-trivial solutions in the computational domain Ω, which implies uniqueness of solutions with a one-term local boundary condition. Adding terms to the local approximation cannot alter this statement. If this is a cutoff mode, then the local boundary condition is exact and higher modes are evanescent. Uniqueness is not an issue if this mode is evanescent. Thus, uniqueness of the original solution is not impaired in all cases, for any number of terms. (In the case of Dirichlet boundary conditions in two dimensions, we substitute μ_1 for μ_0 and repeat the analysis.)

Our interest in local DtN boundary conditions is primarily as the basis of the modified formulation that follows. The one-term local approximations are sufficient for this purpose. Numerical comparisons of global and local DtN conditions have been performed previously [48] and are not repeated here. For completeness, the conclusions of these comparisons are summarized herein.

The global conditions are very robust. Moreover, once they are implemented in a finite element code, one may use them very easily, taking into account any desired number of terms. Their main disadvantage is that they require computations on the global level, which is contrary to the usual architecture of finite element codes.

On the other hand, local boundary conditions have the advantage that they are incorporated in a finite element code in the usual manner, i.e., on the element level. They are also more amenable to parallelization than the nonlocal conditions. The low-order localized conditions are simple, but not always sufficiently accurate, especially for small wave numbers. However, in the propagation regime, they are much more accurate than their nonlocal counterparts *of equal order* in resolving the higher modes in the exact solution. For problems where the first few modes are dominant, or where the wave number is large, they should be satisfactory.

The high-order localized conditions are more accurate. However, only the odd-order ones lead to a stable numerical scheme. Also, they require the use of special finite elements in the layer adjacent to the artificial boundary. The number of element degrees of freedom increases rapidly with the order, considerably increasing the computational effort.

3.4. *Modified DtN Formulations*

The truncated operator is modified so that solutions are unique for any number of terms, based on [26]. The idea is to consider any boundary condition on the artificial boundary, for which the problem in the computational domain is well posed, and add it to the higher modes only. To achieve this goal the modifying boundary operator is added to the global DtN condition and subtracted from it. Only the subtracted part is truncated along with the original operator. We employ the one-term local approximation (valid for variable wave numbers) as the modifying operator. In three dimensions

$$\frac{\partial u}{\partial z}(x, y, z_0) = i\mu_0 u(x, y, z_0) + i\sum_{n=1}^{N-1}(\mu_n - \mu_0)\int_C Y_n(x, y)Y_n(x', y')u(x', y', z_0)\, dx'\, dy'. \tag{57}$$

In two dimensions

$$\frac{\partial u}{\partial z}(y, z_0) = i\mu_0 u(y, z_0) + i\sum_{n=1}^{N-1}(\mu_n - \mu_0)\int_0^b Y_n(y)Y_n(y')u(y', z_0)\, dy' \tag{58}$$

and for Dirichlet boundary conditions in two dimensions

$$\frac{\partial u}{\partial z}(y, z_0) = i\mu_1 u(y, z_0) + i\sum_{n=2}^{N-1}(\mu_n - \mu_1)\int_0^b Y_n(y)Y_n(y')u(y', z_0)\, dy'. \tag{59}$$

Uniqueness is not impaired for any number of terms since the one-term modified condition is identical to the one-term local approximation.

3.5. *Implementation*

DtN boundary conditions are incorporated into finite element computation via the variational form of the boundary-value problem [14, 16, 19, 20, 23, 37, 47], see the third term on the left-hand side of (30). The DtN contribution to the stiffness matrix is a truncation and possible modification of

$$\int_{\mathcal{B}} N_A M N_B\, dC = -i\sum_{n=0}^{\infty}\mu_n I_{An} I_{Bn}, \tag{60}$$

where

$$I_{An} = \int_{\mathcal{B}} N_A Y_n\, dC \tag{61}$$

and N_A are standard finite element shape functions. The DtN contribution preserves the symmetry of the underlying finite element equations but couples all of the degrees of freedom on the artificial boundary.

The cross-sectional eigenvalues μ_n^2 and orthonormal eigenfunctions Y_n, needed to formulate DtN boundary conditions, are presented explicitly in (18) and (19) for the case of constant wave numbers in a strip, and in (9)–(12) for the case of constant wave numbers in rectangular cross sections. (Recall, the double index notation is converted to single index notation by simply ordering the modes with descending values of μ_n^2, starting with $\mu_0 = \mu_{00}$.)

In more general cases the cross-sectional eigenvalue problem is solved numerically for a finite number of eigenpairs. The resulting discrete eigenvalue problem is generally not positive definite since all propagating cross-sectional modes should be included in the DtN map for uniqueness. Care must be taken to compute these modes accurately. A shift of the eigenvalues [36, pp. 574, 575] may be employed in order to make the problem definite and hence more amenable to treatment by commonly used eigenvalue solvers. The size of the discrete eigenvalue problem should be much larger than the number of terms required, which are the terms with the largest eigenvalues. Due to potential deterioration in the quality of approximation of higher modes [51] the roles of the matrices of the discrete eigenvalue problem **K** and **M** may be reversed [36, p. 579] for more accurate numerical solution of the larger eigenvalues and corresponding eigenvectors. A Sturm sequence check [2, p. 943] (also known as spectrum slicing) should be employed to verify that no eigenvalues are missing.

4. NUMERICAL RESULTS

Numerical tests of the performance of the truncated and modified DtN conditions in various wave guide configurations are presented in the following. Convergence tests were performed in [22] and are not repeated here. Convergence rates of 2.006–2.007 in the L_2 norm and 0.981–0.986 in the H^1 semi-norm were obtained in these tests for both global and local DtN conditions. These rates are optimal.

4.1. *Constant Wave Number in a Strip*

The following numerical results are for a two-dimensional unbounded wave guide of constant width b, with Neumann wall conditions (Case 1). A varying Dirichlet boundary condition which satisfies the wall conditions $\frac{1}{2} - \frac{3737}{18}(\frac{y}{b})^2 + \frac{10675}{9}(\frac{y}{b})^3 - \frac{21764}{9}(\frac{y}{b})^4 + \frac{18896}{9}(\frac{y}{b})^5 - \frac{1984}{3}(\frac{y}{b})^6$ is specified on the boundary at $z = 0$, to excite significant contributions to the first three cross-sectional modes. A computational domain, determined by selecting $z_0 = b/4$, is meshed with 40×20 bilinear rectangles.

The cross-sectional eigenvalues μ_n^2 and orthonormal eigenfunctions $Y_n(y)$, needed to formulate DtN boundary conditions, are presented explicitly in (18) and (19) for the case of constant wave numbers in a strip. The criterion for uniqueness is that the number of terms in the truncated DtN operator N be such that $\mu_N^2 \leq 0$ (when the modes are ordered with descending eigenvalues). For constant wave numbers this is equivalent to $N \geq kb/\pi$. This criterion is verified with numerical results from the problem described above, for various wave numbers (Table 1), namely, $N \geq kb/\pi \Longleftrightarrow \mu_N^2 \leq 0$.

TABLE 1
Verifying the Criterion for Uniqueness, Constant Wave Number

kb	kb/π	No. of pos. eigenvalues
2	0.64	1
4	1.27	2
8	2.55	3
12	3.82	4
16	5.09	6
20	6.37	7

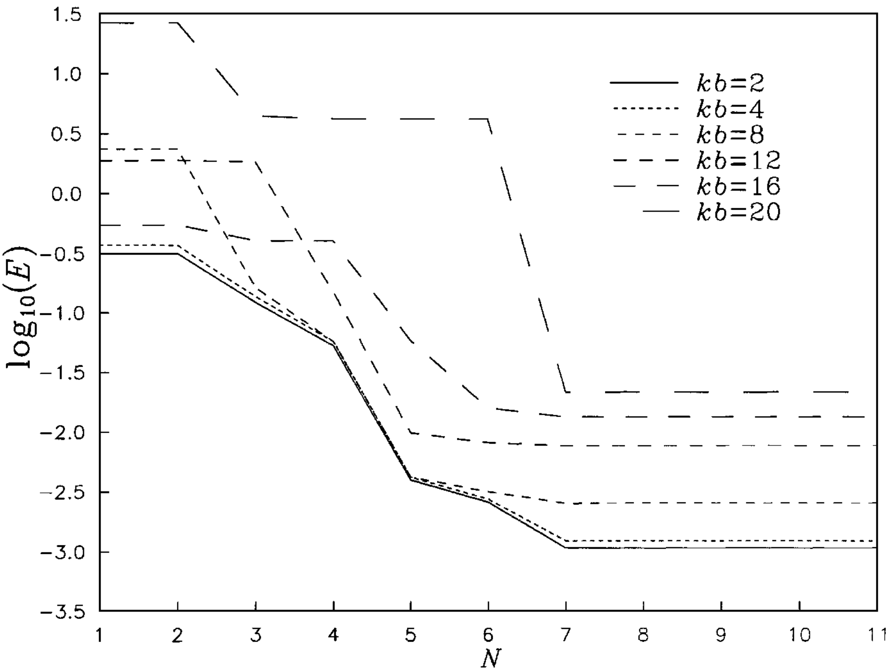

FIG. 3. Dependence of the error on the number of terms in the truncated operator.

The effect of satisfying the criterion for uniqueness with the truncated boundary condition is demonstrated in Fig. 3 for the same wave numbers as in Table 1. The relative error

$$E = \frac{\|u^h - u\|_{\mathcal{B}}}{\|u\|_{\mathcal{B}}} \tag{62}$$

in the $L_2(\mathcal{B})$ norm may be extremely high if the number of terms in the truncated DtN operator is not sufficient for uniqueness. This is particularly evident at $kb = 8$, 12, and 20, with errors on the order of 300% and higher! The somewhat anomalous behavior at $kb = 16$ may be due to its highest propagating mode ($n = 5$) having an eigenvalue close to zero.

As terms are added to the DtN condition the error decreases until it reaches a threshold beyond which adding terms no longer improves the solution. This fact is due to the finite number of significant modes in the boundary data. This behavior holds for all the wave numbers in Fig. 3, as well as for subsequent numerical tests.

The modified boundary condition is unique for any number of terms in the operator. The error with the modified boundary condition remains relatively low (less than 30%) even when the criterion for uniqueness is not satisfied (Fig. 4).

We employ this problem to compare the global DtN conditions to known boundary conditions: the Sommerfeld condition on the artificial boundary

$$\frac{\partial u}{\partial z} - iku = 0, \qquad \text{at } z = z_0 \tag{63}$$

(which is identical to the lowest-order condition of many schemes, including the one-term local DtN conditions) and the second-order Engquist–Majda scheme [9], which is

$$\frac{\partial u}{\partial z} - iku - \frac{i}{2k}\frac{\partial^2 u}{\partial y^2} = 0, \qquad \text{at } z = z_0 \tag{64}$$

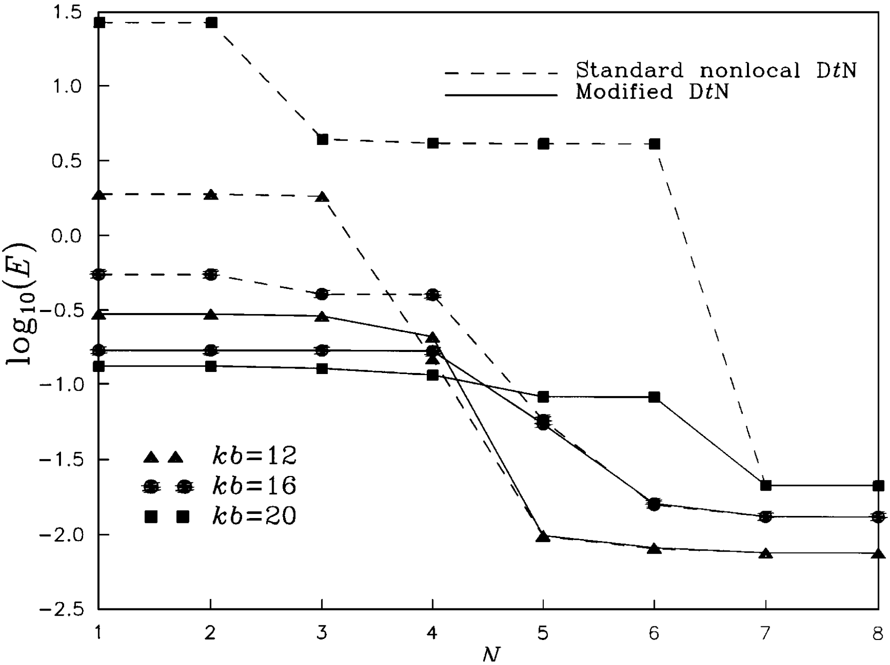

FIG. 4. Comparison of truncated and modified operators.

in the configuration considered. The real parts of the results for $kb = 4$ are compared to the analytical solution in Fig. 5. The Sommerfeld condition and the one-term global DtN condition (which is insufficient for uniqueness) provide poor results. The situation improves considerably for the Engquist–Majda and the three-term global DtN conditions. Three terms are sufficient for uniqueness of DtN in this case (see Table 1), and there is little difference in the performance of truncated and modified DtN, when there are sufficient terms for uniqueness (Fig. 4). Adding terms to the global DtN condition gives results that are barely distinguishable from the analytical solution.

Comparisons to the Bayliss–Turkel conditions [4, 5] were performed in [22] and are not repeated here. Only the first two Bayliss–Turkel boundary conditions are compatible with finite elements. The one-term local DtN condition is much more accurate than the first Bayliss–Turkel condition for all wave numbers. For small wave numbers, the solution obtained with the one-term local DtN condition is also much more accurate than that obtained with the second Bayliss–Turkel condition. In the intermediate range, the second Bayliss-Turkel condition is slightly more accurate. For large wave numbers the errors obtained with the two conditions are similar.

4.2. *Linearly Varying Wave Number in a Strip*

The following results are obtained for the problem described above, with linearly varying wave numbers $k = k_d + (k_u - k_d)y/b$. The cross-sectional eigenvalues μ_n^2 and orthonormal eigenfunctions $Y_n(y)$, needed to formulate DtN boundary conditions, are found numerically in this case, by using a standard eigenvalue solver for a one-dimensional eigenvalue problem discretized with 400 degrees of freedom. A Sturm sequences check [2, p. 943] is employed to verify that no eigenvalues are missing. The accuracy of the modes employed is established by numerical convergence studies. Numerical integration of (61) is performed in each

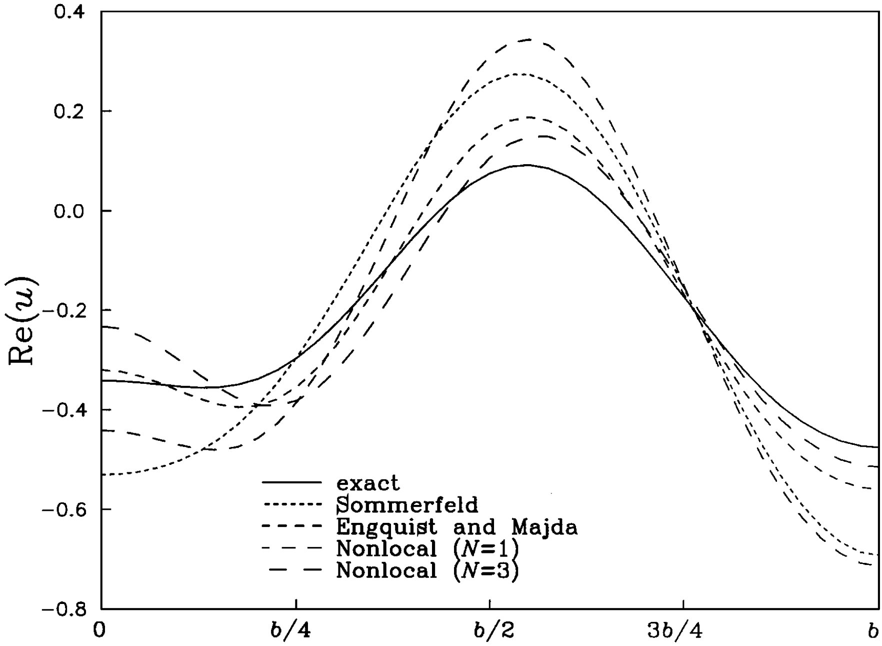

FIG. 5. Comparison of boundary conditions along the artificial boundary.

element by the trapezoidal rule with sufficient points to account for the oscillations of Y_n. The linear variation of k within each element is accounted for in computing the element stiffness matrix.

Recall the criterion for uniqueness, that the number of terms in the truncated DtN operator N be such that $\mu_N^2 \leq 0$ (when the modes are ordered with descending eigenvalues). A conservative estimate for the case of linearly varying wave numbers is $N \geq \max\{k_d, k_u\}b/\pi$. This estimate is verified with numerical results from the problem described above, for various values of the parameters with $k_u > k_d$ (Table 2), namely, $N \geq k_u b/\pi \Longrightarrow \mu_N^2 \leq 0$. Note that the eigenvalue of the most oscillatory mode is bounded by the limit values of the varying wave number $k_d \leq \mu_0 \leq k_u$.

TABLE 2
Verifying the Criterion for Uniqueness, Linearly Varying Wave Number

$k_d b$	$k_u b$	$\mu_0 b$	$k_u b/\pi$	No. of pos. eigenvalues
2	4	3.20	1.27	1
2	8	6.64	2.55	2
2	12	10.34	3.82	3
2	16	14.10	5.09	3
2	20	17.92	6.37	4
6	8	7.34	2.55	3
6	12	10.82	3.82	3
6	16	14.50	5.09	4
6	20	18.24	6.37	5
10	12	11.42	3.82	4
10	16	14.92	5.09	5
10	20	18.60	6.37	5

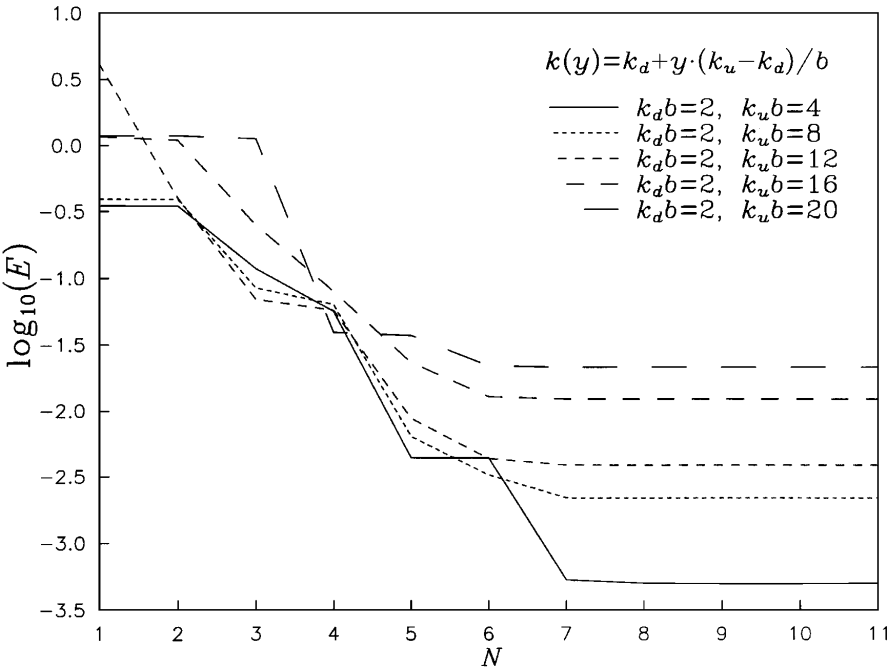

FIG. 6. Dependence of the error on the number of terms in the truncated operator ($k_d b = 2$).

The effect of satisfying the criterion for uniqueness with the truncated boundary condition is demonstrated in Figs. 6–8 for the same wave numbers as in Table 2. The relative error may be quite high if the number of terms in the truncated DtN operator is not sufficient for uniqueness.

4.3. *Constant Wave Number in a Square Cross-section*

The following numerical results are for a three-dimensional unbounded wave guide of square cross section $a = b$, with Neumann wall conditions (Case 1). A varying Dirichlet boundary condition which satisfies the wall conditions $(16(\frac{x}{a})^2 - 32(\frac{x}{a})^3 + 24(\frac{x}{a})^4 - \frac{32}{5}(\frac{x}{a})^5)(4(\frac{y}{b})^2 - \frac{8}{3}(\frac{y}{b})^3) - (4(\frac{x}{a})^2 - \frac{8}{3}(\frac{x}{a})^3)(8(\frac{y}{b})^2 - \frac{32}{3}(\frac{y}{b})^3 + 4(\frac{y}{b})^4)$ is specified on the boundary at $z = 0$, to excite significant contributions to the first three cross-sectional modes. A computational domain, determined by selecting $z_0 = b/2$, is meshed with $14 \times 14 \times 7$ trilinear cubes.

The cross-sectional eigenvalues μ_n^2 and orthonormal eigenfunctions $Y_n(x, y)$, needed to formulate DtN boundary conditions, are presented explicitly in (9)–(12) for the case of constant wave numbers in rectangular cross sections. Recall, this double index notation is converted to single index notation by simply ordering the modes with descending values of μ_n^2, starting with $\mu_0 = \mu_{00}$. Table 3 shows the correspondence of the first nine cross-sectional terms in a square. Due to the symmetry of eigenfunctions in a square, $Y_{mn} = Y_{nm}$ the ordering of terms 1 and 2, terms 4 and 5, and terms 6 and 7 can be reversed.

The criterion for uniqueness is that the number of terms in the truncated DtN operator N be such that $\mu_N^2 \leq 0$. For constant wave numbers in a square cross section, sufficient conditions for the truncated DtN map expressed in terms of a double sum with indices $m = 0, \ldots, M - 1$ and $n = 0, \ldots, N - 1$ are $M^2 + N^2 \geq (ka/\pi)^2$.

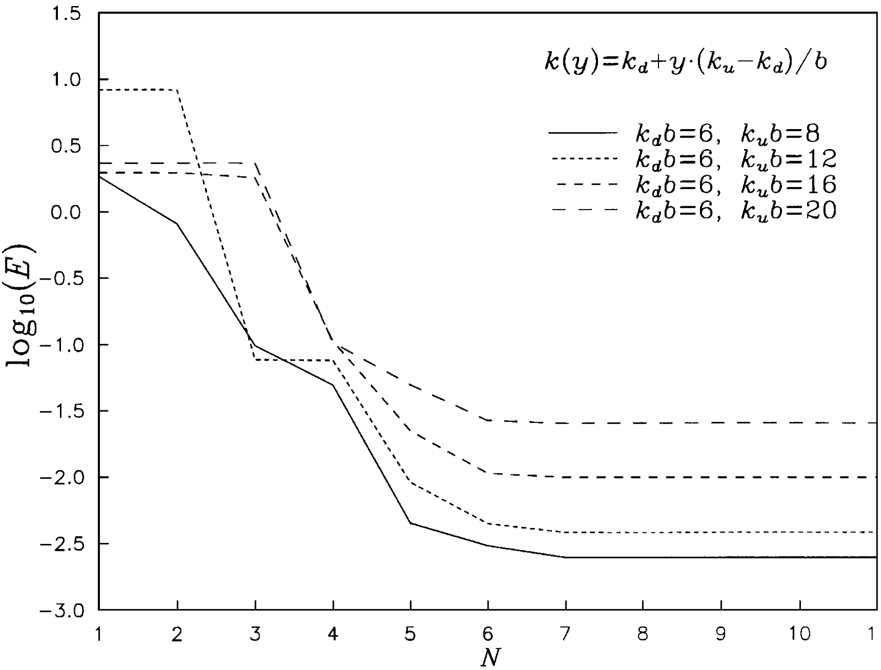

FIG. 7. Dependence of the error on the number of terms in the truncated operator ($k_d b = 6$).

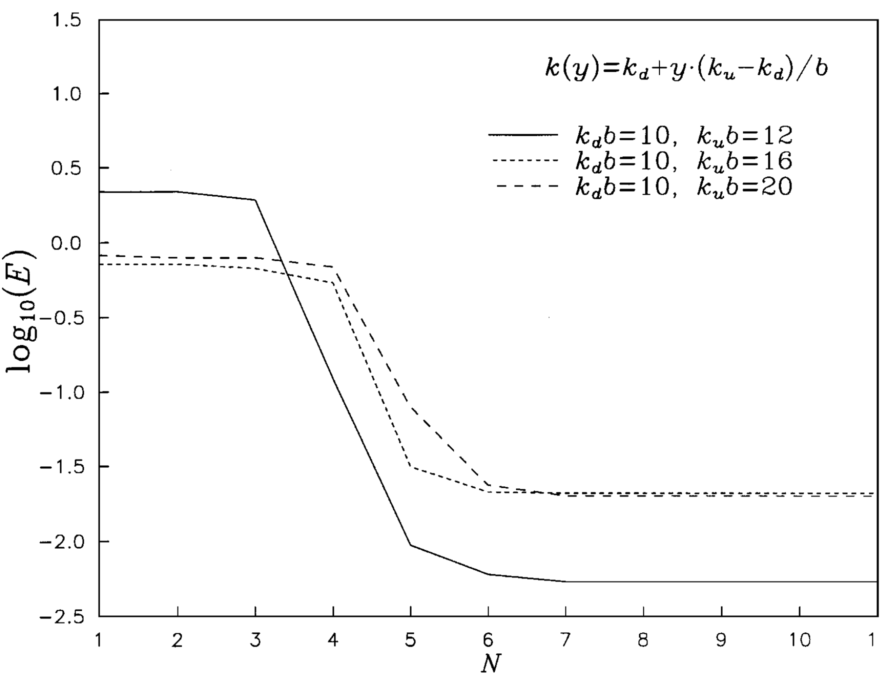

FIG. 8. Dependence of the error on the number of terms in the truncated operator ($k_d b = 10$).

TABLE 3
Correspondence of Double- and Single-Index Notations for Cross-sectional Modes in a Square

(m,n)	n
(0,0)	0
(1,0)	1
(0,1)	2
(1,1)	3
(2,0)	4
(0,2)	5
(2,1)	6
(1,2)	7
(2,2)	8

The effect of satisfying the criterion for uniqueness with the truncated boundary condition is demonstrated in Fig. 9. For wave numbers $k = 0, 2, 4$, and 6 the number of terms required is $N = 1, 4, 6$, and 19 (see, e.g., Table 3). The relative error may be extremely high (approaching 1,000%!) if the number of terms in the truncated DtN operator is not sufficient for uniqueness. The modified boundary condition is unique for any number of terms in the operator. The error with the modified boundary condition remains relatively low (less than 30%) even when the criterion for uniqueness is not satisfied (Fig. 9).

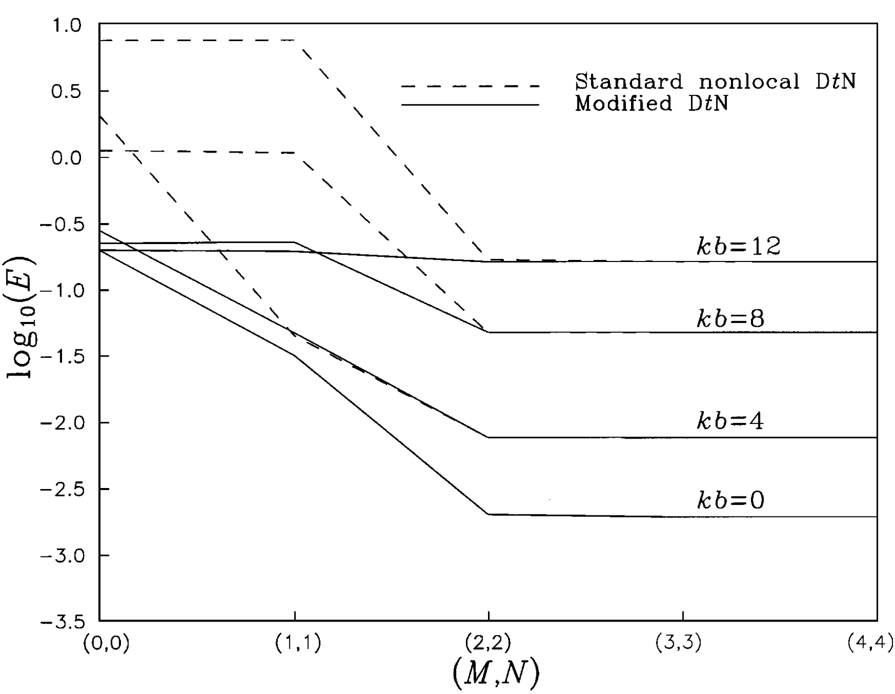

FIG. 9. Dependence of the error on the number of terms in the truncated and modified operators.

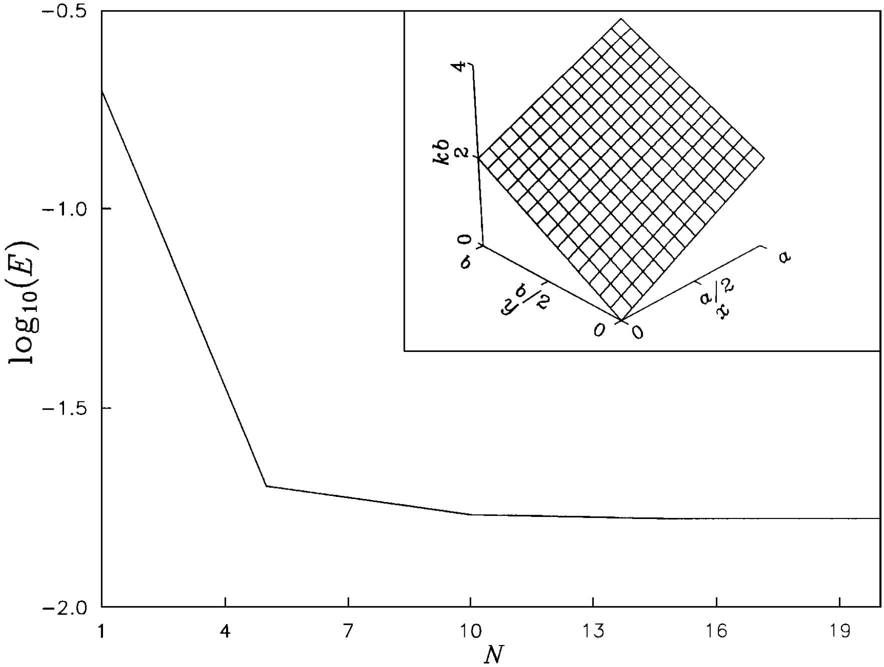

FIG. 10. Dependence of the error (with varying wave number) on the number of terms in the truncated operator.

4.4. *Linearly Varying Wave Number in a Square Cross-section*

The following results are obtained for the problem described above, with a linearly varying wave number $k = k_0(x + y)/a$, where $k_0 b = 2$. The cross-sectional eigenvalues μ_n^2 and orthonormal eigenfunctions $Y_n(x, y)$, needed to formulate DtN boundary conditions, are found numerically in this case, by using a standard eigenvalue solver for a two-dimensional eigenvalue problem discretized with a uniform mesh of 35×35 nodes for a total of 1225 degrees of freedom. A Sturm sequence check [2, p. 943] is employed to verify that no eigenvalues are missing. The accuracy of the modes employed is established by numerical convergence studies. Numerical integration of (61) is performed in each element by the trapezoidal rule with sufficient points to account for the oscillations of Y_n. The linear variation of k within each element is accounted for in computing the element stiffness matrix.

In this problem there is a single positive eigenvalue. Thus, there is always a sufficient number of terms in the DtN boundary condition and the relative error remains relatively low (less then 20%), see Fig. 10.

5. CONCLUSIONS

This work presents the derivation and analysis of DtN formulations for unbounded wave guides in two and three dimensions. DtN boundary conditions, relating the solution to its normal derivative on an artificial boundary, define problems in bounded domains that are suitable for finite element analysis. Explicit expressions are obtained for constant wave numbers in strips and in rectangular cross sections (the extension to circular cross sections is straightforward). The boundary conditions are derived numerically for wave numbers varying in the cross section, and for cross sections of general shape in three dimensions.

The bounded-domain problem obtained by employing the DtN procedure is analyzed in its continuous form, prior to discretization. The DtN operator is expressed in the form of infinite series. The solution of the bounded-domain problem with the full operator is a restriction of the solution to the original problem to the bounded domain. The truncated DtN operator, which is employed in practice, fails to inhibit higher modes, so that nonunique solutions may occur. Simple criteria determine a sufficient number of terms in the truncated operator for unique solutions at any given wave number. Local approximations of the boundary conditions for constant wave numbers yield uniqueness for all wave numbers. A simple modification of the truncated operator by the lowest-order local approximation, which is valid for varying wave numbers, leads to boundary conditions that are unique for any number of terms in the operator.

Numerical results validate the performance of the DtN boundary conditions for wave guides in two and three dimensions and confirm the criteria for uniqueness. In particular, the truncated and modified conditions perform similarly as long as there are sufficient terms for the truncated condition to yield unique solutions. Otherwise, the modified condition is superior, as expected.

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