Propagation in Helmholtz Waveguides using DtN, NtD and Ra,tD Maps: Part I, a Second Order Method

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Abstract

For many wave propagation problems, it is often necessary to solve the variable coefficient Helmholtz equation in a very large domain. The one-way re-formulation based on the Dirichlet-to-Neumann (DtN) map can be used to find the solutions of the Helmholtz equation over a large range distance. It is particularly useful for waveguide problems, since it leads to a numerical algorithm that marches in the range variable. The DtN map satisfies an operator Riccati equation and may blow up even though the original problem is well-posed. In this paper, we develop a method that automatically switches between the DtN and Neumann-to-Dirichlet (NtD) maps, or between the DtN and the Robin-to-Dirichlet (Ra,tD) maps, to avoid the singularities of these operators. When implemented with a truncated local eigenfunction expansion, the operator equations can be efficiently solved.

1 Introduction

For acoustic, electro-magnetic and seismic wave propagation problems of practical interest, it is often necessary to solve the governing equation in a domain that has a length scale much larger than the typical wavelength. Standard numerical techniques such as the finite difference and finite element methods lead to a system of equations with a very large number of unknowns and are not very practical for these large scale problems.

On the other hand, boundaries and different medium properties often lead the waves to propagate in some preferred directions. The length scale along the waveguide is typically very large. The transverse length scale is much smaller, but still larger than the characteristic wavelength. For example, the ocean surface and the relative small sound speed in water (compared with the sea-bed) effectively force the sound waves to propagate in horizontal directions. Low

\textsuperscript{1}This research was partially supported by grant from the Research Grants Council of Hong Kong Special Administrative Region, China (Project No. CityU 1080/99P).

\textsuperscript{2}This research was partially supported by ONR grant #N00014-96-1-0349 and NFS grant #DMS9802309.
frequency sound waves in the ocean could travel hundreds and even thousands of kilometers in
the horizontal (i.e. range) direction.

To take advantage of the difference in range and transverse length scales, one-way re-
formulations that are exactly equivalent to the Helmholtz equation can be used. Such a re-
formulation turns a boundary value problem into an “initial” value problem where the range
variable (along the waveguide) acts as the usual time variable. Numerical computations based
on one-way re-formulations have a memory requirement that is independent of the total range
distance and a computation time that is linearly proportional to the same distance. Fishman
[7] first developed a re-formulation based on a wave-field decomposition and the scattering
operators. A simpler re-formulation based on the Dirichlet-to-Neumann (DtN) map has also
been derived [7, 8, 9, 16]. A detailed numerical implementation of the DtN re-formulation was
developed in [16].

A widely used approach for long range propagation problems in a weakly range dependent
waveguide is to approximate the Helmholtz equation by the one-way Helmholtz equation or
its further approximations [13, 19, 5, 11, 12]. These methods can be efficiently implemented.
However, the one-way Helmholtz equation is truly valid only for range independent media.
Even when the range dependence is weak, if the one-way Helmholtz equation is used in a long
range calculation, the accuracy is questionable. In contrast, the one-way re-formulations used
in this paper give the exact solution of the Helmholtz equation.

The underlying ideas for our approach are as follows. Let \( x \) be the range variable and \( z \)
the depth variable. We then factor the Helmholtz equation as

\[
\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + \kappa^2(x, z) = \left( \frac{\partial}{\partial x} + Q \right) \left( \frac{\partial}{\partial x} - Q \right).
\]

At fixed \( x \), the operator \( Q \) is shown to satisfy a Riccati equation. The outgoing solution, \( u \), of
the Helmholtz equation is then determined by simultaneously solving the Riccati equation for
\( Q \) and the equation \((\partial_x - Q)u = 0\) for \( u \).

Note that for fixed \( x \), the operator \( Q \) is the Dirichlet to Neumann (DtN) map. For most
\( x \), this is a well defined operator. However, even when the solution of the Helmholtz equation
is uniquely defined, if can happen that at some \( x = x_* \) the DtN map, \( Q \), is not defined. In
this case, the map \( Q \) can become singular and the numerical approximation of it can blow up
at \( x = x_* \). This is an artifact of the method; and it creates numerical difficulties. However, in
this paper, we establish that when \( Q \) becomes singular we can switch to another operator in
the neighborhood of a singularity of \( Q \), which is either \( Q^{-1} \), the Neumann to Dirichlet (NtD)
map, or \((Q - aI)^{-1} \), a Robin to Dirichlet (RtD) map with \( a \) a non-zero constant, switching
back to \( Q \) when the singularity is past. Since \( Q^{-1} \) and \((Q - aI)^{-1} \) satisfy Riccati equations,
the computations using the new maps are similar to those for \( Q \). The switch is automatically
handled when the operators are marched in range and the overall computation effort is only
slightly larger than the original method using the DtN map alone.
2 One-way re-formulations

In this paper, we consider the 2-dimensional Helmholtz equation

$$u_{xx} + u_{zz} + \kappa^2(x, z)u = 0$$  \hspace{1cm} (1)

for $-\infty < x < \infty$ and $0 < z < 1$. This is supplemented by the boundary conditions

$$u(x, 0) = 0, \quad u_z(x, 1) = 0.$$  \hspace{1cm} (2)

The wavenumber $\kappa$ is assumed to depend on $x$ and $z$ together only for $0 < x < L$ and

$$\kappa(x, z) = \begin{cases} \kappa_0(z) & x \le 0 \\ \kappa_\infty(z) & x \ge L, \end{cases}$$

where $\kappa_0$, $\kappa_\infty$ are functions of $z$. Under this assumption, it is only necessary to solve the Helmholtz equation in the reduced domain $\Omega = \{(x, z) \mid 0 < x < L, \ 0 < z < 1 \}$.

If there is no incident wave coming from $x = +\infty$, we have the following exact radiation boundary condition at $x = L$

$$u_x = i \sqrt{\partial_z^2 + \kappa^2_\infty(z)} \ u.$$  \hspace{1cm} (3)

The square root operator above is a linear operator that maps $j \phi_j$ to $p_j \kappa_\infty(z)$, where $f_j \phi_j$ and $f_j \phi_j$ are eigenvalues and the corresponding eigenfunctions of the operator $\partial_z^2 + \kappa^2_\infty(z)$, subject to boundary conditions similar to (2), and $\sqrt{\lambda_j} > 0$ when $\lambda_j > 0$ and $\text{Im} \sqrt{\lambda_j} > 0$ when $\lambda_j < 0$.

At $x = 0$, the easiest case is when a starting field is specified:

$$u = u_0(z) \quad \text{at} \quad x = 0,$$  \hspace{1cm} (4)

where $u_0$ is a given function of $z$. Another common situation is when an incident wave $u^{(i)}$ is given for $x \le 0$. Since the waveguide is range independent for $x \le 0$, the incident wave and the reflected wave $u^{(r)}$ satisfy the following two equations, respectively

$$u_x^{(i)} = i \sqrt{\partial_z^2 + \kappa^2_0(z)} \ u^{(i)}, \quad u_x^{(r)} = -i \sqrt{\partial_z^2 + \kappa^2_0(z)} \ u^{(r)}$$

for $x \le 0$. This leads to the following boundary condition for the total wave field $u = u^{(i)} + u^{(r)}$:

$$[\partial_x + i \sqrt{\partial_z^2 + \kappa^2_0(z)}] u = 2i \sqrt{\partial_z^2 + \kappa^2_0(z)} \ u^{(i)} \quad \text{at} \quad x = 0.$$  \hspace{1cm} (5)

Finally, the wave field could be generated by a source. If the source is distributed at the vertical line at $x = 0$, the right hand side of the Helmholtz equation (1) should be replaced by $\delta(x)f(z)$, where $f$ is the given distribution. The source term creates a discontinuity for $u_x$, that is, $u_x|_{x=0}^{0+} = f(z)$. Since the medium is $x$-independent for $x \le 0$, we have $u_x|_{x=0}^{0-} = -i \sqrt{\partial_z^2 + \kappa^2_0(z)} \ u|_{x=0}$.

Since $\sqrt{\partial_z^2 + \kappa^2_0(z)}u$ is continuous at $x = 0$, this gives rise to the boundary condition:

$$u_x|_{x=0}^{0+} = f(z) - i \sqrt{\partial_z^2 + \kappa^2_0(z)} \ u|_{x=0}.$$  \hspace{1cm} (6)
If the source is located inside the range dependent region, say at $x = x_s$, for $0 < x_s < L$, the problem must be solved in two regions $0 < x < x_s$ and $x_s < x < L$ with the following matching conditions at $x = x_s$:
\[ u|_{x_s^-} = 0, \quad u_x|_{x_s^+} = f(z), \]
and the exact outgoing radiation condition at $x = 0$:
\[ u_x = -i\sqrt{\partial_z^2 + \kappa_0^2(z)} u. \]

Our problem is characterized by the existence of three distinct length scales
\[ \frac{1}{\kappa} << 1 << L. \]
Namely, the typical wavelength $O(1/\kappa)$ is much smaller than the transverse length scale (normalized as 1), which is still much smaller than the range distance $L$. Standard numerical methods such as the finite difference and finite element methods must resolve the details of the wave field by using a few grid points (or basis functions) for each wavelength. This could lead to very large, indefinite and non-symmetric linear systems that are difficult to solve. These methods are also constrained by the large memory requirement.

To avoid the difficult boundary value problem of the Helmholtz equation, it is common to use the one-way Helmholtz equation
\[ u_x \approx i\sqrt{\partial_z^2 + \kappa^2(x, z)} u \]
(7)
or its further approximations, under the assumption that the range dependence is weak. Since only a first derivative in $x$ is involved, equation (7) can be efficiently solved by marching forward in $x$. However, the one-way Helmholtz equation is only valid when the waveguide is range independent. For weakly range dependent media, if equation (7) is used over a large range distance, the result could be inaccurate.

The approach we follow in this paper is to use one-way reformulations that are exactly equivalent to the original Helmholtz equation. The idea is to factor the Helmholtz operator as
\[ \partial_x^2 + \partial_z^2 + \kappa^2(x, z) = (\partial_x + Q)(\partial_x - Q) \]
determine the outgoing solution, $u$, using only the factor $\partial_x - Q$ and hence solving the evolution equation
\[ u_x = Qu \]
(8)
instead of $(\partial_x^2 + \partial_z^2 + \kappa^2(x, z))u = 0$. In the range independent case, i.e., $\kappa^2 = \kappa_0^2(z)$, (8) becomes
\[ u_x = i\sqrt{\partial_z^2 + \kappa_0^2(z)} u, \]
(9)
and the Helmholtz equation can be solved by marching forward in $x$ using (9). In the range dependent case, the operator $Q$ which for fixed $x$ is the Dirichlet to Neumann (DtN) map satisfies the operator Riccati equation
\[ \frac{dQ}{dx} = -(\partial_z^2 + \kappa^2(x, z)) - Q^2, \]
(10)
where when $x > L$, $Q$ is independent of $x$ and is equal to $Q(L)$ which is
\[ Q(L) = i\sqrt{\partial_z^2 + \kappa_L^2(z)}. \] (11)

The goal, then, in the range dependent case is to solve (8) and (10) simultaneously. Note that the Riccati equation (10) is more stable if we march backward in $x$ (from $x = L$ to $x = 0$) and this strongly influences our numerical implementation.

To calculate our solution we define the fundamental solution operator, $Y(x)$, by
\[ Y(x)u(x,z) = u(L,z) \]
with
\[ Y(L) = I, \] (12)
where $I$ is the identity operator. We have established, see [16], that $Y$ satisfies the equation
\[ \frac{dY}{dx} = -YQ. \] (13)

For stability reasons, we then solve (10) and (13) from $x = L$ back to $x = 0$ starting at $x = L$ with (11) and (12) and obtaining $Y(0)$ and $Q(0)$ (or $Q(0^+)$ if a source is given at $x = 0$). If $Q$ is well defined for all values of $x$, $0 < x < L$, to complete our calculation to find $u(L,z)$, we compute
\[ u(L,z) = Y(0)u(0,z), \] (14)
where
\[ u(0,z) = u_0(z), \] if (4) holds, \[ Q(0) + i\sqrt{\partial_z^2 + \kappa_0^2(z)} \] \[ u(0,z) = 2i\sqrt{\partial_z^2 + \kappa_0^2(z)} u^{(i)}(0,z), \] if (5) holds, \[ Q(0^+) + i\sqrt{\partial_z^2 + \kappa_0^2(z)} \] \[ u(0,z) = f(z), \] if (6) holds. \[ \] (15) (16) (17)

Note that we can determine $u(\hat{x},z)$ for any $0 < \hat{x} < L$, if that is needed, simply by restarting our calculation for $Y$ with $Y(\hat{x}) = I$. Calling this solution $\hat{Y}$, we obtain
\[ u(\hat{x},z) = \hat{Y}(0)u(0,z). \]

A significant saving in required computer memory is obtained if the solution $u$ is needed only at a limited number of points $0 < \hat{x}^1 < \hat{x}^2 < \ldots < \hat{x}_p = L$.

The goal of this paper is to take care of the case where $Q$ may not be well defined at all values of $x$, $0 < x < L$. The approach in that case is to switch to either $Q^{-1}$, (NtD), or $(Q-aI)^{-1}$, (RtD), where $a$ is a non-zero constant, in the neighborhood of a singularity of $Q$. Before explaining the switching method, we first explain how the solution of the Helmholtz equation can be obtained if the maps $Q^{-1}$ or $(Q-aI)^{-1}$ are themselves well-defined for all values of $x$, $0 < x < L$. 

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In the first case, letting $H = Q^{-1}$ we would obtain that $H$ satisfies the following Riccati equation and initial condition (at $x = L$)

$$\frac{dH}{dx} = I + H \left[ \partial_z^2 + \kappa^2(x, z) \right] H,$$

$$H(L) = -i \left[ \partial_z^2 + \kappa_{\infty}^2(z) \right]^{-1/2},$$

further with $v = u_x$ and the fundamental solution operator, $W$, satisfying

$$W(x)v(x, z) = u(L, z),$$

then also satisfies

$$\frac{dW}{dx} = W \left[ \partial_z^2 + \kappa^2(x, z) \right] H,$$

$$W(L) = -i \left[ \partial_z^2 + \kappa_{\infty}^2(z) \right]^{-1/2}.$$ Again we solve from $x = L$ to $x = 0$ to obtain $W(0)$ and $H(0)$ (or $H(0^+)$ if a source is located at $x = 0$). Finally, to obtain $u(L, z)$ from $v(0, z)$ using (20), we calculate

$$H(0)v(0, z) = u_0(z),$$

$$[I + i \sqrt{\partial_z^2 + \kappa_{0}^2(z)} H(0)] v(0, z) = 2i \sqrt{\partial_z^2 + \kappa_{0}^2(z)} u^{(i)}(0, z),$$

$$[I - i \sqrt{\partial_z^2 + \kappa_{0}^2(z)} H(0^+)] v(0, z) = f(z),$$

In the second case, letting $J_a = (Q - aI)^{-1}$ and the fundamental solution operator $M_a$ be defined by

$$J_a(x)(u_x - au) = u,$$

$$M_a(x)(u_x - au)(x, z) = u(L, z),$$

we solve the Helmholtz equation from $x = L$ to $x = 0$ to find $J_a(0)$ (or $J_a(0^+)$ if a source is located at $x = 0$) and $M_a(0)$ using

$$\frac{dJ_a}{dx} = I + 2a J_a + J_a \left[ \partial_z^2 + \kappa^2(x, z) + a^2 \right] J_a,$$

$$\frac{dM_a}{dx} = M_a \left[ aI + \left( \partial_z^2 + \kappa^2(x, z) + a^2 \right) J_a \right],$$

$$J_a(L) = \left[ i \left( \partial_z^2 + \kappa_{\infty}^2(z) \right) \right]^{1/2} - aI,$$

$$M_a(L) = \left[ i \left( \partial_z^2 + \kappa_{\infty}^2(z) \right) \right]^{1/2} - aI.$$ We note that $J_0 = H$. Finally to obtain $u(L, z)$ from $(u_x - au)|_{x=0}$ using (27), we calculate

$$J_a(0)(u_x - au)|_{x=0} = u_0(z),$$

$$[I + (aI + iB(0)) J_a(0)] (u_x - au)|_{x=0} = 2iB(0)u^{(i)}(0, z),$$

$$[I + (aI - iB(0)) J_a(0^+)] (u_x - au)|_{x=0} = f(z),$$

6
where \( B(0) = \sqrt{\partial_z^2 + \kappa_0^2(z)} \).

Note that if all the maps \( Q, H \) or \( J_a \) are well-defined in \( 0 < x < L \), then the Helmholtz equation can be solved using any one of the above three one-way re-formulations. Note also that we can find the fundamental solution operator \( Y \) from \( W, H \) or \( M_a, J_a \) by

\[
Y = WH = M_a J_a,
\]

or we can obtain \( W \) or \( M_a \) from \( Y, Q \) using

\[
W = YQ, \quad M_a = Y(Q - aI).
\]

The advantage of the DtN, NtD or R\textsubscript{ntD} re-formulations is their simplicity. However, the maps \( Q, H \) or \( J_a \) may not be well defined for all \( x \) in the interval \( (0, L) \). This is related to the possibility that a non-zero solution \( u, u_x \) or \( u_x - au \) may vanish at some \( x \), for all \( z \) in \( (0, 1) \).

Should this happen, \( Q, H \) and \( J_a \), respectively, can not be defined at \( x \). To be more specific, recall that \( Q, H \) and \( J_a \) are linear operators. In the case that a non-zero solution, \( u \), satisfies \( u(x, z) = 0 \) for all \( z \in (0, 1) \), if \( Q \) is well defined then \( u_x = Qu = 0 \) for all \( z \in (0, 1) \). In a later paper, we will prove that this implies that \( u \equiv 0 \) which yields a contradiction. Hence \( Q \) cannot be well defined at \( x = x_\star \). A similar argument can be made if \( u_x \) or \( u_x - au \) vanish at some \( x \), for all \( z \in (0, 1) \).

The objective of this paper is to develop a one-way method that couples \( Q \) and \( H \) or \( Q \) and \( J_a \) (also \( Y \) and \( W \) or \( Y \) and \( M_a \), if needed) to overcome this difficulty. In a later paper, we will prove that at any \( x = x_\star \), it is always possible to choose a constant \( a \), so that at least one of the maps \( Q, H, J_a \) is well defined at \( x = x_\star \).

### 3 Non-uniqueness and blow-ups

To further explain the blowup of \( Q \), suppose that for a fixed value of \( x = x_\star \), there is a unique solution for the problem

\[
\left[ \partial_x^2 + \partial_z^2 + \kappa^2(x, z) \right] u = 0 \quad x_\star < x < \infty, \quad 0 < z < 1,
\]

\[
u(x, 0) = u_x(x, 1) = 0 \quad x_\star < x < \infty
\]

\[
u_x = i\sqrt{\partial_z^2 + \kappa_\infty^2(z)} u \quad L \leq x < \infty, \quad 0 < z < 1,
\]

\[
u(x_\star, z) = f(z) \quad 0 < z < 1,
\]

where \( f \) is fixed but arbitrary. Letting \( g_f = u_x(x_\star, z) \), the DtN map \( Q(x_\star) \) is then defined by

\[
Q(x_\star)f = g_f.
\]

(Note that the uniqueness assumption implies \( f = 0 \) yields \( g_f = 0 \).) If, however, the eigenvalue problem

\[
- \left[ \partial_x^2 + \partial_z^2 + \kappa^2(x, z) \right] u = \mu u \quad x_\star < x < \infty, \quad 0 < z < 1,
\]

\[
u(x, 0) = u_x(x, 1) = 0 \quad x_\star < x < \infty
\]

\[
u_x = i\sqrt{\partial_z^2 + \kappa_\infty^2(z)} u \quad L \leq x < \infty, \quad 0 < z < 1,
\]

\[
u(x_\star, z) = 0 \quad 0 < z < 1,
\]
has $\mu = 0$ as an eigenvalue, then (37-40) will not have a unique solution. In this case, $Q$ is not well defined at $x = x_*$ and the effect of this is that when we compute our numerical approximate for $Q$ from $x = L$ to $x = x_*$ by solving the Riccati equation for $Q$, that approximate blows up at $x = x_*$. To further emphasize our point, in general, when we consider the Helmholtz equation with starting field (4), the problem (1)-(4) is assumed to have a unique solution. However, even with this uniqueness assumption for the problem (1)-(4), the subproblem (37)-(40) still may not have a unique solution. In other words, the DtN map may be well defined for most values of $x$, including $x = 0$, but still may not be defined at some $x_* \in (0, L)$. [In a later paper, we will present a proof that the DtN map is well defined for all but a finite number of values of $x$ in $(0, L)$.]

To better illustrate this loss of uniqueness, we consider the special case of a $z$-independent medium, where the wavenumber is given by $\kappa(x, z) = \kappa(x)$. For $x \geq L$, $\kappa$ is simply a constant $\kappa_\infty$. This is a separable problem. A solution is given by

$$u_j(x, z) = v_j(x) \sin(m_j z),$$

where $m_j = (j - \frac{1}{2})\pi$, if $v_j$ satisfies the second order equation

$$v''_j + (\kappa^2(x) - m_j^2)v_j = 0.$$ 

If $\kappa_\infty < m_j$, $v_j$ is an exponentially decaying function of $x$ for $x > L$, corresponding to an evanescent mode. However, if for some region of $x$, $\kappa(x) > m_j$, the function $v_j$ could be oscillatory for $x < L$ and $v_j$ could vanish at some values of $x$. A simple example that can be easily worked out is when $\kappa$ is a step function that assumes a value larger than $\kappa_\infty$ for smaller $x$ values. If $x_*$ is a zero of $v_j$ for some $j$, then the DtN map at $x_*$ can not be defined.

When one encounters the non-uniqueness for a Dirichlet boundary condition at $x = x_*$, it is frequently the case that the problem (37)-(39) together with the Neumann condition

$$u_x(x_*, z) = g(z) \quad 0 < z < 1,$$

has a unique solution. In this case the NtD operator $H(x_*)$ is well defined. It maps the $x$-derivative of a solution of the Helmholtz equation that satisfies (2)-(3) to the solution itself at $x_*$. To further illustrate the connection with eigenvalue problems, if (41)-(44) has $\mu = 0$ as an eigenvalue, then also the eigenvalue problem

$$Hg = \tau g$$

has the eigenvalue $\tau = 0$. In the case when $Q$ is not well defined at $x = x_*$ and $H$ is well defined at $x = x_*$, it is our intent then to perform our calculation from $x = L$ to $x = 0$ by switching from $Q$ to $H$ in the neighborhood of $x = x_*$, switching back to $Q$ outside of the neighborhood of $x_*$. This procedure can be repeated in the neighborhood of each point where $Q$ is not well defined as long as $H$ is well defined at these same points.

However, this is not the end of the story because it is possible to have an $x_*$ for which $\mu = 0$ is an eigenvalue both for (41)-(44) and for the eigenvalue problem (41)-(43) together with

$$u_x(x_*, z) = 0.$$

(46)
In this case, neither $Q$ nor $H$ are well defined. As an example, we consider the special case where $\kappa$ is simply a step function of $x$ (and $\kappa$ is $z$ independent), say

$$
\kappa(x, z) = \begin{cases} 
\kappa_\infty & \text{for } x > L \\
\kappa_0 & \text{for } x < L.
\end{cases}
$$

For $\kappa_\infty = \pi$ and $\kappa_0 \approx 8.3458$, then $x_* \approx L - 0.9806$ is such a location. In fact, the Helmholtz equation has special solutions

$$
u_j(x, z) = v_j(x) \sin[(j - 0.5)\pi z] \quad \text{for } j = 1, 2, \ldots$$

which satisfy the conditions (2,3) and

$$v'_2(x_*) = v_3(x_*) = 0.$$

Therefore, neither $Q$ nor $H$ can be defined at $x_*$. For this problem, there are three propagating modes for $x < L$ and one propagating mode for $x > L$, the functions $v_2$ and $v_3$ decay exponentially as $x \to +\infty$.

It is possible to show, however, that if $Q$ is not well defined at $x = x_*$, then there is always a constant $a$ for which $J_a$ is well defined. It is our intent then to perform our numerical calculations by solving (10), (13) until our approximate to $Q$ blows up (or is not well defined) at some $x = x_*$, then to switch to solving (18), (21) for $H, W$ in a neighborhood of $x_*$ if $H$ is well defined at $x_*$, and if $H$ is also not well defined at $x_*$, switch to solving (28), (29) for $J_a$, $M_a$ in a neighborhood of $x_*$. Outside the neighborhood of points where our approximate to $Q$ blows up (or is not well defined), we will solve (10),(13) for $Q, Y$.

We emphasize that the operators $Q, H$ or $J_a$ are not well defined if any outgoing solution of the Helmholtz equation satisfies $u = 0$, $u_x = 0$ or $u_x - au = 0$, respectively, at $x = x_*$, for all $z \in (0,1)$. It is not necessary, in fact not possible, that the solution of our original problem (1), (2), (3) and either (4), (5) or (6) satisfy this property if it is unique in the whole waveguide and not identically zero.

We note also that solutions of the Helmholtz equation which do satisfy $u = 0$ at $x = x_*$ for all $z \in (0,1)$ decay exponentially for $x > L$. To see this, let $\phi_j$ be the normalized eigenfunction of $\partial_x^2 + \kappa_\infty^2(z)$ corresponding to the eigenvalue $\lambda_j$, namely

$$
\left[ \frac{d^2}{dz^2} + \kappa_\infty^2(z) \right] \phi_j(z) = \lambda_j \phi_j(z), \quad \int_{0}^{1} |\phi_j(z)|^2 dz = 1.
$$

The boundary conditions for $\phi_j$ are similar to (2), that is $\phi_j(0) = 0$, $\phi_j(z)(1) = 0$. If we expand $u(L, z)$ by

$$
u = \sum_{j=1}^{\infty} c_j \phi_j(z)
$$

and $u$ satisfies (1), (2), (3) and $u(x_*, z) = 0$ for all $z \in (0,1)$ then integrate $\nabla[u_{xx} + u_{zz} + \kappa^2 u]$ over the rectangle $\{(x, z) \mid x_* < x < L, 0 < z < 1\}$ to obtain

$$0 = \int_{x_*}^{L} \nabla[u_{xx} + u_{zz} + \kappa^2 u] \, dx \, dz = i \sum_{j=1}^{\infty} \sqrt{\lambda_j} |c_j|^2 + \int \left( \kappa^2 |u|^2 + |\nabla u|^2 \right) \, dx \, dz.$$
The coefficients corresponding to propagating modes \( (\lambda_j > 0) \) must vanish, since the imaginary part of the above equation must be zero. Hence

\[
u(x, z) = \sum_{\lambda_j > 0} c_j e^{-\sqrt{|\lambda_j|}(x-L)} \phi_j(z) \quad \text{for} \quad x > L.
\]

A similar argument can be made if \( u_x = 0 \) or \( u_x - au = 0 \) at \( x = x_* \) for all \( z \in (0,1) \) and real \( a \).

4 Coupled formulation based on DtN, NtD and \( R_a \) maps

The basic equations for finding the exact solution to the Helmholtz equation using the maps \( Q, Y \), the maps \( H, W \) or the maps \( J_a, M_a \) are given in section 2. Further the formulas to switch from \( Q, Y \) to either \( H, W \) or \( J_a, M_a \), or to switch back, are given by

\[
H = Q^{-1}, \quad J_a = (Q - aI)^{-1} \quad Q = H^{-1}, \quad J_a^{-1} + aI = Q
\]

together with (35) and (36).

Following the method developed in [14, 15], we discretize the range \( x \) from 0 to \( L \) by

\[
0 = x_0 < x_1 < x_2 < ... < x_m = L, \quad h_j = x_j - x_{j-1}, \quad x_{j-1/2} = \frac{x_{j-1} + x_j}{2},
\]

and approximate the square root operator \( \sqrt{\partial^2_z + \kappa^2(x, z)} \) by its midpoint value

\[
B_j = \sqrt{\partial^2_z + \kappa^2(x_{j-1/2}, z)} \quad \text{for} \quad x_{j-1} < x < x_j, \quad j = 1, 2, ..., m.
\]

Further requiring that \( u \) and \( u_x \) are continuous in the waveguide yields that \( Q, Y \) and their numerical approximates are continuous there. In addition, we use the connection with the Lyapunov operator equation, see [2], which when \( B \) is constant is

\[
P_x = -iBP - PiB. \tag{47}
\]

The importance of this equation is that, when \( B \) is constant and

\[
P(x_j) = P_j
\]

then the Lyapunov equation has the exact solution

\[
P(x) = e^{-i(x-x_j)B} P_j e^{-i(x-x_j)B}, \quad x_{j-1} < x < x_j. \tag{48}
\]

Further it is straightforward to show that in the same interval

\[
Q(x) = iBS
\]

where

\[
S = (I - P)(I + P)^{-1}
\]
is a solution of the operator Riccati equation for $Q$. Expressing $P$ in terms of $B$ and $Q$ we can write

$$P = (iB + Q)^{-1}(iB - Q).$$

Hence starting with

$$Q_m = i\sqrt{\partial_z^2 + \kappa_\infty^2(z)}, \quad Y_m = I$$

and letting $Q_j \approx Q(x_j)$, $Y_j \approx Y(x_j)$, $j = 0, 1, 2, ..., m$, we use the following formulas to calculate $Q_{j-1}$, $Y_{j-1}$ from $Q_j$, $Y_j$:

$$B_j = \sqrt{\partial_z^2 + \kappa^2(x_{j-1/2}, z)}$$

$$P_j = (iB_j + Q_j)^{-1}(iB_j - Q_j)$$

$$P_{j-1} = e^{ih_j B_j} P_j e^{ih_j B_j}$$

$$S_j = (I - P_{j-1})(I + P_{j-1})^{-1}$$

$$Q_{j-1} = iB_j S_j$$

$$Y_{j-1} = Y_j(I + P_j) e^{ih_j B_j} (I + P_{j-1})^{-1}.$$  

Note that our calculations are done so that $Q$ and $Y$ are continuous at $x = x_j$, but that in general $P_j \neq P_j$, $j = 1, 2, ..., m - 1$, since in the range dependent case usually $B_j \neq B_{j-1}$.

We remark that the advantage of the exact representation $Q = iBS = iB(I - P)(I + P)^{-1}$ with $P$ given by (48) is that if $\kappa^2(x, z)$ is independent of $x$ in a large interval $\hat{x} < x < \hat{x}$ then it is possible to take a \textquotedblleft large range step\textquotedblright in this interval utilizing the exact formula. It is straightforward to verify that the solution $P$ of the Lyapunov equation can also generate a solution of the operator Riccati equation for $H$ and $J_a$ using the relations

$$H = -i(I + P)(I - P)^{-1}B^{-1}$$

$$J_a = (I + P)([iB + aI] - (iB + aI)P)^{-1}. $$

Hence if approximates to the DtN map, $Q$, and $Y$ are calculated at $x = x_k$ as $Q_k$, $Y_k$, then we can switch to calculate with the NtD map, $H$ (if it is defined) and $W$ from $x_k$ back to $x_{k-1}$ by setting

$$H_k = Q_k^{-1}, \quad W_k = Y_k Q_k$$

and with $H_{j-1}$ and $W_{j-1}$ determined from $H_j$ and $W_j$ for $j = k, k-1, ..., k-l+1$ by the formulas

$$B_j = \sqrt{\partial_z^2 + \kappa^2(x_{j-1/2}, z)}$$

$$P_j = (iH_j B_j + I)\^{-1}(iH_j B_j - I)$$

$$P_{j-1} = e^{ih_j B_j} P_j e^{ih_j B_j}$$

$$S_j^{-1} = (I + P_{j-1})(I - P_{j-1})^{-1}$$

$$H_{j-1} = -iS_j^{-1} B_j^{-1}$$

$$W_{j-1} = W_j B_j(I - P_j) e^{ih_j B_j} (I + P_{j-1})^{-1}B_j^{-1}. $$
To switch back to $Q, Y$ at $x = x_{k-l}$, we use the formulas
\[ Q_{k-l} = H_{k-l}^{-1}, \quad Y_{k-l} = W_{k-l}H_{k-l}. \]

Likewise, if approximates to the DtN map, $Q$, and $Y$ are calculated at $x = x_k$ as $Q_k, Y_k$, then we can switch to calculate the RaT map, $J_a$ (if it is defined) and $M_a$ from $x_k$ back to $x_{k-l}$ by setting
\[ J_{a,k} = (Q_k - aI)^{-1}, \quad M_{a,k} = Y_k(Q_k - aI) \]
and with $J_{a,j-1}, M_{a,j-1}$ determined from $J_{a,j}, M_{a,j}$ for $j = k, k-1, ..., k-l+1$ by
\[
B_j = \sqrt{\partial_x^2 + \kappa^2(x_{j-1/2}, z)} \quad (62) \\
P_j = (iJ_{a,j}B_j + aJ_{a,j} + I)^{-1}(iJ_{a,j}B_j - aJ_{a,j} - I) \quad (63) \\
P_{j-1} = e^{ih_jB_j}P_je^{ih_jB_j} \quad (64) \\
J_{a,j-1} = (I + P_{j-1})[iB_j(I - P_{j-1}) - a(I + P_{j-1})]^{-1} \quad (65) \\
M_{a,j-1} = M_{a,j}[iB_j(I - P_j) - a(I + P_j)]e^{ih_jB_j}[iB_j(I - P_{j-1}) - a(I + P_{j-1})]^{-1}. \quad (66)
\]

To switch back to $Q, Y$ at $x = x_{k-l}$, we use the formulas
\[ Q_{k-l} = J_{a,k-l}^{-1} + aI, \quad Y_{k-l} = M_{a,k-l}J_{a,k-l}. \]

Because $P$ is the exact solution of the Lyapunov equation, all our formulas are exact for the range independent piece $(x_{j-1}, x_j)$, where $\kappa(x, z)$ is replaced by $\kappa(x_{j-1/2}, z)$. Notice that $P_j, P_{j-1}$ in the above three sets of formulas are the same, $S_j$ in DtN and NtD formulas is also the same. Further observe that $B_j$ is always defined and $B_j^{-1}$ is defined as long as all eigenvalues of the operator $\partial_x^2 + \kappa^2(x_{j-1/2}, z)$ are non-zero.

If the operator $\partial_x^2 + \kappa^2(x_{j-1/2}, z)$ (or $B_j$) has no zero eigenvalue, then the places where $Q_{j-1}$ (or $H_{j-1}$) are not defined coincide with the places where $S_j$ (or $S_j^{-1}$) is singular. On the other hand, when the operator $B_j$ has a zero eigenvalue, it is usually the case that both $Q_{j-1}$ and $H_{j-1}$ are still well defined, but $S_j$ is singular (caused by the zero eigenvalue of $B_j$) and $S_j^{-1}$ has a zero eigenvalue. However, it is also possible that $Q_{j-1}$ or/and $H_{j-1}$ are not well defined. Since the operators $S_j$ and $S_j^{-1}$ play pivotal rules in our step-wise matching formulas, we choose a switch strategy based on their singularity and the eigenvalue of $\partial_x^2 + \kappa^2(x_{j-1/2}, z)$ closest to zero.

To implement our method, we already have the eigenvalues of $\partial_x^2 + \kappa^2$, then we start with (49)-(55) and calculate $S_j$ and a function $\rho$ of $S_j$ or $S_j^{-1}$ (for example, some kind of norm) that can be used as a measure of whether or not $S_j$ or $S_j^{-1}$ are singular. Let $\lambda_s$ be the eigenvalue of $\partial_x^2 + \kappa^2(x_{j-1/2}, z)$ closest to 0. Selecting $E, F, \epsilon > 0$, we use the following criteria to determine when to switch operators:

1. If $\rho(S_j) \leq \min\{\rho(S_j^{-1}), E\}$, calculate using the DtN formulation;
2. If $\rho(S_j^{-1}) < \min\{\rho(S_j), E\}$ and $|\lambda_s| > \epsilon$, calculate using the NtD formulation;
3. If $\rho(S_j) > E$ and either $\rho(S_j^{-1}) > E$ or $|\lambda_\nu| \leq \epsilon$, then calculate the eigenvalues for

$$Q_{j-1}g = \nu g$$

Choosing $a$ so that the distance to any eigenvalue of $Q_{j-1}$ is greater than $F$, then calculate with the R$_{a,t}$D reformulation.

The function $\rho$ should increase when its argument operator is “more singular”. However, it is not desirable to choose a $\rho$ that takes too much time to compute. In the fully discretize version, when the operators are approximated by matrices, it is sufficient to use the Frobenius norm of the matrices for $\rho$. In practice, we choose $\rho$ as the matrix Frobenius norm (after the operators are approximated by matrices) and take $E = 3\rho(I)$ and $F = 1$.

Notice that we use the Frobenius norm for $S$ and $S_1$ instead of the Frobenius norm for $Q$ and $H$. The reason is that in our implementation, the Frobenius norm of $S$ and $S_1$ more clearly exhibits the $1/|x - x_*|$ blowup expected at the point $x_*$ where $Q$ or $H$ become singular. The Frobenius norm for $Q$ and $H$ are already so large for all values of $x$ that when the blowup of these same norms is seen, it is very narrowly supported and can be difficult to detect, which at least partially explains why we calculate the norms of $S$ and $S_1$ to detect when to make a switch. We exhibit the blowup of $Q$ and $H$ in Section 6.

We comment again that by choosing $S$ and $S_1$ to detect singularities, we do occasionally detect additional singularities produced because $B$ has a zero eigenvalue. In this case, the blowup of the Frobenius norm of $S$ exhibits $|x - x_*|^{-1/2}$ behavior.

5 Discretization

With the discretization of range $x$, the differential equations for the operators have been reduced to approximate iteration formulas in the last section. For actual numerical computation, the transverse variable $z$ must also be discretized. This leads to matrix approximations for the operators. The marching formulas obtained in the last section can be conveniently evaluated if an eigenvalue decomposition of the transverse operator $\partial_z^2 + \kappa^2(x_{j-1/2}, z)$ is calculated first. It also allows us to project the operators into the subspace spanned by a relatively small number of modes, giving rise to much smaller matrix representations of the operators.

Corresponding to the boundary conditions (2), we discretize the $z$ axis by $z_j = j\delta$, for $j = 1, 2, ..., N$ with $\delta = 1/(N + \frac{1}{2})$. The second derivative operator $\partial_z^2$ is then approximated by the following matrices $D_2$ and $D_4$, for second and fourth orders of accuracy, respectively:

$$D_2 = \frac{1}{\delta^2} \begin{bmatrix} -2 & 1 & \cdots & \cdots & 1 \\ 1 & \ddots & \ddots & \cdots & \ddots \\ \ddots & \ddots & -2 & 1 \\ \cdots & \cdots & \ddots & -2 & 1 \\ 1 & \cdots & \cdots & 1 & -1 \end{bmatrix}, \quad D_4 = 12 \begin{bmatrix} 10 & 1 & \cdots & \cdots & 1 \\ 1 & \ddots & \ddots & \cdots & \ddots \\ \ddots & \ddots & 10 & 1 \\ \cdots & \cdots & \ddots & 10 & 1 \\ 1 & \cdots & \cdots & 1 & 11 \end{bmatrix}^{-1} D_2.$$ 

Let $A_{j-1/2}$ be the $N \times N$ matrix corresponding to a fourth order approximation of $\partial_z^2 + \kappa^2(x_{j-1/2}, z)$.
\( \kappa^2(x_{j-1/2}, z) \), i.e.,

\[
A_{j-1/2} = D_4 + \begin{bmatrix} \kappa_1^2 & \kappa_2^2 & \cdots & \kappa_n^2 \\
\end{bmatrix},
\]

where \( \kappa_k = \kappa(x_{j-1/2}, z_k) \). The eigenvalue decomposition of \( A_{j-1/2} \) is essential for a simple implementation of the operator marching formulas. Let

\[
A_{j-1/2} = V_j \Lambda_j V_j^T,
\]

where \( V_j \) is the orthogonal matrix of the eigenvectors and \( \Lambda_j \) is the diagonal matrix of the eigenvalues. The formulas for the DtN formulation is now reduced to the following:

\[
\begin{align*}
\tilde{Q}_j &= V_j^T Q_j V_j, \\
\tilde{P}_j &= (i \sqrt{\Lambda_j} + \tilde{Q}_j)^{-1} (i \sqrt{\Lambda_j} - \tilde{Q}_j), \\
\tilde{P}_{j-1} &= e^{ih_j \sqrt{\Lambda_j}} \tilde{P}_j e^{ih_j \sqrt{\Lambda_j}}, \\
\tilde{S}_j &= (I - \tilde{P}_{j-1})(I + \tilde{P}_{j-1})^{-1}, \\
Q_{j-1} &= i V_j \sqrt{\Lambda_j} \tilde{S}_j V_j^T, \\
Y_{j-1} &= Y_j V_j (I + \tilde{P}_j) e^{ih_j \sqrt{\Lambda_j}} (I + \tilde{P}_{j-1})^{-1} V_j
\end{align*}
\]

Since \( \Lambda_j \) is a diagonal matrix, the matrices \( \sqrt{\Lambda} \) and \( e^{ih \sqrt{\Lambda}} \) are also diagonal matrices which can be easily calculated. The notation \( Q_j, Q_{j-1}, Y_j \) and \( Y_{j-1} \) are now used to represent \( N \times N \) matrices approximating \( Q \) and \( Y \) at \( x_j \) and \( x_{j-1} \), corresponding to the \( N \) discrete points of \( z \). However, the matrices \( \tilde{P}_j, \tilde{P}_{j-1}, \) and \( \tilde{S}_j \) are not the discrete version of \( P \) and \( S \), since a similarity transform with the matrix \( V_j \) has been removed.

Similarly, for the NtD formulation, the fully discretized marching formulas are

\[
\begin{align*}
\tilde{H}_j &= V_j^T H_j V_j, \\
\tilde{P}_j &= (i \tilde{H}_j \sqrt{\Lambda_j} + I)^{-1} (i \tilde{H}_j \sqrt{\Lambda_j} - I) \\
\tilde{P}_{j-1} &= e^{ih_j \sqrt{\Lambda_j}} \tilde{P}_j e^{ih_j \sqrt{\Lambda_j}}, \\
\tilde{S}_j^{-1} &= (I + \tilde{P}_{j-1})(I - \tilde{P}_{j-1})^{-1} \\
H_{j-1} &= -i V \tilde{S}_j^{-1} \sqrt{\Lambda_j}^{-1} V_j^T, \\
W_{j-1} &= W_j V_j \sqrt{\Lambda_j} (I - \tilde{P}_j) e^{ih \sqrt{\Lambda_j}} (I - \tilde{P}_{j-1})^{-1} \sqrt{\Lambda_j}^{-1} V_j^T,
\end{align*}
\]

and for the RnDtD formulation, the fully discretized marching formulas are

\[
\begin{align*}
\tilde{J}_{a,j} &= V_j^T J_{a,j} V_j \\
\tilde{B}_j &= \sqrt{\Lambda_j} \\
P_j &= (i \tilde{J}_{a,j} \sqrt{\Lambda_j} + a \tilde{J}_{a,j} + I)^{-1} (i \tilde{J}_{a,j} \sqrt{\Lambda_j} - a \tilde{J}_{a,j} - I) \\
\tilde{P}_{j-1} &= e^{ih_j \sqrt{\Lambda_j}} \tilde{P}_j e^{ih_j \sqrt{\Lambda_j}}
\end{align*}
\]
\[ J_{a,j-1} = V_j (I + \tilde{P}_j) \left[ i \sqrt{\Lambda_j (I - \tilde{P}_j)} - a (I + \tilde{P}_j) \right]^{-1} V_j^T \]
\[ M_{a,j-1} = M_j V_j \left[ i \sqrt{\Lambda_j (I - \tilde{P}_j) - a (I + \tilde{P}_j)} \right] e^{ih_j \sqrt{\Lambda_j}} \left[ i \sqrt{\Lambda_j (I - \tilde{P}_j - 1) - a (I + \tilde{P}_j - 1)} \right]^{-1}. \]

The above scheme approximates the operators by \( N \times N \) matrices and requires \( O(N^3) \) operations in each step. Significant speedup is possible if we project the operators into the subspace spanned by the eigenfunctions corresponding to the \( n \) largest eigenvalues of the transverse operator \( \partial_x^2 + \kappa^2 \), where \( n \) can be much smaller than \( N \). This corresponds to the coupled mode method \([17, 18, 3, 4, 1]\) where the solution of the Helmholtz equation is approximated by an expansion in terms of the \( n \) eigenfunctions. For the waveguides of interest, there are relatively few propagating modes (corresponding to the positive eigenvalues of \( \partial_x^2 + \kappa^2 \)), the coefficients of the evanescent modes are typically very small. Usually, the integer \( n \) can be taken as slightly larger than the number of propagating modes.

For the matrix \( A_{j-1/2} \) (approximating \( \partial_x^2 + \kappa^2(x_{j-1/2}, z) \)), only the \( n \) largest eigenvalues and the corresponding eigenvectors are needed. That is

\[ A_{j-1/2} V_j^n = V_j^n A_j^n \]

where \( A_j^n \) is the \( n \times n \) diagonal matrix of the eigenvalues, \( V_j^n \) is the \( N \times n \) matrix of the corresponding eigenvectors. In the step from \( x_j \) to \( x_{j-1} \), if the DtN formulation is used, our objective is to calculate the matrices \( \hat{Q}_{j-1} \) and \( \hat{Y}_{j-1} \), such that

\[ Q_{j-1} V_j^n \approx V_j^n \hat{Q}_{j-1}, \quad Y_{j-1} V_j^n \approx V_j^n \hat{Y}_{j-1}. \]

We realize that the input \( \hat{Q}_j \) and \( \hat{Y}_j \) are \( n \times n \) matrices related to the \( n \) eigenvectors of \( A_{j+1/2} \) (which approximates the operator \( \partial_x^2 + \kappa^2(x_{j+1/2}, z) \)) and that when we step from the interval \( (x_j, x_{j+1}) \) back to \( (x_{j-1}, x_j) \) it will be necessary to make the representation relative to the eigenvectors of \( A_{j-1/2} \). To do this, let \( V_{j+1}^n \) be the matrix of the \( n \) eigenvectors of \( A_{j+1/2} \). To relate \( V_{j+1}^n \) to \( V_j^n \), we introduce an \( n \times n \) matrix \( Z \), such that

\[ V_{j+1}^n \approx V_j^n Z. \]

This leads to \( Z = (V_j^n)^T V_{j+1}^n \). From \( Q_j V_{j+1}^n \approx V_{j+1}^n \hat{Q}_j \), we obtain \( Q_j V_j^n \approx V_j^n \hat{Q}_j \), with \( \hat{Q}_j = Z \hat{Q}_j Z^{-1} \). This gives us a representation of \( Q_j \) relative to the eigenvectors of \( A_{j-1/2} \). The remaining steps are similar as before. We have the following formulas for the DtN re-formulation

\[ Z = (V_j^n)^T V_{j+1}^n \]
\[ \hat{Q}_j = Z \hat{Q}_j Z^{-1}, \]
\[ \hat{P}_j = (i \sqrt{\Lambda_j} + \hat{Q}_j)^{-1} (i \sqrt{\Lambda_j - \hat{Q}_j}), \]
\[ \tilde{S}_j = (I - \tilde{P}_{j-1})(I + \tilde{P}_{j-1})^{-1}, \]
\[ \tilde{Q}_{j-1} = i \sqrt{\Lambda_j} \tilde{S}_j, \]
\[ \hat{Y}_{j-1} = Z \hat{Y}_j Z^{-1} (I + \hat{P}_j) e^{ih_j \sqrt{\Lambda_j}} (I + \hat{P}_{j-1})^{-1}. \]
For the NtD re-formulation, the formulas are as follows:

\[
Z = (V^n_j)^T V^n_{j+1} \\
\hat{H}_j = Z\hat{H}_j Z^{-1} \,, \\
\hat{P}_j = (i\hat{H}_j \sqrt{\Lambda^n_j} + I)^{-1} (i\hat{H}_j \sqrt{\Lambda^n_j} - I) \\
\hat{P}_{j-1} = e^{ih_j \sqrt{\Lambda^n_j}} \hat{P}_j e^{ih_j \sqrt{\Lambda^n_j}} \\
\hat{S}_j^{-1} = (I + \hat{P}_{j-1}) (I - \hat{P}_{j-1})^{-1} \\
\hat{H}_{j-1} = -i\hat{S}_j^{-1} \sqrt{\Lambda^n_j}^{-1} \\
\hat{W}_{j-1} = ZW_j Z^{-1} \sqrt{\Lambda^n_j} (I - \hat{P}_j) e^{ih_j \sqrt{\Lambda^n_j}} (I - \hat{P}_{j-1})^{-1} \sqrt{\Lambda^n_j}^{-1} .
\]

And for the RₜD formulation, the formulas utilizing the local eigenfunction expansion are:

\[
Z = (V^n_j)^T V^n_{j+1} \\
\hat{J}_{a,j} = Z\hat{J}_j Z^{-1} \,, \\
\hat{B}_j = \sqrt{\Lambda^n_j} \\
\hat{P}_j = (i\hat{J}_{a,j} \sqrt{\Lambda^n_j} + a\hat{J}_{a,j} + I)^{-1} (i\hat{J}_{a,j} \sqrt{\Lambda^n_j} - a\hat{J}_{a,j} - I) \\
\hat{P}_{j-1} = e^{ih_j \sqrt{\Lambda^n_j}} \hat{P}_j e^{ih_j \sqrt{\Lambda^n_j}} \\
\hat{J}_{a,j-1} = (I + \hat{P}_{j-1}) \left[ i\sqrt{\Lambda^n_j} (I - \hat{P}_{j-1}) - a(I + \hat{P}_{j-1}) \right]^{-1} \\
\hat{M}_{a,j-1} = Z \hat{M}_{a,j} Z^{-1} \left[ i\sqrt{\Lambda^n_j} (I - \hat{P}_j) - a(I + \hat{P}_j) \right] e^{ih_j \sqrt{\Lambda^n_j}} . \\
\cdot \left[ i\sqrt{\Lambda^n_j} (I - \hat{P}_{j-1}) - a(I + \hat{P}_{j-1}) \right]^{-1}
\]

The switch between the DtN, NtD and RₜD formulations is based on the matrices \( S \) and \( S^{-1} \). The Frobenius norm has been used to define the function \( \rho \) as in section 4. Notice that the switch criterion can also use other matrices, for example, \( (I + \hat{P}_{j-1})^{-1} \) and \( (I - \hat{P}_{j-1})^{-1} \).

6 Numerical examples

The numerical method described in this paper has been implemented and tested on a number of examples. The first example has the following formula for the wavenumber

\[
\kappa^2(x, z) = \kappa^2_\infty \left[ 1 - \epsilon \left( 1 - \tanh (\sigma (x/L - 0.5)) \sin^2(\pi z) \right) \right] .
\]

We take the following parameter values

\[
\kappa_\infty = \frac{50 \pi}{3}, \quad \sigma = 15, \quad \epsilon = -0.1, \quad L = 10
\]

and solve the Helmholtz equation for \( 0 < x < L \) and \( 0 < z < 1 \) with the boundary conditions (2) and the radiation condition (3). For this example, there are 17 propagating modes at \( x = L \) and 18 propagating modes at \( x = 0 \). We expect strong back-scattering for incident waves that has a large component in the 18-th mode. As shown in Figure 1(a), the DtN map has three
Figure 1: (a). Frobenius norm of a $50 \times 50$ matrix approximating the DtN map for the first example; (b). Frobenius norms of the $20 \times 20$ matrices $\hat{S}$ (solid) and $\hat{S}^{-1}$ (dotted).
singularities for \(0 < x < L\). The variable \(z\) is discretized with \(N = 50\) and the operator \(Q\) is approximated by a \(50 \times 50\) matrix in the full matrix approach. Frobenius norm of the matrix approximating \(Q\) is shown with the range \(x\). This graph is obtained with the step size \(h = 1/32\), thus a total of 320 range steps is involved. Note again that the Frobenius norm of \(Q\) is very large even when it is not singular. The result of this is that the singularities are narrowly supported and can be hard to detect.

In the truncated local eigenfunction expansion approach, we take \(n = 20\) for the number of retained modes. The Frobenius norms of \(\hat{S}\) and \(\hat{S}^{-1}\) are shown in Figure 1(b), since they are used to determine when to calculate with \(Q\), \(H\) or \(J_a\). Observe that the norm of \(\hat{S}\) (\(\hat{S}\) is a \(20 \times 20\) matrix) is significantly less than the norm of the approximate for \(Q\) and the singularities develop more gradually and are easier to detect. Since the DtN map blows up at three values of \(x\), we expect the NtD or Ra tD map to be used at least three times. When the NtD or Ra tD maps are used we explicitly calculate \((\hat{S}^{-1})^{-1}\) and its norm in order to determine when we switch back to the DtN formulation. The case \(h = 1/32\) gives rise to the following switches:

\[
\begin{array}{cccccccc}
 x & 9.8125 & 3.7188 & 3.1250 & 2.5625 & 2.0312 & 1.5000 & 0.9688 & 0.4375 \\
 switch & Q \to H & H \to Q & Q \to H & H \to Q & Q \to H & H \to Q & Q \to H & H \to Q \\
\end{array}
\]

Although \(Q\) has no singularity in the interval \((3.7188, 9.8125)\), the NtD map has been used there, since the norm of \(\hat{S}^{-1}\) is smaller than the norm of \(\hat{S}\) on that interval. Notice that the norm of \(\hat{S}\) has a local maximum near \(x = 4\) which corresponds to a zero eigenvalue of \(\partial_z^2 + \kappa^2\), not a singularity of \(Q\).

To complete the example we need to choose one of our three conditions at \(x = 0\). We use the boundary condition (5), that is, we assume there is an incident field at \(x = 0\). The incident wave is chosen to be exactly the 18-th local mode at \(x = 0\), that is, the 18-th eigenfunction of the operator \(\partial_z^2 + \kappa_0^2(z)\) subject to the boundary conditions \(\phi(0) = \phi_2(1) = 0\). Then expressing \(u\) at \(x = 0\) as the sum of the incident and reflected waves, \(u = u^{(i)} + u^{(r)}\), we solve

\[
\left[ Q(0) + i\sqrt{\partial_z^2 + \kappa_0^2(z)} \right] [u^{(i)} + u^{(r)}] = 2i\sqrt{\partial_z^2 + \kappa_0^2(z)} u^{(i)}
\]

for \(u^{(r)}\). Letting \(r_{18,18}^{(h)}\) be the coefficient of the 18-th mode in the local eigenfunction representation of \(u^{(r)}\), we consider \(r_{18,18}^{(h)}\), the coefficient that results from the computation based on the range step size \(h\) and obtain the result in Table 1. Using the reflection coefficient calculated with \(h = 1/256\) as the “exact” solution, we plot the “error” as a function of \(h\) in Figure 2. More precisely, we use logarithmic scales and plot \(\log_2 |r_{18,18}^{(h)} - r_{18,18}^{(1/256)}|\) against \(\log_2(1/h)\). It is clear from Figure 2 that our range discretization scheme has second order accuracy.

For the second example, we consider a Helmholtz waveguide with

\[
\kappa^2(x, z) = \kappa_0^2 \left[ 1 - \epsilon \sin \left( \frac{\pi x^2}{2L^2} \right) \sin^2 \left( \frac{\pi (1 - z)}{2} \right) \right]
\]

for \(0 < x < L\) and \(0 < z < 1\). Outside the interval \((0, L)\), the waveguide is range independent:

\[
\kappa^2(x, z) = \begin{cases} 
\kappa_0^2 & \text{for } x < 0, \\
\kappa_0^2 [1 - \epsilon \sin^2 (0.5\pi(1 - z))] & \text{for } x > L.
\end{cases}
\]

18
<table>
<thead>
<tr>
<th>$h$</th>
<th>$r_{18,18}^{(h)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.5385 + 0.7168 i</td>
</tr>
<tr>
<td>1/2</td>
<td>0.5910 + 0.6819 i</td>
</tr>
<tr>
<td>1/4</td>
<td>0.5070 + 0.7475 i</td>
</tr>
<tr>
<td>1/8</td>
<td>0.4802 + 0.7861 i</td>
</tr>
<tr>
<td>1/16</td>
<td>0.4740 + 0.7884 i</td>
</tr>
<tr>
<td>1/32</td>
<td>0.4724 + 0.7894 i</td>
</tr>
<tr>
<td>1/64</td>
<td>0.4720 + 0.7896 i</td>
</tr>
<tr>
<td>1/128</td>
<td>0.4719 + 0.7897 i</td>
</tr>
<tr>
<td>1/256</td>
<td>0.4718 + 0.7897 i</td>
</tr>
</tbody>
</table>

Table 1: Reflection coefficient $r_{18,18}$ calculated with different values of $h$.

Figure 2: Error in $r_{18,18}$ versus $h$ in logarithm scale. The horizontal axis is $\log_2(1/h)$, the vertical axis is $\log_2 |r_{18,18}^{(h)} - r_{18,18}^{(1/256)}|$. 
For this example, we demonstrate the accuracy obtained using the local eigenfunction expansion by comparing the calculation using the local eigenfunction expansion with the calculation using the full $N \times N$ matrix representation throughout the waveguide.

For $\kappa_0 = 5\pi$ and $\epsilon = 0.4$, the waveguide supports 5 propagating modes in the left ($x < 0$) and 4 propagating modes in the right ($x > L$). For $L = 15$, the DtN map has 21 singularities as shown in Figure 3, where the Frobenius norms of the $6 \times 6$ matrices $\hat{S}$ and $\hat{S}^{-1}$ are shown. This example is calculated with the switched DtN, NtD and RntD method using both the full matrix approximation and the truncated local eigenfunction expansion. We choose $N = 40$, where $N$ is the number of points used to discretize $z$. Since there are only 4 or 5 propagating modes, it is sufficient to take $n = 6$ in the local eigenfunction expansion calculation and it has led to a significant speedup in computing time. At $x = 0$, writing $u = u^{(i)} + u^{(r)}$ and $u^{(r)} = R(0)u^{(i)}$, where $R(0)$ is the reflection operator at $x = 0$ which maps the incident wave $u^{(i)}$ to the reflected wave $u^{(r)}$, we can use (16) to show that

$$R(0) = [i\sqrt{\partial_z^2 + \kappa_0^2(z)} + Q(0)]^{-1}[i\sqrt{\partial_z^2 + \kappa_0^2(z)} - Q(0)]$$

and then represent $R(0)$ using the local eigenfunction expansion with $n = 6$ or alternatively

---

Figure 3: Frobenius norms of the $6 \times 6$ matrix $\hat{S}$ (solid) and $\hat{S}^{-1}$ (dotted) for the second example.
using the full matrix approach for $N = 40$. We choose to compare the calculations of $R(0)$, since an accurate $R(0)$ is needed to obtain an accurate $u(0,z)$.

The first six diagonal elements of the reflection coefficient matrix $R(0)$ are nearly identical using both approaches. In Table 2, the left column lists the six diagonal elements of the reflection coefficient matrix obtained by the full matrix approach with $N = 40$ and $h = 1/64$. The right column lists the difference (in absolute value) between these coefficients and the ones calculated with $n = 6$ by the truncated eigenfunction expansion method (for the same $N$ and $h$). Notice that the full matrix approach corresponds to $n = N$. We observe that the 5th diagonal element is large indicating substantial backscattering and this is consistent with the fact that only 4 propagating modes are supported when $x > L$. However, we emphasize that for all the diagonal elements we have an acceptable relative accuracy with the truncated approach that retains 6 modes. While these terms are obtained with a fixed $h$, we also compare the results for different step sizes. In Figure 4, we compare the real and imaginary parts of the numerical solutions for a reflected wave calculated with $h = 1/2$ and $h = 1/128$. This is generated by choosing the fifth propagating mode in the local eigenfunction expansion at $x = 0$ as the incident wave. In other words, the incident wave is

$$u^{(i)} = \sin(4.5\pi z)e^{ix\sqrt{\kappa^2 - (4.5)^2}} = \sin(4.5\pi z)e^{i\sqrt{4.75}\pi x} \text{ for } x < 0.$$  

The slight difference between the numerical solutions can hardly be noticed.

Continuing with the second example, we utilize the operators $Y$, $W$ and $M_\alpha$, and also show the results of the calculation of the solution of the Helmholtz equation at $x = L$, where instead of the incident field we now choose a starting field at $x = 0$ which is

$$u_0(z) = \sum_{j=1}^{6} \frac{1}{j} \sin \left( 0.45 \left( j - \frac{1}{2} \right) \pi \right) \sin \left( \left( j - \frac{1}{2} \right) \pi z \right).$$  

(69)

The real and imaginary parts of $u(L,z)$ in this case are shown in Figure 5. The numerical solutions are obtained with $h = 1$ and $h = 1/64$, but the difference is quite small.

To compare with other methods, we note that the widely used Parabolic Equation methods are approximations to the one-way Helmholtz equation (7) which itself is only an approximation to the solution to the Riccati equation (it assumes that $Q_x = 0$) when $\kappa(x,z)$ depends on $x$. For
Figure 4: Comparison of numerical results for $\text{Re}\ u^{(r)}$ and $\text{Im}\ u^{(r)}$ at $x = 0$ calculated with $h = 1/2$ (the circles) and $h = 1/128$ (the solid lines) for the reflection of the 5th mode.

Figure 5: Real and imaginary parts of $u(L,z)$ calculated with $h = 1$ (the circles) and $h = 1/64$ (the solid lines), for example 2 and the boundary condition (69).
the above example, we compare the square root operator in Eq. (7) with the operator $Q$ in the exact one-way evolution equation (8) at $x = 0$. Expanded in the eigenfunctions of $\partial_z^2 + \kappa^2(0, z)$, the operator $iB(0) = i\sqrt{\partial_z^2 + \kappa^2(0, z)}$ is diagonal. The DtN operator $Q(0)$ is symmetric but not diagonal when it is expanded in the same eigenfunctions. However, the off-diagonal entries are small. The first 6 diagonal entries for $iB(0)$ and $Q(0)$ are listed in the following table:

<table>
<thead>
<tr>
<th>$iB(0)$</th>
<th>$Q(0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>15.6292i</td>
<td>0.0000 + 15.6292i</td>
</tr>
<tr>
<td>14.9844i</td>
<td>0.0000 + 14.9846i</td>
</tr>
<tr>
<td>13.6035i</td>
<td>0.0002 + 13.6034i</td>
</tr>
<tr>
<td>11.2179i</td>
<td>-0.0005 + 11.2175i</td>
</tr>
<tr>
<td>6.8478i</td>
<td>-2.9528 + 0.0000i</td>
</tr>
<tr>
<td>-7.1954</td>
<td>-7.1956 + 0.0000i</td>
</tr>
</tbody>
</table>

Table 3: First 6 diagonal entries for $iB(0)$ and $Q(0)$ expanded in the local eigenfunctions.

We point out that the main difference is in the fifth row corresponding to the fact that there is a propagating mode at $x = 0$ that becomes evanescent at $x = L$. Because of the reflection, this mode no longer propagates and it behaves like a standing wave reflecting the scattering within the waveguide. The off-diagonal entries in the eigenfunction representation of $Q(0)$ give an indication of the effect of scattering which results in the interaction between propagating and evanescent modes. The relatively large entries are close to the diagonal and we list some entries here:

<table>
<thead>
<tr>
<th>$(i, j)$</th>
<th>$(i, j)$ entry of $Q(0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1, 2)</td>
<td>1.5623E-5 + 1.5117E-5i</td>
</tr>
<tr>
<td>(2, 3)</td>
<td>-6.1938E-5 - 1.7540E-5i</td>
</tr>
<tr>
<td>(3, 4)</td>
<td>-1.1083E-5 + 1.3923E-4i</td>
</tr>
<tr>
<td>(4, 5)</td>
<td>9.1330E-4 + 2.0233E-3i</td>
</tr>
<tr>
<td>(5, 6)</td>
<td>-3.4433E-4 + 9.1050E-12i</td>
</tr>
</tbody>
</table>

Table 4: Some off-diagonal entries of $Q(0)$ expanded in local eigenfunctions.

For a third example, we consider the plane-parallel range-dependent waveguide benchmark problem addressed at the 112th and 113th meetings of the Acoustic Society of America [10, 20]. The wavenumber is given by

$$\kappa^2(x, z)/\kappa_\infty^2 = 1 + \sigma_1^2e^{-2\pi x} + \sigma_2^2e^{-4\pi x} - \sigma_1e^{-\pi x}(1 - \sigma_2e^{-2\pi x})\cos(\pi z)$$

$$-2\sigma_2e^{-2\pi x}\cos(2\pi z),$$

where $\kappa_\infty$, $\sigma_1$ and $\sigma_2$ are parameters. Corresponding to a waveguide with a depth of 500 meters, a sound source frequency of 25 Hz and a reference sound speed of 1500 meters per second, we
have $\kappa_\infty = 50\pi/3$. The other two parameters are chosen to be 
$$\sigma_1 = 0.032\pi, \quad \sigma_2 = 0.032\pi.$$ 

The waveguide has 17 propagating modes and an analytic solution was found by DeSanto[6]: 
$$u(x, z) = \sum_{j=1}^{\infty} a_j \sin[m_j \eta(x, z)]e^{i \sqrt{\kappa_\infty - m_j^2} \xi(x, z)}$$  \hspace{1cm} (70) 
where $m_j = (j-1/2)\pi$ and 
$$\xi(x, z) = x + \frac{\sigma_1}{\pi} e^{-\pi x} \cos(\pi z) + \frac{\sigma_2}{2\pi} e^{-2\pi x} \cos(2\pi z),$$ 
$$\eta(x, z) = z - \frac{\sigma_1}{\pi} e^{-\pi x} \sin(\pi z) - \frac{\sigma_2}{2\pi} e^{-2\pi x} \sin(2\pi z).$$ 

For comparison with our numerical solutions, we follow [16] and assume that only the first 17 coefficients in (70) are non-zero. These 17 coefficients are listed in the Appendix of [16]. The starting field $u(0, z)$ is then obtained from the analytic formula (70) and used in our numerical computation.

Since the given $\kappa^2$ has an exponential dependence on $x$, smaller step sizes are needed near $x = 0$. In the following calculation, we choose the step size to be negative powers of 2 only and be bounded by 1/4, with the further requirement that 
$$(e^{-\pi x_{j-1}} - e^{-\pi x_j})h^2 < 10^{-5}, \quad \text{for} \quad h = x_j - x_{j-1}.$$ 
For the range distance of $L = 10$, we have a total of $m = 116$ steps. In Table 3, we list the $L^2$, $L^1$ and $L^\infty$ relative errors at ten values of $x$ for $N = 180$, where $N$ is the number of points used in a 4th order finite difference approximation to the depth operator $\partial_z^2 + \kappa^2(x, z)$. The relative errors are defined as 
$$E_2 = \frac{||u - \tilde{u}||_2}{||u||_2}, \quad E_1 = \frac{||u - \tilde{u}||_1}{||u||_1}, \quad E_\infty = \frac{||u - \tilde{u}||_\infty}{||u||_\infty},$$ 
where $u$ and $\tilde{u}$ are the exact and numerical solutions, respectively, and the norms are defined for functions of $z$ on the interval $(0, 1)$. Clearly, four significant digits are obtained in this computation. This is consistent with our previously published result in [16] where the implementation of our calculation is different than in this paper. We remark that the published results for the Parabolic Equation (PE) method which uses 
$$u_x \approx i \sqrt{\partial_z^2 + \kappa^2(x, z)} \ u$$ 
have errors around 7%.

Note that in our first three examples, the R_{atD} formulation is only needed at those places where $\partial_z^2 + \kappa^2$ has a zero eigenvalue, since the minimum of $\rho(S)$ and $\rho(S^{-1})$ is always less than the bound $E$ which is set as $3\rho(I)$. In our fourth example we present a case where a switch to the R_{atD} formulation is needed because both $\rho(S)$ and $\rho(S^{-1})$ are both larger than $E$. We consider the problem with 
$$\kappa(x, z) = \begin{cases} 
\kappa_0, & x \leq 3, \\
\frac{1}{2}(\kappa_0 - \kappa_\infty) \cos[\frac{\pi}{2}(x - 3)] + \frac{1}{2}(\kappa_0 + \kappa_\infty), & 3 < x < 5, \\
\kappa_\infty, & x \geq 5.
\end{cases} \hspace{1cm} (71)$$
Table 5: Relative errors of the numerical solution for Example 3.

<table>
<thead>
<tr>
<th>x</th>
<th>$E_2(x)$</th>
<th>$E_1(x)$</th>
<th>$E_\infty(x)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>7.104E-4</td>
<td>7.049E-4</td>
<td>8.364E-4</td>
</tr>
<tr>
<td>2</td>
<td>4.588E-4</td>
<td>4.748E-4</td>
<td>4.105E-4</td>
</tr>
<tr>
<td>3</td>
<td>4.701E-4</td>
<td>4.699E-4</td>
<td>3.784E-4</td>
</tr>
<tr>
<td>4</td>
<td>4.777E-4</td>
<td>4.848E-4</td>
<td>4.534E-4</td>
</tr>
<tr>
<td>5</td>
<td>4.876E-4</td>
<td>4.685E-4</td>
<td>5.565E-4</td>
</tr>
<tr>
<td>6</td>
<td>5.000E-4</td>
<td>5.147E-4</td>
<td>6.126E-4</td>
</tr>
<tr>
<td>7</td>
<td>5.147E-4</td>
<td>5.587E-4</td>
<td>3.385E-4</td>
</tr>
<tr>
<td>8</td>
<td>5.315E-4</td>
<td>5.342E-4</td>
<td>6.126E-4</td>
</tr>
<tr>
<td>9</td>
<td>5.503E-4</td>
<td>5.155E-4</td>
<td>6.393E-4</td>
</tr>
<tr>
<td>10</td>
<td>5.708E-4</td>
<td>5.591E-4</td>
<td>6.199E-4</td>
</tr>
</tbody>
</table>

For a full matrix approximation with $N = 50$, the minimum of $\|S\|_F$ and $\|S^{-1}\|_F$ (the Frobenius norm) reaches 44.96 at $x = 0.8281$. Since this value is larger than our threshold $E = 3\|I\|_F = 3\sqrt{50} \approx 21.21$, the RαtD formulation will be used near $x = 0.8281$. For a calculation with the range step size $h = 5/640$ (for $L = 5$ and $m = 640$), the RαtD formulation is actually used for 2 steps at $x = 106h$ and $x = 107h$. Meanwhile, the operator $\partial_x^2 + \kappa^2$ has a zero eigenvalue near $x = 4.266$ and the RαtD formulation is also used there for one step. In Figure (6), we plot the Frobenius norms of $S$ and $S^{-1}$ calculated with our algorithm that automatically switches between the three formulations.

7 Connection with Invariant Imbedding

If we decompose the solution, $u$, of the Helmholtz equation into a right going wave $u^{(+)}$ and a left going wave $u^{(-)}$ with $u = u^{(+)} + u^{(-)}$ and assume

$$u_x = iB(x)u^{(+)} - iB(x)u^{(-)},$$

where $B(x) = \sqrt{\partial_x^2 + \kappa^2(x,z)}$, one can use scattering operators, see Fishman [7], to re-formulate the Helmholtz equation as a first order system for $u^{(+)}$ and $u^{(-)}$, which is

$$\frac{\partial}{\partial x} \begin{bmatrix} u^{(+)} \\ u^{(-)} \end{bmatrix} = \begin{bmatrix} iB(x) - \alpha(x) & \alpha(x) \\ \alpha(x) & -iB(x) - \alpha(x) \end{bmatrix} \begin{bmatrix} u^{(+)} \\ u^{(-)} \end{bmatrix},$$

where $\alpha(x) = B^{-1}(x)B'(x)/2$. If we define the reflection operator by

$$R(x)u^{(+)}(x,z) = u^{(-)}(x,z),$$

it can be established that $R$ satisfies the Riccati equation

$$\frac{dR}{dx} = \alpha(x) - [iB(x) + \alpha(x)] R - R [iB(x) - \alpha(x)] - R\alpha(x)R. \quad (71)$$
Figure 6: Frobenius norms of the $50 \times 50$ matrices $S$ (solid) and $S^{-1}$ (dotted) for example 3.

with $R(L) = 0$ and the right-going component $u^{(+)}$ of the wave field satisfies the evolution equation

$$u^{(+)}_x = [iB(x) - \alpha(x)(I - R(x))] u^{(+)}.$$  

If we define a transmission operator $T$ for $u^{(+)}$ by

$$T(x)u^{(+)}(x, z) = u^{(+)}(L, z),$$

then $T$ satisfies

$$\frac{dT}{dx} = -T[iB(x) - \alpha(x)(I - R(x))].$$  \hspace{1cm} (72)$$

with $T(L) = I$.

Note that the differential equation for $R$ when $\kappa^2$ is independent of $x$ is

$$\frac{dR}{dx} = -iBR - RiB$$

which is the same equation as the Lyapunov equation (47). Further even when $\kappa^2$ is dependent on $x$, we can establish the connection between $R$ and $Q$, $R$ and $H$, or $R$ and $J_a$ at $x = 0$ to be

$$R(0) = [iB(0) + Q(0)]^{-1}[iB(0) - Q(0)]$$

$$= -[I + iH(0)B(0)]^{-1}[I - iH(0)B(0)]$$

$$= [J_a(0)(iB(0) + aI) - I]^{-1}[J_a(0)(iB(0) - aI) - I],$$

where $B(0) = \sqrt{\partial^2_x + \kappa_0^2(z)}$. When the incident field, $u^{(i)} = u^{(+)}$, at $x = 0$ is given, then the backscattered field, $u^{(r)} = u^{(-)}$, can be determined by

$$u^{(r)} = [R(0)]^{-1}u^{(i)}$$
a relation that has already been utilized implicitly in Section 6. Finally, the relation between $T$ and $Q$, $Y$, $T$ and $H$, $W$, or $T$ and $J_a$, $M_a$ at $x = 0$ is

\[
T(0) = Y(0)[R(0) + I]^{-1} = W(0)H^{-1}(0)[R(0) + I]^{-1} = M_aJ_a^{-1}[R(0) + I]^{-1}
\]

where in each expression the appropriate formula for $R(0)$ (from above) is used.

8 Conclusions

In this paper, we have developed a numerical method for two dimensional plane parallel Helmholtz waveguides based on the DtN, NtD and R$_a$tD maps. One-way re-formulations of the Helmholtz equation in terms of these operators are useful for large scale range dependent wave propagation problems. The DtN re-formulation is natural and very simple, but the DtN map may encounter singularities in the waveguide. These singularities correspond to the non-uniqueness with a Dirichlet boundary condition given at these locations.

Standard numerical schemes that solve the Riccati equation of the DtN map may have difficulties at the singularities. The “large range step” method is more robust, since it can jump over a singularity that lies between two nearby grid points of $x$. This is so, because the exact solution is used in each panel, say from $x_j$ to $x_{j-1}$, to find the relationship between the operators at $x_j$ and $x_{j-1}$. Nevertheless, it is possible that a singularity is at a grid point, thus the DtN map is not even defined there. A numerical computation that involves a singularity which is is very close to a grid point can also lead to some loss of precision.

In this paper, we develop a method that switches to the NtD operator or R$_a$tD operator when the DtN map is close to singular. However, the NtD map or R$_a$tD alone can not solve the problem, since each of these operators can also have singularities. Our method is to switch between the three operators so that the singularities are avoided. In a separate paper, we will prove that it is always possible to choose $a$, so that at each $x$ at least one of the operators DtN, NtD or R$_a$tD is nonsingular.

Automatic switching between the three formulations is designed based on some associate operators used in the “large range step” method, which calculates the operators at $x_{j-1}$ from the operators at $x_j$ using the exact solution of the Helmholtz equation with $\kappa(x, z)$ approximated by $\kappa(x_{j-1/2}, z)$. This method utilizes the exact solution representation of the Lyapunov equation. The advantage of the large range step method is that when the range dependence is weak, the range step size can be large (compared with the typical wavelength). On the other hand, if a finite difference method is used for the range derivative, the step size is restricted by a fraction of the wavelength. Note that we can improve the accuracy by adapting the fourth order method for DtN formulation developed in [15] to NtD and R$_a$tD maps and implementing our switching technique. This we will do in Part II of this pair of papers.
References


