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A FOURTH ORDER DERIVATIVE-FREE OPERATOR MARCHING METHOD FOR HELMHOLTZ EQUATION IN WAVEGUIDES*

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Abstract

A fourth-order operator marching method for the Helmholtz equation in a waveguide is developed in this paper. It is derived from a new fourth-order exponential integrator for linear evolution equations. The method improves the second-order accuracy associated with the widely used step-wise coupled mode method where the waveguide is approximated by segments that are uniform in the propagation direction. The Helmholtz equation is solved using a one-way reformulation based on the Dirichlet-to-Neumann map. An alternative version closely related to the coupled mode method is also given. Numerical results clearly indicate that the method is more accurate than the coupled mode method while the required computing effort is nearly the same.

Mathematics subject classification: 65N99, 78A50.
Key words: Helmholtz equation, Waveguides, Dirichlet-to-Neumann map, Operator marching.

1. Introduction

For acoustic [1], microwave and optical waveguides [2], it is often necessary to solve the Helmholtz equation

$$u_{xx} + u_{zz} + \kappa^2(x, z)u = 0 \tag{1.1}$$

in a domain which has an extended length scale in one direction, say x. Here, x is the variable along the axis of the waveguide (*i.e.*, the main propagation direction), z is the transverse variable and the wavenumber κ varies with both x and z. Typically, the original waveguide is infinite in the x direction, but we assume that the x-dependent part of the waveguide is finite. That is, κ is x-independent when $x < 0$ and $x > L$ for some $L > 0$. For a given incident wave in $x < 0$, the problem is to calculate the reflected wave for $x < 0$ and the transmitted wave for $x > L$. This is a boundary value problem and the solution can be highly oscillatory if κ is large. Finite difference [3–5] and finite element [6–9] methods have been used to solve this problem. In particular, highly accurate solutions can be obtained by the adaptive finite element method [10, 11]. However, the problem is difficult to solve by a direct discretization of the Helmholtz equation when $L \gg 1$. The finite difference and finite element methods give rise to large linear systems that are difficult to solve, because the coefficient matrix is complex, non-Hermitian and indefinite.

Typically, we are interested in waveguides that change slowly in the propagation direction. That is, the variation of κ with x is small over the scale of a typical wavelength (*i.e.*, $1/\kappa$). In this case, approximate one-way models [1] which have a first-order derivative in x are widely

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used. These one-way models can be efficiently solved by marching forward in the x direction. However, for problems where the reflected waves are important and when the overall change of the waveguide (over a large propagation distance) is significant, it is still necessary to solve the Helmholtz equation. Standard discretization schemes of the Helmholtz equation require that a step size in the x-direction be smaller than a fraction of the typical wavelength. For slowly varying waveguides, it is possible to develop more efficient numerical methods [12] where the step size in x is only restricted by the variation of the waveguide in the x direction. In the step-wise coupled mode method [1, 2, 13], the waveguide is approximated by a sequence of x-invariant segments. For the segment from x_{j-1} to $x_j = x_{j-1} + h$, the wavenumber $\kappa(x, z)$ is approximated by $\kappa(x_{j-1/2}, z)$, where $x_{j-1/2} = x_j - h/2$, and the solution is expanded in the eigenfunctions of the operator $\partial_z^2 + \kappa^2(x_{j-1/2}, z)$. When κ has a weak dependence on x, the segment length h can be larger than a typical wavelength. Notice that this is a second-order method, so that the numerical solution should have an $\mathcal{O}(h^2)$ error. But the coefficient in the error term vanishes when the waveguide becomes x-independent.

The second-order methods developed in [14] is equivalent to the step-wise coupled mode method, but it uses a one-way reformulation of the Helmholtz equation in terms of the Dirichlet-to-Neumann map. The advantage of such a one-way operator marching scheme is that the required computer memory is independent of the total distance in the x direction, *i.e.* L. On the other hand, the required computer memory of the coupled mode method depends linearly on L. The two methods require nearly the same computing effort in terms of the floating point operations. The fourth-order method developed in [14] reduces the $\mathcal{O}(h^2)$ error of the coupled mode method to $\mathcal{O}(h^4)$ and it preserves the property that h can be larger than a typical wavelength when κ varies with x slowly. However, this method needs to evaluate the derivatives of κ. This can be very inconvenient, for example, when κ itself is calculated from a coordinate transform when the original waveguide has a more complicated geometry [15]. Based on a fourth-order Magnus method [16] for linear evolution equations, we derived another fourth-order operator marching method for the Helmholtz equation in [17]. The method does not require the derivative of κ, but it cannot be applied to the more general Helmholtz equation as in [15] due to the existence of a commutator in the fourth-order Magnus method [16].

In this paper, we develop a new derivative-free fourth-order operator marching method that can be applied to the more general case. It is based on a new fourth-order exponential integrator for linear evolution equations. This exponential integrator may be useful in other applications and its fourth-order of accuracy is proved in this paper. While there are many high order numerical methods for linear evolution equations, only a few methods can be used to derive efficient operator marching schemes for the Helmholtz equation. The new fourth-order operator marching method is given using a one-way reformulation based on the Dirichlet-to-Neumann map, but we also present a version of this method which is similar to the standard step-wise coupled mode method [1, 2, 13]. Although the fourth-order methods in [14, 17] also have variants similar to the widely used coupled mode methods, this connection has not been revealed before. Numerical examples are used to illustrate the fourth-order accuracy of the proposed method.

2. One-way Re-formulations

The waveguide is assumed to be x-invariant for $x < 0$ and $x > L$; thus, we let

$$\kappa = \kappa_0(z) \quad \text{for} \quad x < 0, \quad \kappa = \kappa_\infty(z) \quad \text{for} \quad x > L.$$

For simplicity, we assume that the domain is bounded between $z = 0$ and $z = 1$ and u satisfies some simple homogeneous boundary conditions, such as

$$u(x, 0) = u_z(x, 1) = 0. \tag{2.1}$$

For $x < 0$, the transverse operator has eigenvalues λ_k and eigenfunctions ϕ_k (for $k = 1, 2, \cdots$) satisfying

$$\left[\frac{d^2}{dz^2} + \kappa_0^2(z)\right] \phi_k(z) = \lambda_k \phi_k(z), \quad \phi_k(0) = \phi_k'(1) = 0.$$

The wave field in the region $x < 0$ can be written as $u = u^+ + u^-$, where

$$u^+ = \sum_{k=1}^{\infty} a_k \phi_k(z) e^{i\sqrt{\lambda_k}x}, \quad u^- = \sum_{k=1}^{\infty} b_k \phi_k(z) e^{-i\sqrt{\lambda_k}x},$$

for some coefficients $\{a_k, b_k\}$. Here, u^+ and u^- represent wave field components that propagate in the increasing and decreasing x directions, respectively. If we define the square root operator $B_0 = \sqrt{\partial_z^2 + \kappa_0^2(z)}$ as a linear operator satisfying

$$B_0\, \phi_k = \sqrt{\lambda_k}\, \phi_k, \quad k = 1, 2, 3, \cdots,$$

then

$$u_x^+ = iB_0 u^+, \quad u_x^- = -iB_0 u^-.$$

Typically, we assume that u^+ (the incident wave) is given in $x < 0$. Then u^- is the reflected wave to be determined. This gives rise to

$$u_x + iB_0 u = 2iB_0 u^+, \quad x < 0. \tag{2.2}$$

Similarly, we can define the square root operator $B_\infty = \sqrt{\partial_z^2 + \kappa_\infty^2(z)}$ for $x > L$ and decompose the wave field as $u = u^+ + u^-$. We allow only waves propagating towards $x = +\infty$ in the region $x > L$, *i.e.*, $u^- = 0$, then $u = u^+$ satisfies

$$u_x = iB_\infty u, \quad x > L. \tag{2.3}$$

Various numerical methods have been developed to solve the boundary value problem (1.1)-(2.3). When L is extremely large, it is advantageous to use a one-way reformulation, so that the problem can be solved within a computer memory that is independent of L. Fishman [18] proposed a one-way reformulation based on the scattering operators, but the approach based on the Dirichlet-to-Neumann (DtN) map [19] is simpler. Define the DtN map Q and the fundamental solution operator Y (at a fixed x) by

$$Q(x)u(x, z) = u_x(x, z), \quad Y(x)u(x, z) = u(L, z), \tag{2.4}$$

where u is an arbitrary solution of the Helmholtz equation (1.1) satisfying the boundary conditions (2.1) and (2.3). The operators Q and Y act on functions of z, and they satisfy the following differential equations [19]:

$$\frac{dQ}{dx} = -Q^2 - [\partial_z^2 + \kappa^2(x, z)], \tag{2.5}$$

$$\frac{dY}{dx} = -YQ(x), \tag{2.6}$$

and the following "initial" conditions:

$$Q(L) = iB_\infty, \quad Y(L) = I,$$

where I is the identity operator. The above condition on $Q(L)$ is obtained from (2.3). This is an initial value for the two operators Q and Y, it can be solved from $x = L$ to $x = 0$. Once $Q(0)$ and $Y(0)$ are calculated, we can find the reflected and transmitted waves. From (2.2), $u(0, z)$ satisfies

$$[Q(0) + iB_0]u(0, z) = 2iB_0u^+(0-, z).$$

Thus, $u^-(0-, z) = u(0, z) - u^+(0-, z)$ is the reflected wave at $x = 0-$. The transmitted wave can be simply obtained from

$$u(L, z) = Y(L)u(0, z).$$

To solve equations (2.5) and (2.6), the operators Q and Y must be approximated by matrices. If the transverse variable z is discretized by N points, the operators are reduced to $N \times N$ matrices. This can be rather expensive, since N maybe quite large. A more efficient approach [19] is to represent the operators in a local eigenfunction expansion. For a waveguide with a relatively small number of propagating modes, the operators can be approximated by $n \times n$ matrices, where n is an integer that is slightly larger than the number of propagating modes. Typically, n is much smaller than N.

With a proper matrix representation of the operators, equations (2.5) and (2.6) can be solved by standard ODE solvers. However, these methods do not take advantage of the fact that the waveguide is slowly varying in x. The step size would be restricted even if the waveguide happens to be x-invariant. Our methods (developed in [14] and in the next section) overcome this restriction and they allow large step sizes in x for slowly varying waveguides.

3. Discretization Schemes

The Helmholtz equation (1.1) can be written as a first-order system

$$\frac{\partial \vec{y}}{\partial x} = A(x)\vec{y}, \tag{3.1}$$

where

$$\vec{y} = \begin{bmatrix} u \\ u_x \end{bmatrix}, \quad A(x) = \begin{bmatrix} 0 & I \\ -\partial_z^2 - \kappa^2(x, z) & 0 \end{bmatrix}. \tag{3.2}$$

For (3.1), we have the following second-order midpoint exponential method

$$\vec{y}_j = e^{hA_{j-1/2}}\ \vec{y}_{j-1}, \tag{3.3}$$

where $\vec{y}_j \approx \vec{y}(x_j)$, $\vec{y}_{j-1} \approx \vec{y}(x_{j-1})$, $A_{j-1/2} = A(x_{j-1/2})$ for $x_{j-1} = x_j - h$ and $x_{j-1/2} = x_j - h/2$. Since $\kappa_{j-1/2}(z) = \kappa(x_{j-1/2}, z)$ is used to approximate $\kappa(x, z)$, it is equivalent to replacing the Helmholtz equation by

$$u_{xx} + u_{zz} + \kappa^2_{j-1/2}(z)u = 0 \quad \text{for} \quad x_{j-1} < x < x_j.$$

The second-order method developed in [14] is based on (3.3). A fourth-order generalization of (3.3) was developed in [20] and it gives rise to the fourth-order operator marching method for the Helmholtz equation in [14]. However, this fourth-order Helmholtz solver requires the

derivatives of κ. This is not convenient, since the derivatives of κ are often not available. In the following, we derive a derivative-free fourth-order operator marching method for the Helmholtz equation based on the following new fourth-order exponential method:

$$\vec{y}_j = e^{\frac{h}{12}(A_j - A_{j-1})} e^{\frac{h}{6}(A_{j-1} + 4A_{j-1/2} + A_j)} e^{\frac{h}{12}(A_{j-1} - A_j)} \vec{y}_{j-1}. \tag{3.4}$$

The local truncation error of the above method is derived in the Appendix.

For the Helmholtz equation given in (3.1), the exponential method (3.4) gives rise to

$$\begin{bmatrix} u_j \\ Q_j u_j \end{bmatrix} = \exp\left(\begin{bmatrix} 0 & 0 \\ -s_{j-1/2} & 0 \end{bmatrix}\right) \exp\left(h \begin{bmatrix} 0 & I \\ -\partial_z^2 - \gamma_{j-1/2} & 0 \end{bmatrix}\right) \exp\left(\begin{bmatrix} 0 & 0 \\ s_{j-1/2} & 0 \end{bmatrix}\right) \begin{bmatrix} u_{j-1} \\ Q_{j-1} u_{j-1} \end{bmatrix},$$

where $s_{j-1/2}$ and $\gamma_{j-1/2}$ are the following functions of z:

$$s_{j-1/2} = \frac{h}{12}(\kappa_j^2 - \kappa_{j-1}^2), \quad \gamma_{j-1/2} = \frac{1}{6}(\kappa_{j-1}^2 + 4\kappa_{j-1/2}^2 + \kappa_j^2). \tag{3.5}$$

The first and the third exponentials are easy to evaluate. We have

$$\exp\left(\begin{bmatrix} 0 & 0 \\ -s_{j-1/2} & 0 \end{bmatrix}\right) = \begin{bmatrix} I & 0 \\ -s_{j-1/2} & I \end{bmatrix} = \begin{bmatrix} I & 0 \\ s_{j-1/2} & I \end{bmatrix}^{-1}.$$

Therefore,

$$\begin{bmatrix} u_j \\ (Q_j + s_{j-1/2}) u_j \end{bmatrix} = \exp\left(h \begin{bmatrix} 0 & I \\ -\partial_z^2 - \gamma_{j-1/2} & 0 \end{bmatrix}\right) \begin{bmatrix} u_{j-1} \\ (Q_{j-1} + s_{j-1/2}) u_{j-1} \end{bmatrix}.$$

Similar to the derivation in [14], we end up with the following set of formulas:

$$B = \sqrt{\partial_z^2 + \gamma_{j-1/2}}, \tag{3.6}$$

$$R = (iB + Q_j + s_{j-1/2})^{-1}(iB - Q_j - s_{j-1/2}), \tag{3.7}$$

$$P = e^{ihB} R e^{ihB}, \tag{3.8}$$

$$Q_{j-1} = iB(I - P)(I + P)^{-1} - s_{j-1/2}, \tag{3.9}$$

$$Y_{j-1} = Y_j (I + R) e^{ihB} (I + P)^{-1}. \tag{3.10}$$

This gives rise to a set of relationships between (Q_j, Y_j) and (Q_{j-1}, Y_{j-1}), leading to a fourth-order method for solving (2.5) and (2.6). This method reproduces the exact relationships between these operators if κ is x-independent in the interval. When κ varies with x slowly, the step size h can often be much larger than the typical wavelength.

To use the above algorithm, we represent the operators Q_{j-1} and Y_{j-1} by $n \times n$ matrices resulting from a truncated expansion in the eigenfunctions of the transverse operator $\partial_z^2 + \gamma_{j-1/2}(z)$. The details are similar to the fourth-order method developed in [14].

The method can be generalized to the following more general Helmholtz equation:

$$u_{xx} + \alpha(x, z) u_{zz} + \beta(x, z) u_z + \kappa^2(x, z) u = 0. \tag{3.11}$$

Such an equation is obtained when the original Helmholtz equation (1.1) is considered in a waveguide with a curved boundary which is flattened by a local orthogonal transform [15]. For

Eq. (3.11), the linear evolution equation (3.1) now involves an operator A defined as in (3.2) with ∂_z^2 replaced by $\alpha\partial_z^2 + \beta\partial_z$. With the following modifications

$$B = \frac{1}{\sqrt{6}}\left[(\alpha_{j-1} + 4\alpha_{j-1/2} + \alpha_j)\partial_z^2 + (\beta_{j-1} + 4\beta_{j-1/2} + \beta_j)\partial_z + \kappa_{j-1}^2 + 4\kappa_{j-1/2}^2 + \kappa_j^2\right]^{1/2},$$
$$s_{j-1/2} = \frac{1}{12}\left[(\alpha_j - \alpha_{j-1})\partial_z^2 + (\beta_j - \beta_{j-1})\partial_z + \kappa_j^2 - \kappa_{j-1}^2\right],$$

the main steps of the method (3.7)-(3.10) remain valid. On the other hand, it is difficult to generalize the Magnus method [17] to Eq. (3.11), since it involves the commutator $A(\xi_1)A(\xi_2) - A(\xi_2)A(\xi_1)$, where ξ_1 and ξ_2 are two different values in (x_{j-1}, x_j).

4. Relating to the Coupled Mode Method

A widely used version of the coupled mode method [13] starts from a discretization of the waveguide,

$$0 = x_0 < x_1 < x_2 < \cdots < x_m = L$$

and replaces the wavenumber $\kappa(x, z)$ in each interval by an x-independent function of z, that is

$$\kappa(x, z) \approx \kappa(x_{j-1/2}, z) = \kappa_{j-1/2}(z), \qquad x_{j-1} < x < x_j. \tag{4.1}$$

The solution is then expanded in the local eigenfunctions of the transverse operator $\partial_z^2 + \kappa_{j-1/2}^2(z)$ and the coefficients are solved from a large linear system of equations. Because of the midpoint approximation (4.1), the method has a second-order of accuracy. In this section, we describe how the coupled mode method can be modified to achieve a fourth-order of accuracy.

In the section $x_{j-1} < x < x_j$, the eigenvalue problem is

$$\left[\frac{d^2}{dz^2} + \kappa_{j-1/2}^2(z)\right]\phi_k^{(j)}(z) = \lambda_k^{(j)}\phi_k^{(j)}(z), \quad 0 < z < 1, \tag{4.2}$$

$$\phi_k^{(j)}(0) = \frac{d\phi_k^{(j)}}{dz}(1) = 0. \tag{4.3}$$

Assuming that the eigenfunctions are normalized as

$$\int_0^1 \phi_k^{(j)}\phi_s^{(j)}dz = \begin{cases} 1 & \text{if } k = s, \\ 0 & \text{if } k \neq s, \end{cases}$$

we may write down the solution in this section as

$$u(x, z) = \sum_{k=1}^{\infty}\left[a_k^{(j)}e^{i\beta_k^{(j)}(x - x_{j-1})} + b_k^{(j)}e^{-i\beta_k^{(j)}(x - x_j)}\right]\phi_k^{(j)}(z), \tag{4.4}$$

where $\beta_k^{(j)} = \sqrt{\lambda_k^{(j)}}$. To simplify the notation, we introduce the quantity

$$p_k^{(j)} = e^{i\beta_k^{(j)}(x_j - x_{j-1})}.$$

For $x < 0$, we let $\kappa_{-1/2}(z) = \kappa(0-, z)$ and define eigenfunctions (for $j = 0$) as before. Then expand the solution as

$$u(x, z) = \sum_{k=1}^{\infty}\left[a_k^{(0)}e^{i\beta_k^{(0)}x} + b_k^{(0)}e^{-i\beta_k^{(0)}x}\right]\phi_k^{(0)}(z),$$

where $a_k^{(0)}$ is a coefficient of the given incident wave in $x < 0$, $b_k^{(0)}$ is a reflection coefficient. The above can be consistent with (4.4), if we let $x_{-1} = 0$. In this case, $p_k^{(0)} = 1$. Similarly for $x > L$, we let $\kappa_{m+1/2}(z) = \kappa(L+, z)$, define the eigenfunctions for $j = m + 1$ as in (4.2) and expand the solution as

$$u(x,z) = \sum_{k=1}^{\infty} \left[a_k^{(m+1)} e^{i\beta_k^{(m+1)}(x-L)} + b_k^{(m+1)} e^{-i\beta_k^{(m+1)}(x-L)} \right] \phi_k^{(m+1)}(z).$$

The coefficient $a_k^{(m+1)}$ is a transmission coefficient and $b_k^{(m+1)} = 0$ because only outgoing waves are allowed for $x > L$. The above can be consistent with (4.4), if we let $x_{m+1} = L$. Thus, $p_k^{(m+1)} = 1$.

At x_j $(j = 0, 1, \cdots, m)$, u and u_x are continuous. This gives rise to

$$p_k^{(j)} a_k^{(j)} + b_k^{(j)} = \sum_{s=1}^{\infty} v_{ks}^{(j)} \left[a_s^{(j+1)} + p_s^{(j+1)} b_s^{(j+1)} \right], \tag{4.5}$$

$$\beta_k^{(j)} \left[p_k^{(j)} a_k^{(j)} - b_k^{(j)} \right] = \sum_{s=1}^{\infty} v_{ks}^{(j)} \beta_s^{(j+1)} \left[a_s^{(j+1)} - p_s^{(j+1)} b_s^{(j+1)} \right], \tag{4.6}$$

for $k = 1, 2, 3, \cdots$, where

$$v_{ks}^{(j)} = \int_0^1 \phi_k^{(j)} \phi_s^{(j+1)} dz.$$

In practice, we can truncate the expansion (4.4) to n terms and solve the coefficients (for $k = 1, 2, \cdots, n$) from the above system.

Our fourth-order method starts with a slightly different eigenvalue problem in each segment. Eq. (4.2) is replaced by

$$\left[\frac{d^2}{dz^2} + \gamma_{j-1/2}(z) \right] \phi_k^{(j)}(z) = \lambda_k^{(j)} \phi_k^{(j)}(z), \quad 0 < z < 1, \tag{4.7}$$

where

$$\gamma_{j-1/2}(z) = \frac{1}{6} \left(\kappa_{j-1}^2(z) + 4\kappa_{j-1/2}^2(z) + \kappa_j^2(z) \right).$$

The expansion (4.4) can still be used if we use the new $\phi_k^{(j)}$ and $\beta_k^{(j)}$. At x_j, we have the continuity of u and (4.5) is still valid. However, the continuity of u_x should be interpreted as

$$\left[u_x - s_{j-1/2} u \right]_{x=x_j-} = \left[u_x - s_{j+1/2} u \right]_{x=x_j+}, \tag{4.8}$$

where

$$s_{j-1/2} = \frac{h}{12}(\kappa_j^2 - \kappa_{j-1}^2), \quad s_{j+1/2} = \frac{h}{12}(\kappa_{j+1}^2 - \kappa_j^2).$$

This gives rise to

$$\begin{aligned} \beta_k^{(j)} \left[p_k^{(j)} a_k^{(j)} - b_k^{(j)} \right] = & \sum_{s=1}^{\infty} v_{ks}^{(j)} \beta_s^{(j+1)} \left[a_s^{(j+1)} - p_s^{(j+1)} b_s^{(j+1)} \right] \\ & + i \sum_{s=1}^{\infty} w_{ks}^{(j)} \left[a_s^{(j+1)} + p_s^{(j+1)} b_s^{(j+1)} \right], \end{aligned} \tag{4.9}$$

where

$$w_{ks}^{(j)} = \int_0^1 \delta_j(z) \phi_k^{(j)} \phi_s^{(j+1)} dz, \quad \delta_j(z) = s_{j+1/2} - s_{j-1/2} = \frac{h}{12}(\kappa_{j+1}^2 - \kappa_{j-1}^2).$$

The coefficients $a_k^{(j)}$ and $b_k^{(j)}$ are then solved from (4.5) and (4.9).

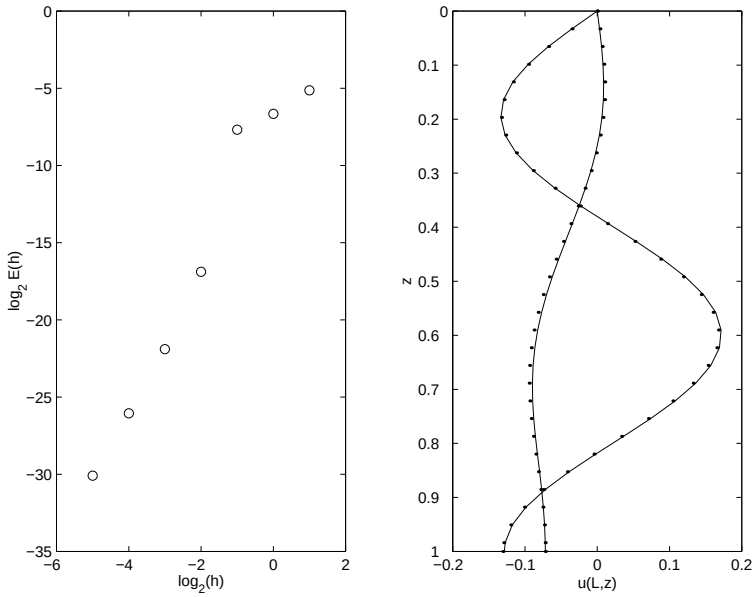

Fig. 5.1. (a). Relative errors of $u(L,z)$ for various values of h; (b). Comparison of $u(L,z)$ for $h=2$ and $h=1/128$.

5. Numerical Examples

As an example, we consider a waveguide where

$$\kappa^2(x,z) = 100\left[1+0.05e^{-20(x/L-0.5)^2}\sin^2(\pi z)\right].$$

We take $L=10$ and discretize z by $N=30$ points, namely, $z_j = j/(N+0.5)$ for $j=1,2,\cdots,N$. A fourth-order finite difference scheme is used to approximate the operator ∂_z^2. In the first case, we calculate the solution at $x=L$ based on the following Dirichlet boundary condition at $x=0$

$$u(0,z) = \sum_{j=1}^{7} \sin(m_j z_0)\sin(m_j z)/\sqrt{\kappa_0^2 - m_j^2} \quad \text{for} \quad m_j = (j-1/2)\pi, \quad z_0 = 0.65.$$

Various values of the step size h (for discretizing x) are used and the numerical solutions are compared with the "exact" solution to find the relative error (denoted by $E(h)$) in the L^2 norm. The relative errors for $h = 2, 1, 1/2, 1/4, \cdots, 1/32$ are shown in Fig. 5.1(a), using a logarithmic scale. It gives a clear indication that the method is indeed fourth-order. The large stepping capacity is also quite clear. In fact, as it is illustrated in Fig. 5.1(b), the result obtained with $h=2$ is already quite accurate.

In the second case, we calculate the back-scattered wave generated by the following incident wave

$$u^{(i)}(0,z) = \sin(2.5\pi z).$$

This corresponds to the third propagating mode in the waveguide (away from the distortion near $x = L/2$). Since the waveguide has a very gradual variation in the x direction, the back-scattered wave is quite weak. However, we are able to obtain a fairly accurate solution with $h=1/8$. In Fig. 5.2, the numerical solution obtained with $h=1/8$ is compared with a much more accurate solution calculated with $h=1/256$. Notice that the magnitude is only

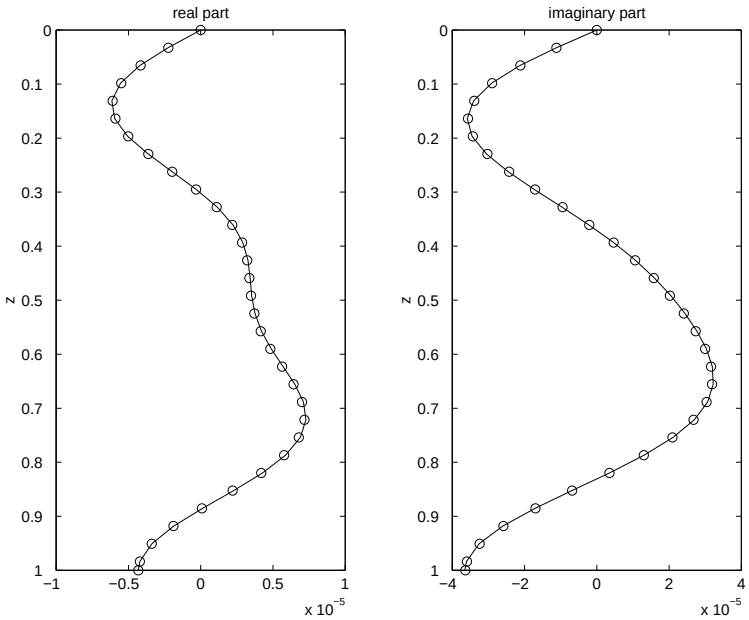

Fig. 5.2. A comparison of the back-scattered waves calculated with step size $h = 1/8$ (small circles) and $h = 1/128$ (solid line).

around 10^{-5}. Using the numerical solution obtained with $h = 1/256$ as the "exact" solution, we compute the relative errors for a few values of h. The results are listed in the following table:

h	$1/8$	$1/16$	$1/32$	$1/64$
$E(h)$	2.01×10^{-2}	1.11×10^{-3}	6.75×10^{-5}	4.19×10^{-6}

6. Conclusions

A numerical method is developed for the Helmholtz equation in a slowly varying waveguide. In the propagation direction x, the method has a fourth-order of accuracy and it also preserves exact solutions when the waveguide is x-independent. In general, the step size in x is not restricted by the wavelength of the field and it can be large, when the x-dependence is weak. The method is derived from the fourth-order derivative-free exponential method (3.4) for linear evolution equations. In our implementation, a one-way re-formulation of the Helmholtz equation in terms of the Dirichlet-to-Neumann map is used. This gives rise to a fourth-order operator marching method that does not require the derivatives of κ. We also present our method as a simple modification of the standard step-wise coupled mode method [13]. Numerical examples are used to demonstrate the fourth-order accuracy when the step size in x is reduced and also the good accuracy obtained with larger step sizes in x when the dependence on x is weak.

Appendix

For the linear system of ordinary differential equations

$$y' = A(t)y, \tag{6.1}$$

the solution is highly oscillatory if the matrix A has an eigenvalue with a large imaginary part. Exponential methods have the advantage that a larger step size h is possible when A varies with t slowly. For a step from t_j to $t_{j+1} = t_j + h$, we show that the method

$$y_{j+1} = e^{\frac{h}{12}[A_{j+1}-A_j]} e^{h[A_j+4A_{j+1/2}+A_{j+1}]/6} e^{\frac{h}{12}[A_j-A_{j+1}]}\, y_j, \tag{6.2}$$

has a fourth-order accuracy, where A_j, $A_{j+1/2}$ and A_{j+1} denote the matrix A evaluated at t_j, $t_{j+1/2}$ and t_{j+1}, respectively.

To find the local truncation error, we let $y(t_{j+1})$ be the exact solution of (6.1) starting with the initial condition $y(t_j) = y_j$. Based on the Taylor expansions of $y(t_j)$ and $y(t_{j+1})$ around $t_{j+1/2}$, we obtain [20]:

$$y(t_{j+1}) = \left(I + hC_1 + h^2C_2 + h^3C_3 + h^4C_4 + h^5C_5 + \cdots\right) y_j,$$

where

$$\begin{aligned}
C_1 &= A,\\
C_2 &= \frac{A^2}{2},\\
C_3 &= \frac{A^3}{6} + \frac{A'' + 2A'A - 2AA'}{24},\\
C_4 &= \frac{A^4}{24} + \frac{1}{48}\left(A''A + AA'' + 2A'A^2 - 2A^2A'\right),\\
C_5 &= \frac{1}{1920}\Big[A^{(4)} + 4(A'''A - AA''' + A'A'' - A''A')\\
&\quad +8(2A''A^2 + AA''A + 2A^2A'' + A'^2A + AA'^2 - 2A'AA')\\
&\quad +24(A'A^3 - A^3A') + 8A(A'A - AA')A + 16A^5\Big],
\end{aligned}$$

where A and its derivatives are all evaluated at the midpoint $t_{j+1/2}$. On the other hand, for y_{j+1} given in (6.2), we have

$$y_{j+1} = \left(I + hC_1 + h^2C_2 + h^3C_3 + h^4C_4 + h^5\hat{C}_5 + \cdots\right) y_j,$$

where

$$\begin{aligned}
\hat{C}_5 = {} & \frac{1}{120}A^5 + \frac{1}{72}(A'A^3 - A^3A') + \frac{1}{24}(A^2A'' + A''A^2 + AA''A)\\
& + \frac{1}{288}(A'^2A + AA'^2 - 2A'AA' + A'A'' - A''A' + A'''A - AA''') + \frac{1}{1152}A^{(4)}.
\end{aligned}$$

Therefore, the local truncation error is

$$\begin{aligned}
y(t_{j+1}) - y_{j+1} = -\frac{h^5}{720}\Big[& A'A^3 - A^3A' + A'A'' - A''A' + A'''A - AA'''\\
& -\frac{1}{2}(A'^2A + AA'^2 - 2A'AA') + 24(A^2A'' + A''A^2) + 27AA''A\\
& -3A(A'A - AA')A + \frac{1}{4}A^{(4)}\Big] y_j + \cdots.
\end{aligned}$$

A variant of the scheme (6.2) is

$$y_{j+1} = \frac{I + \frac{h}{24}(A_{j+1} - A_j)}{I - \frac{h}{24}(A_{j+1} - A_j)}\, e^{\frac{h}{6}(A_j+4A_{j+1/2}+A_{j+1})}\, \frac{I + \frac{h}{24}(A_j - A_{j+1})}{I - \frac{h}{24}(A_j - A_{j+1})}\, y_j. \tag{6.3}$$

This corresponds to replacing $\exp[\pm\frac{h}{12}(A_{j+1} - A_j)]$ by its [1/1] Padé approximants. The error introduced here is $\mathcal{O}(h^6)$. Therefore, (6.3) is also a fourth-order method and its local truncation error is exactly the same as (6.2).

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