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POLLUTION-FREE FINITE DIFFERENCE SCHEMES FOR NON-HOMOGENEOUS HELMHOLTZ EQUATION

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Abstract. In this paper, we develop pollution-free finite difference schemes for solving the non-homogeneous Helmholtz equation in one dimension. A family of high-order algorithms is derived by applying the Taylor expansion and imposing the conditions that the resulting finite difference schemes satisfied the original equation and the boundary conditions to certain degrees. The most attractive features of the proposed schemes are: first, the new difference schemes have a $2n-$order of rate of convergence and are pollution-free. Hence, the error is bounded even for the equation at high wave numbers. Secondly, the resulting difference scheme is simple, namely it has the same structure as the standard three-point central differencing regardless the order of accuracy. Convergence analysis is presented, and numerical simulations are reported for the non-homogeneous Helmholtz equation with both constant and varying wave numbers. The computational results clearly confirm the superior performance of the proposed schemes.

Key words. Helmholtz equation, Finite difference method, Convergence analysis, High wave number, Pollution-free, High-order schemes.

1. Introduction

In the study of time-harmonic wave propagations in one dimension, if we assume the wave has a steady-state and its circular frequency is fixed, we obtain the Helmholtz equation. The model equation to be investigated in this paper is given by:

$$-u_{xx}(x) - k^2u(x) = f(x), \ x \in (0, 1), \tag{1}$$

$$u(0) = 0, \tag{2}$$

$$u_x(1) - iku(1) = 0, \tag{3}$$

where $k = \omega/c$ is the wave number with ω being the circular frequency, c and f represents the speed of sound and the forcing term, respectively.

The Helmholtz equation arises in many problems related to wave propagations, such as acoustic, electromagnetic wave scattering and geophysical applications. It has been accepted that it is a difficult computational problem to develop efficient and accurate numerical schemes to solve the Helmholtz equation at high wave numbers.

The foremost difficulty in the numerical solution for the Helmholtz equation is to eliminate or minimize the "pollution effect" which causes a serious problem as the wave number k increases [10, 17, 25]. When the wave number is small, there is no difficulty to obtain accurate numerical solution for the Helmholtz equation. However, the accuracy of the computed solution deteriorates rapidly for problems at high wave numbers. Thus, eliminating or improving the pollution term will be a

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crucial issue in developing efficient and accurate numerical schemes for (1)-(3). To overcome this difficulty, many literatures have been reported in the past decades, and the reader is referred to [21, 22, 29, 34, 35, 41, 45, 5, 6, 16, 4] for the finite difference method and [3, 1, 2, 10, 15, 17, 20, 23, 24, 25, 26, 27, 28, 37, 39] for the finite element approximation. In fact, the following two issues are critical to the "pollution effect". First, when approximating the Helmholtz equation numerically, the "numerical wave number" $\tilde{k}$ from a resulting computational scheme will disperse in the non-dispersive media and they may not be the same as the wave number k from the original equation, which results the numerical dispersion. It is well-known that for the standard finite difference method, the difference

$$|\tilde{k} - k| \le C_1 k^3 h^2, \tag{4}$$

and for the fourth order compact scheme proposed in [21]

$$|\tilde{k} - k| \le C_1 k^5 h^4, \tag{5}$$

where C_1 is a general constant independent of $k, \tilde{k}$ and the mesh size h. Hereafter, we use C_1 to denote a general constant independent of $k, \tilde{k}$ and the mesh size h, but it may take different values at its different occurrences. For the p-version finite element method (see [25]), we have

$$|\tilde{k} - k| \le C_1 k \Big(\frac{hk}{2p}\Big)^{2p}. \tag{6}$$

Ainsworth [2] improved the estimate for the p-version finite element method result:

$$|\tilde{k} - k| \le C_1 k \Big(\frac{p!}{(2p)!}\Big)^2 \Big(\frac{hk}{2p+1}\Big)^{2p}. \tag{7}$$

Recently, Zhu et al. [37] reported a better estimate by using the continuous interior penalty finite element method

$$|\tilde{k} - k| \le C_1 kh. \tag{8}$$

The above results reveal the relationship between the original wave number k and the "numerical wave number" $\tilde{k}$. For a fixed kh, we observe that the difference increases as k increases for all methods.

Another important consequence is that the "pollution effect" has a direct impact on the error estimate. In the finite difference approach, Singer and Turkel [35] proposed a fourth order scheme based on the Pade approximation. Higher order difference schemes had also been investigated in [22, 29, 34, 35, 41]. However, the error estimates have not been analyzed. Recently, Fu presented the error estimate for a compact fourth order finite difference method in [21]. Although it has been claimed that the developed compact scheme is independent of the wave number, numerical simulations reveal that all finite difference methods referred above depend on the wave number and the "pollution effect" will become more serious as k increases. For the finite element method, stabilities and error estimates are analyzed for the problem (1)-(3) with PML boundary in [23]. In [10], Babuška et al. developed a generalized finite element method such that the pollution effect is minimal. Let h be the step size and assume that kh is fixed, Ihlenburg and Babuška proposed the $h-p$ version finite element method in [25, 27, 28], the error estimates and dispersion analysis confirm that the "pollution effect" can be reduced as p increases or h decreases. This estimate is further improved in [15]. Recently, the continuous interior penalty finite element method has been proposed in [37]. Although a modified finite element method is considered in [39], a physical spline finite element method is investigated in [20] and a least squares finite element method with high degree element shape functions is suggested in [24], however, no theoretical result is presented and the numerical experiments suggest that the "pollution effect" cannot be entirely eliminated in these references. The error estimate results reported in the references are summarized as follows: under certain conditions, it holds that, for the standard finite difference method,

$$\frac{||u-U||}{||u||} \leq C_1 k^2 (kh)^2, \tag{9}$$

and for the fourth order compact scheme,

$$\frac{||u-U||}{||u||} \leq C_1 k^2 (kh)^4, \tag{10}$$

and for the $p-$version finite element method (see [25, 27]),

$$\frac{||(u-U)'||}{||u'||} \leq C_1 \Big(\Big(\frac{kh}{2p}\Big)^p + k \Big(\frac{kh}{2p}\Big)^{2p} \Big), \tag{11}$$

and for the continuous interior penalty finite element method (see [37]),

$$\frac{||(u-U)'||}{||u'||} \leq C_1 kh, \tag{12}$$

by choosing a specific range of values for the stabilization parameter, where $||\cdot||$ is the L^2-norm, u' denotes the first derivative of u, u and U is the solution of the problem (1)-(3) and its numerical approximation, respectively. By assuming $p > C_1 \ln k$, Melenk and Sauter [15] improved the error estimate for the $p-$version finite element method, and show that

$$\frac{||u-U||_{\mathcal{H}}}{||u||_{\mathcal{H}}} \leq C_1 \Big(\frac{h}{p} + \Big(\frac{kh}{\sigma p}\Big)^p \Big), \tag{13}$$

where σ is a positive constant, and $||u||_{\mathcal{H}} = \big(||u'||^2 + k^2 ||u||^2 \big)^{1/2}$. From the above estimates, we note that the error estimates for the finite element method are better than that of the finite difference method.

It is now clear that to ensure the bound of asymptotic error estimates of the numerical schemes, we need to impose $k^\beta (kh)^\gamma = \text{constant}, \beta > 0, \gamma \geq 0$. For the standard finite differences, $\beta = 2, \gamma = 2$, and $\beta = 1, \gamma = 2$ for the finite element method with P_1 element. This implies that a very fine mesh is needed for problems at high wave numbers, since we require $h \sim O(1/k^2)$ or $h \sim O(1/k^{3/2})$ for the finite difference or the finite element methods. Consequently, this restriction leads to an enormous linear system.

The other difficulty in solving the Helmholtz problem numerically is that the resulting linear system is indefinite and very ill-conditioned. Numerous computational methods have been reported in the literatures, and the reader is referred to multilevel and preconditioned methods in [7, 32, 38]. However, since we consider one dimensional problems in this paper, the resulting matrix has a simple tri-diagonal structure which can be solved efficiently by a direct method. For this reason, the development on the linear solvers will not be discussed here.

To develop efficient and robust numerical schemes for the Helmholtz equation, it is import to first study the problem in one dimension. Indeed, many papers devoting to the one dimensional Helmoholtz equation have been published, see [14, 19, 23, 27, 28, 31, 37, 38, 39, 41]. It should be mentioned that for problems in two or three dimension in the polar or spherical coordinate, the solution can be obtained by solving a sequence of one dimensional equations (see [9, 12, 25, 33]); When dealing with higher dimensional problems in the Cartesian coordinate using a directional splitting method [43, 44], it is also important to have an efficient algorithm for the one dimensional equation. Moreover, accurate algorithms in one dimension are very helpful when considering boundary conditions in two dimensional problems. For example, the discrete singular convolution method proposed in [42] is an essentially pollution-free scheme on the domain for the two dimensional problem, but its superiority is not easily to extend to treat the boundary condition. In this case, the new approach introduced in this paper can offer an effective implementation for the boundary. When applying a domain decomposition method for a two dimensional Helmholtz equation [13], a sequence of one dimensional problems are solved on the interface.

Replacing the weight in the standard central difference quotients with optimal parameters, a new finite difference scheme was proposed in [29] for the homogeneous Helmholtz equation. The difference approximation satisfied the original equation exactly for all interior points. However, the exact solution of the problem cannot be reproduced if the standard finite difference scheme is implemented for the boundary conditions. Recently, Wong and Li [41] derived a special finite difference scheme for the radiation boundary condition. It has been shown that for a one dimensional homogeneous Helmholtz equation, the exact solution can be computed regardless the value of kh. Extending the ideas presented in [29, 41], we now propose new finite difference schemes which are capable of dealing with the non-homogeneous Helmholtz equation in one dimension. In developing the new schemes, we only need to assume $kh \le C_0$ with C_0 being a positive constant. However, the value of C_0 could be greater than 1, and this is confirmed by numerical simulation results. We will show that the new scheme does not produce numerical dispersion, that is

$$k - \tilde{k} = 0. \tag{14}$$

Furthermore, there is no restriction between the wave number k and the mesh size h, and the resulting difference schemes are pollution free with a $2n-$order convergence and the relative error in L^2-norm satisfies:

$$\frac{||u-U||}{||u||} \le C_1(kh)h^{2n-1}. \tag{15}$$

Comparing (14) with (4)-(8), and (15) with (9)-(13), respectively, a significant improvement is achieved by using the new method. Not only the numerical wave number $\tilde{k}$ is exactly equal to the original wave number k, but also the relative error approaches zero with fixed kh. Another attractive feature of this new scheme is that it has the same simple structure as the standard central differencing. Unlike other high order compact difference schemes [21, 22, 34, 35], the effect of the higher order accuracy is implemented by including more terms in the right hand side of the linear system.

The remaining article is organized as follows. In Section 2, we present the details on the derivation of the new schemes. The rate of convergence and the numerical dispersion are discussed in Section 3. To verify the theoretical predictions, numerical simulations are reported in Section 4 and the test cases include the Helmholtz equation with constant and varying wave numbers. Finally, conclusions and future work are presented in Section 5.

2. New finite difference schemes

We now derive the new finite difference schemes for the Helmholtz equation (1)-(3).

2.1. Approximation for the interior points. Using a uniform mesh size $0 < h < 1$, we have $N = \frac{1}{h}$. Let the grid point in the computational domain be defined as $x_i = ih(i \in Z, 0 < i \leq N)$. By applying the Taylor expansion, the values at the points $x_i + h$, x_i and $x_i - h$ will be used to approximate the second derivative $u_{xx}(x_i)$, such that

$$
\begin{aligned}
u(x_i+h) =& u(x_i) + hu^{(1)}(x_i) + \frac{h^2}{2!}u^{(2)}(x_i) + \frac{h^3}{3!}u^{(3)}(x_i) + \cdots \\
&+ \frac{h^n}{n!}u^{(n)}(x_i) + \cdots , \qquad (16)
\end{aligned}
$$

$$
\begin{aligned}
u(x_i-h) =& u(x_i) - hu^{(1)}(x_i) + \frac{h^2}{2!}u^{(2)}(x_i) - \frac{h^3}{3!}u^{(3)}(x_i) + \cdots \\
&+ (-1)^n\frac{h^n}{n!}u^{(n)}(x_i) + \cdots , \qquad (17)
\end{aligned}
$$

where $u^{(n)}(x_i)$ denotes the $n-$th derivative of $u(x)$ at the point $x_i (n \in Z)$. By adding (16) and (17), we get

$$
\begin{aligned}
u(x_i+h) + u(x_i-h) =& 2\Big[u(x_i) + \frac{h^2}{2!}u^{(2)}(x_i) + \frac{h^4}{4!}u^{(4)}(x_i) + \frac{h^6}{6!}u^{(6)}(x_i) + \cdots \\
&+ \frac{h^{2n}}{(2n)!}u^{(2n)}(x_i) + \cdots\Big]. \qquad (18)
\end{aligned}
$$

From the original equation (1), we have

$$
\begin{aligned}
u^{(2)}(x_i) &= (-1)k^2u(x_i) + (-1)f(x_i), \\
u^{(4)}(x_i) &= (-1)^2k^4u(x_i) + (-1)f^{(2)}(x_i) + (-1)^2k^2f(x_i), \\
u^{(6)}(x_i) &= (-1)^3k^6u(x_i) + (-1)f^{(4)}(x_i) + (-1)^2k^2f^{(2)}(x_i) + (-1)^3k^4f(x_i), \\
&\ \vdots \\
u^{(2n)}(x_i) &= (-1)^nk^{2n}u(x_i) + (-1)f^{(2n-2)}(x_i) + \cdots + (-1)^{n-1}k^{2n-4}f^{(2)}(x_i) \\
&\quad + (-1)^nk^{2n-2}f(x_i), \\
&\ \vdots
\end{aligned}
$$

Using the above equations and the trigonometric function theory, the equation (18) can be rewritten as

$$
\begin{aligned}
&u(x_i+h) + u(x_i-h) \\
=& 2\Big[\Big(1 - \frac{(kh)^2}{2!} + \frac{(kh)^4}{4!} - \frac{(kh)^6}{6!} + \cdots + (-1)^n\frac{(kh)^{2n}}{(2n)!} + \cdots\Big)u(x_i) \\
&+ (-1)\frac{h^2}{2!}f(x_i) + (-1)\frac{h^4}{4!}f^{(2)}(x_i) + (-1)^2\frac{k^2h^4}{4!}f(x_i) + (-1)\frac{h^6}{6!}f^{(4)}(x_i) \\
&+ (-1)^2\frac{k^2h^6}{6!}f^{(2)}(x_i) + (-1)^3\frac{k^4h^6}{6!}f(x_i) + \cdots + (-1)\frac{h^{2n}}{(2n)!}f^{(2n-2)}(x_i) \\
&+ \cdots + (-1)^{n-1}\frac{k^{2n-4}h^{2n}}{(2n)!}f^{(2)}(x_i) + (-1)^n\frac{k^{2n-2}h^{2n}}{(2n)!}f(x_i) + \cdots\Big] \\
=& 2\big[\cos(kh)u(x_i) + F(f(x_i))\big], \qquad (19)
\end{aligned}
$$

where $F(f(x_i)) = \sum_{m=0}^{+\infty} Y_m = Y_0 + Y_1 + \cdots + Y_{n-1} + \cdots$, and

$$\begin{aligned} Y_0 =&(-1)\frac{h^2}{2!}f(x_i) + (-1)^2\frac{k^2h^4}{4!}f(x_i) + (-1)^3\frac{k^4h^6}{6!}f(x_i) + \cdots \\ &+ (-1)^n\frac{k^{2n-2}h^{2n}}{(2n)!}f(x_i) + \cdots, \\ Y_1 =&(-1)\frac{h^4}{4!}f^{(2)}(x_i) + (-1)^2\frac{k^2h^6}{6!}f^{(2)}(x_i) + \cdots + (-1)^{n-1}\frac{k^{2n-4}h^{2n}}{(2n)!}f^{(2)}(x_i) + \cdots, \\ &\vdots \\ Y_{n-1} =&(-1)\frac{h^{2n}}{(2n)!}f^{(2n-2)}(x_i) + (-1)^2\frac{k^2h^{2(n+1)}}{(2(n+1))!}f^{(2n-2)}(x_i) + \cdots, \\ &\vdots \end{aligned}$$

Since

$$\begin{aligned} k^2Y_0 =&(-1)\frac{(kh)^2}{2!}f(x_i) + (-1)^2\frac{(kh)^4}{4!}f(x_i) + (-1)^3\frac{(kh)^6}{6!}f(x_i) + \cdots \\ &+ (-1)^n\frac{(kh)^{2n}}{(2n)!}f(x_i) + \cdots \\ =&-f(x_i) + f(x_i) + (-1)\frac{(kh)^2}{2!}f(x_i) + (-1)^2\frac{(kh)^4}{4!}f(x_i) + (-1)^3\frac{(kh)^6}{6!}f(x_i) \\ &+ \cdots + (-1)^n\frac{(kh)^{2n}}{(2n)!}f(x_i) + \cdots \\ =&[\cos(kh) - 1]f(x_i), \end{aligned}$$

it yields that

$$Y_0 = \frac{[\cos(kh) - 1]}{k^2}f(x_i). \tag{20}$$

Assume $f(x) \in C^\infty$, if $kh \to 0$, expanding $\cos(kh)$ by the Taylor formula at the point 0, we have

$$\begin{aligned} &\frac{\cos(kh) - 1}{k^2}f(x_i) \\ =&\big[(-1)\frac{h^2}{2!} + (-1)^2\frac{k^2h^4}{4!} + \cdots + (-1)^n\frac{k^{2n-2}h^{2n}}{(2n)!} + \cdots\big]f(x_i) = O(h^2), \end{aligned}$$

If kh is not small enough (meaning $\cos(kh)$ cannot be expanded at the point 0), we can consider that $kh = C_0$ where C_0 is a positive constant. It then follows that $\cos(kh) - 1$ is a bounded constant and $k = C_0/h$, which also yields

$$\frac{\cos(kh) - 1}{k^2}f(x_i) = O(h^2).$$

Therefore, it always holds that

$$Y_0 = \frac{[\cos(kh) - 1]}{k^2}f(x_i) = O(h^2). \tag{21}$$

By applying a similar process as deriving (21), it is not hard to verify that

(22)

$$Y_1 = (-1)\frac{[\cos(kh) - 1 + \frac{(kh)^2}{2!}]}{k^4} f^{(2)}(x_i) = O(h^4),$$

$$\vdots$$

(23)

$$Y_{n-1} = (-1)^{n-1}\frac{\left[\cos(kh) - 1 + \frac{(kh)^2}{2!} - \cdots + (-1)^n \frac{(kh)^{2n-2}}{(2n-2)!}\right]}{k^{2n}} f^{(2n-2)}(x_i) = O(h^{2n}),$$

$$\vdots$$

Now, by combining the above equations with (19), we have

$$-u_{i+1} + 2\cos(kh)u_i - u_{i-1} = -2F(f_i), \tag{24}$$

where $u_i = u(x_i) = u(ih)$ and $f_i = f(x_i) = f(ih)$.

Replacing u_{i+1}, u_i and u_{i-1} with U_{i+1}, U_i and U_{i-1} in (24), respectively, the new finite difference schemes for any interior grid point x_i can be constructed from

$$-U_{i+1} + 2\cos(kh)U_i - U_{i-1} = -2F_n(f_i) + O(h^{2n+2}), \tag{25}$$

where U_i is the approximation of u_i, $U = \{U_i\}_{i=1}^N$ and

$$F_n(f_i) = \sum_{m=0}^{n-1} Y_m = Y_0 + Y_1 + \cdots + Y_{n-1}.$$

The new scheme is accurate of $2n-$order depending on how many terms are included in the summation for $F_n(f_i)$. For example, the new scheme is of second order if we only take Y_0 in $F_n(f_i)$. By including two terms $Y_0 + Y_1$, it leads to a fourth order scheme. It should be noted that, unlike the usual high order compact difference scheme in which the complexity of the resulting scheme increases as the order increases, the proposed new schemes always have a simple structure as the three-point central differencing.

Remark 1: 1). By taking the first two terms on the right hand side of (18), then substituting the results into (1) and replacing u_{i+1}, u_i and u_{i-1} with U_{i+1}, U_i and U_{i-1} , we derive the standard finite difference scheme:

$$-U_{i+1} + (2 - k^2h^2)U_i - U_{i-1} = h^2 f_i. \tag{26}$$

2). By including the first three terms on the right hand side of (18), and applying (1), it leads to the fourth order compact scheme [21]:

$$\begin{aligned}\big(-1 - \frac{k^2h^2}{12}\big)U_{i+1} + \big(2 - k^2h^2 + \frac{k^2h^2}{6}\big)U_i + \big(-1 - \frac{k^2h^2}{12}\big)U_{i-1} \\ = h^2\big(f_i + \frac{h^2}{12} f_i^{(2)}\big).\end{aligned} \tag{27}$$

2.2. Approximation for the boundary points. We now construct the new finite difference schemes for the boundary points. Since at $x = 0$, we have the Dirichlet boundary condition, we will only focus on developing the new schemes for the radiation condition (3).

Using the same approach as for the interior points described in the previous section, we apply the Taylor expansion and derive the relation between $u(x_i + h), u(x_i - h)$ and $u(x_i)$ for $x_i = 1$. Now, By subtracting (16) with (17), it gives

$$\begin{aligned} u(x_i+h)-u(x_i-h) =& 2\Big[hu^{(1)}(x_i)+\frac{h^3}{3!}u^{(3)}(x_i)+\frac{h^5}{5!}u^{(5)}(x_i)+\cdots \\ &+\frac{h^{2n+1}}{(2n+1)!}u^{(2n+1)}(x_i)+\cdots\Big]. \end{aligned} \tag{28}$$

By the application of the original equation (1), we have

$$\begin{aligned} u^{(3)}(x_i) &= (-1)k^2u^{(1)}(x_i)+(-1)f^{(1)}(x_i), \\ u^{(5)}(x_i) &= (-1)^2k^4u^{(1)}(x_i)+(-1)f^{(3)}(x_i)+(-1)^2k^2f^{(1)}(x_i), \\ &\vdots \\ u^{(2n+1)}(x_i) &= (-1)^nk^{2n}u^{(1)}(x_i)+(-1)f^{(2n-1)}(x_i)+\cdots+(-1)^nk^{2n-2}f^{(1)}(x_i), \\ &\vdots \end{aligned}$$

Putting the above equations into (28) and using the trigonometric function theory, we get

$$\begin{aligned} &u(x_i+h)-u(x_i-h) \\ =&2\Big[\Big(h-\frac{k^2h^3}{3!}+\frac{k^4h^5}{5!}-\cdots+(-1)^n\frac{k^{2n}h^{2n+1}}{(2n+1)!}+\cdots\Big)u^{(1)}(x_i) \\ &+(-1)\frac{h^3}{3!}f^{(1)}(x_i) \\ &+(-1)\frac{h^5}{5!}f^{(3)}(x_i)+(-1)^2\frac{k^2h^5}{5!}f^{(1)}(x_i) \\ &+\cdots \\ &+(-1)\frac{h^{2n+1}}{(2n+1)!}f^{(2n-1)}(x_i)+\cdots+(-1)^n\frac{k^{2n-2}h^{2n+1}}{(2n+1)!}f^{(1)}(x_i) \\ &+\cdots\Big]. \end{aligned} \tag{29}$$

Therefore,

$$k[u(x_i+h)-u(x_i-h)] =2\big[\sin(kh)u^{(1)}(x_i)+B(f(x_i))\big], \tag{30}$$

where $B(f(x_i)) = \sum_{m=1}^{+\infty} Z_m = Z_1 + Z_2 + \cdots + Z_n + \cdots$, and

$$\begin{aligned} Z_1 &= (-1)\frac{kh^3}{3!}f^{(1)}(x_i)+(-1)^2\frac{k^3h^5}{5!}f^{(1)}(x_i)+\cdots+(-1)^n\frac{k^{2n-1}h^{2n+1}}{(2n+1)!}f^{(1)}(x_i)+\cdots, \\ Z_2 &= (-1)\frac{kh^5}{5!}f^{(3)}(x_i)+(-1)^2\frac{k^3h^7}{7!}f^{(3)}(x_i)+\cdots+(-1)^{n-1}\frac{k^{2n-3}h^{2n+1}}{(2n+1)!}f^{(3)}(x_i)+\cdots, \\ &\vdots \\ Z_n &= (-1)\frac{kh^{2n+1}}{(2n+1)!}f^{(2n-1)}(x_i)+\cdots, \\ &\vdots \end{aligned}$$

By similar argument for (20)-(23), it is easy to verify that

$$Z_1 = \frac{\sin(kh) - kh}{k^2} f^{(1)}(x_i) = O(h^2), \tag{31}$$

$$Z_2 = (-1)\frac{\sin(kh) - kh + \frac{(kh)^3}{3!}}{k^4} f^{(3)}(x_i) = O(h^4), \tag{32}$$

$$\vdots$$

$$Z_n = (-1)^{n-1}\frac{\sin(kh) - kh + \frac{(kh)^3}{3!} + \cdots + \frac{(kh)^{2n-1}}{(2n-1)!}}{k^{2n}} f^{(2n-1)}(x_i) = O(h^{2n}), \tag{33}$$

$$\vdots$$

Taking the above relations into (30), the approximation for the boundary condition (3) is given by

$$u(x_i + h) - u(x_i - h) = \frac{2\big[\sin(kh)u^{(1)}(x_i) + B(f(x_i))\big]}{k}. \tag{34}$$

Consider u_N is the boundary point at $x = 1$, then we have

$$-u_{N+1} + 2i\sin(kh)u_N + u_{N-1} = -\frac{2B(f_N)}{k}. \tag{35}$$

The new finite difference scheme for the boundary equation (3) has the form

$$-U_{N+1} + 2i\sin(kh)U_N + U_{N-1} = -\frac{2B_n(f_N)}{k} + O(h^{2n+2}), \tag{36}$$

where

$$B_n(f_i) = \sum_{m=1}^{n} Z_m = Z_1 + Z_2 + \cdots + Z_n.$$

The new scheme (36) is $2n-$order convergent on the boundary. The order of convergence depends on the terms included in the summation for $B_n(f_i)$. For example, by taking one term Z_1 or two terms $Z_1 + Z_2$, it will lead to a second order or a fourth order scheme. If $f(x)$ is not sufficiently smooth, we can replace $f^{(n)}$ with the corresponding interpolation in (25) and (36).

Hence, by combining (25), (2) and (36), the new finite difference (NFD) schemes of $2n-$order for the problem (1)-(3) are given as follows:

NFD:

$$-U_{j+1} + 2\cos(kh)U_j - U_{j-1} = -\,2F_n(f_j),\ 0 < j \le N, \tag{37}$$

$$U_0 = 0, \tag{38}$$

$$-U_{N+1} + 2i\sin(kh)U_N + U_{N-1} = -\,\frac{2B_n(f_N)}{k}. \tag{39}$$

Remark 2: 1). By using (2) and taking the first term on the right hand side of (28) and by (18), it gives the standard finite difference (SFD) scheme for the problem (1)-(3):

SFD:

$$-U_{j+1} + (2 - k^2h^2)U_j - U_{j-1} = h^2 f_j,\ 0 < j \le N, \tag{40}$$

$$U_0 = 0, \tag{41}$$

$$-U_{N+1} + 2khiU_N + U_{N-1} = 0. \tag{42}$$

2). From the equation (27) and taking the first three terms on the right hand side of (28), and using (1) and (3), the fourth order compact finite difference (CFD) scheme is expressed as (see [21]):

CFD:

$$\big(-1-\frac{k^2h^2}{12}\big)U_{j+1}+\big(2-k^2h^2+\frac{k^2h^2}{6}\big)U_j+\big(-1-\frac{k^2h^2}{12}\big)U_{j-1}$$

$$=h^2\big(f_j+\frac{h^2}{12}f_j^{(2)}\big),\ 0<j\le N, \tag{43}$$

$$U_0=0, \tag{44}$$

$$-U_{N+1}+\frac{12khi}{6+k^2h^2}U_N+U_{N-1}=\frac{12khi}{6+k^2h^2}\frac{h^2}{6}f_N^{(1)}. \tag{45}$$

Remark 3: Since (2) is a Dirichlet boundary, we can also substitute it into the problem directly in the finite difference method when it is non-homogenous. On the other hand, using a similar derivation, we can construct the new finite difference schemes for a general mixed boundary condition

$$u_x(x_i)+g_1u(x_i)=g_2, \tag{46}$$

where g_1, g_2 are constant functions. Notice that, (46) reduces to the Neumann condition when $g_1=0$. By the use of (34), we have

$$u(x_i+h)-u(x_i-h)=\frac{2\big[\sin(kh)u^{(1)}(x_i)+B(f(x_i))\big]}{k}$$

$$=-\frac{2\sin(kh)g_1}{k}u(x_i)+\frac{2\big[\sin(kh)g_2+B(f(x_i))\big]}{k}.$$

Thus, the NFD scheme for (46) can be expressed by

$$-U_{N+1}-\frac{2\sin(kh)g_1}{k}U_N+U_{N-1}=-\frac{2\big[\sin(kh)g_2+B_n(f_N)\big]}{k}+O(h^{2n+2}).$$

3. Convergence order and numerical dispersion analysis

To study the proposed new finite difference schemes, we carry out the convergence and dispersion analysis.

3.1. Convergence order. Let $||\cdot||$ and $|\cdot|$ denote the L^2 and $L^\infty-$norm, respectively. First, we recall the stability results for the problem (1)-(3), which have been investigated by Ihlenburg [25]. Hereafter, we always suppose k is sufficiently large.

Lemma 3.1.[25] *Suppose that u is the solution of the problem (1)-(3) and f is sufficiently smooth, then we have the following stability estimates*

$$||u||\le\frac{1}{k}||f||, \tag{47}$$

$$||u^{(1)}||\le||f||, \tag{48}$$

$$||u^{(2)}||\le C_1k||f||, \tag{49}$$

where C_1 is a general positive constant independent of $k, u, u^{(n)}$, but depends on f and the domain.

For the new finite difference schemes, the following theorem holds.

Theorem 3.1. *Suppose that u is the solution of the problem (1)-(3), f is smooth enough and kh is sufficiently small, then the approximation* $U = \{U_i\}_{i=1}^N$ *generated by the new finite difference scheme has a unique solution, and the following error estimates hold*

$$||u - U|| \leq C_1 h^{2n}, \tag{50}$$

$$\frac{||u - U||}{||u||} \leq C_1 k h^{2n}. \tag{51}$$

Proof. Recall that the mesh size $h = 1/N$, and the resulting discrete linear system is given by

$$DU = b,$$

where D is a tri-diagonal matrix and b is a vector with respect to $f(x)$. When $kh \to 0$, the coefficient matrix D tends to the following matrix

$$\begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 2 & -1 \\ 0 & 0 & 0 & \cdots & -2 & 2 \end{pmatrix}_{N\times N}. \tag{52}$$

The matrix (52) is positive definite which implies that the new method has a unique solution under the condition that kh is sufficiently small.

Setting $e_i = u_i - U_i$, considering (24) and (35), the error vector $E = \{e_i\}_{i=1}^N$ satisfies

$$DE = T^n, \tag{53}$$

where $T^n = (T_1^n, T_2^n, \cdots, T_N^n)^T$ is the error with

$$T_i^n = 2(F(f_i) - F_n(f_i)), \ 1 \leq i \leq N-1,$$

$$T_i^n = 2(F(f_i) - F_n(f_i)) - \frac{2(B(f_i) - B_n(f_i))}{k}, \ i = N.$$

Obviously, it holds that

$$T_i^n = O(h^{2n+2}), \ 1 \leq i \leq N. \tag{54}$$

The eigenvalues of the matrix (52) are given by (see [36, 21]):

$$\lambda_j = 2 - 2\cos\frac{j\pi}{N} = 4\sin^2\frac{j\pi h}{2},$$

and the corresponding eigenvectors, for $j = 1, \cdots, N$, have the following form:

$$\zeta_j = (\zeta_{1,j}, \zeta_{2,j}, \cdots, \zeta_{N,j})^T, \ \zeta_{l,j} = \sin\frac{lj\pi}{N}, \ l = 1, \cdots, N.$$

As h is sufficiently small, it gives

$$\min_{1\leq j\leq N} \lambda_j = 4\sin^2\frac{\pi h}{2} \sim \pi^2 h^2. \tag{55}$$

Setting

$$E = \sum_{j=1}^{N} a_j \zeta_j, \ ||E||^2 = \sum_{j=1}^{N} |a_j|^2 ||\zeta_j||^2, \tag{56}$$

where a_j is the coefficient of the component ζ_j, and taking the inner product with E, we derive from (53) that

$$(DE, E) = (T^n, E). \tag{57}$$

When $kh \to 0$, applying (55), (56) and the Cauchy inequality, we have for the left hand side term of (57)

$$\begin{aligned}(DE, E) &= (D\sum_{j=1}^{N} a_j\zeta_j, \sum_{j=1}^{N} a_j\zeta_j) \to (\sum_{j=1}^{N} \lambda_j a_j\zeta_j, \sum_{j=1}^{N} a_j\zeta_j)\\ &= \sum_{j=1}^{N} \lambda_j |a_j|^2 ||\zeta_j||^2 \geq C_1\pi^2 h^2 \sum_{j=1}^{N} |a_j|^2 ||\zeta_j||^2 = C_1\pi^2 h^2 ||E||^2,\end{aligned}$$

and for the right hand side term of (57)

$$(T^n, E) \leq ||T^n|| ||E||.$$

Taking the above two inequalities into (57) and using (54), it yields

$$||E|| \leq C_1 h^{-2} ||T^n|| \leq C_1 h^{2n},$$

which implies (50).

The relative error (51) can easily be deduced using (50) and (47) in Lemma 3.1. Thus, we complete the proof.

From Theorem 3.1, we can see that the new schemes are very efficient for problems with high wave numbers k since C_1 is a constant independent of $k, u, u^{(n)}$. Furthermore, by taking more terms in the summation for the right hand side of (37) and (39), the relative error will approach zero for any k as $n \to \infty$. This is the most important and attractive feature of the developed new schemes. Moreover, Theorem 3.1 suggests that, if n is taken sufficiently large, the approximation solution U will be very close to the exact solution u. In particular, if there exists a nonnegative integer m, such that $f^{(n)}(x) = 0$ when $n > m$, or when $f(x)$ is a constant (i.e. $m = 0$), then (54) implies that the errors $T_1^n = T_2^n = \cdots = T_N^n = 0$. Consequently, we have $||u - U|| \leq C_1 h^{\infty}$, i.e., the computed solution U produces the exact solution u.

Remark 4: It is noted that the convergence order of the standard finite difference and the compact difference methods are derived under the assumption that $u(x)$ or $u^{(n)}(x)$ are bounded [21, 22, 30, 34, 35, 40]. However, the stabilities of $u(x), u^{(n)}(x)$ depend on the wave number k as suggested in Lemma 3.1. Hence, we expect the performance will be deteriorated rapidly when k is large.

1). For the standard finite difference method, it is not correct to assume that $||u^{(4)}(x_i)|| \leq C, 0 < i \leq N$ on the right hand side of the error estimate, where C is a constant. In fact, the original problem (1) suggests that $||u^{(4)}(x_i)|| \leq k^4||u(x_i)|| + k^2||f(x_i)|| + ||f^{(2)}(x_i)||$. Using (47), the truncation error is given by $O(k^3h^2)$ for the standard finite difference scheme. The following error estimates hold for the standard finite difference scheme:

$$||u - U|| \leq C_1||u^{(4)}(x)||h^2 \leq C_1 k^3 h^2, \tag{58}$$

$$\frac{||u - U||}{||u||} \leq C_1 k^4 h^2. \tag{59}$$

2). For the fourth order compact finite difference scheme, we have

$$\begin{aligned}||u^{(6)}(x_i)|| &= ||(-1)^3k^6u(x_i) + (-1)f^{(4)}(x_i) + (-1)^2k^2f^{(2)}(x_i) + (-1)^3k^4f(x_i)|| \\ &\le C_1k^6||u(x_i)|| \\ &\le C_1k^5.\end{aligned}$$

Hence, the error estimates are:

$$||u - U|| \le C_1k^5h^4, \tag{60}$$

$$\frac{||u-U||}{||u||} \le C_1k^6h^4. \tag{61}$$

3). For the finite element method with P_1 element, the error estimates are given by [25]):

$$||u - U|| \le C_1k^2h^2, \tag{62}$$

$$\frac{||u-U||}{||u||} \le C_1k^3h^2. \tag{63}$$

It is clear that significant improvements are achieved for the convergence results using the new schemes as stated in (37)-(39). Although we assume that $kh \to 0$ in the derivation of the error estimates for the new schemes, the value of kh used in actual computations does not need to be very small. For some cases which will be reported in the next section, accurate numerical solutions could be computed even when $kh = 5$ or larger.

3.2. Numerical dispersion analysis. The "pollution effect" can be investigated through numerical dispersion analysis. When solving the Helmholtz equation numerically, the wave number resulted from a numerical scheme may be different from the original wave number. In a simple word, to achieve an accurate computed solution, one should expect the numerical wave number should be close to the original wave number.

A simple way to determine the numerical wave number is given by Ihlenburg, and the details can be found in [25, 26]. Assuming a uniform mesh is used, and the discrete linear system is given by the tri-diagonal matrix with the following structure

$$\begin{pmatrix} 2S(kh) & R(kh) & 0 & \cdots & 0 & 0 \\ R(kh) & 2S(kh) & R(kh) & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 2S(kh) & R(kh) \\ 0 & 0 & 0 & \cdots & 2R(kh) & 2S(kh) - 2i\sin(kh) \end{pmatrix}_{N\times N}, \tag{64}$$

where $2S(kh)$ and $R(kh)$ denote the coefficients of the main and off-diagonal terms.

Let $\tilde{k}$ be the numerical wave number, then it is shown in [25, 26] that

$$\cos(\tilde{k}h) = -\frac{S(kh)}{R(kh)}. \tag{65}$$

For the new finite difference schemes, we have $S(kh) = \cos(kh)$ and $R(kh) = -1$. Hence,

$$\cos(\tilde{k}h) = -\frac{S(kh)}{R(kh)} = \cos(kh). \tag{66}$$

Therefore,

$$\tilde{k} = k. \tag{67}$$

Consequently, there is no numerical dispersion by applying the new schemes for solving the problem (1)-(3) numerically.

Remark 5: 1). For the standard finite difference scheme (40)-(42), we have $S(kh) = 1 - \frac{k^2h^2}{2}$ and $R(kh) = -1$ in (64). The numerical wave number satisfies

$$\cos(\tilde{k}h) = -\frac{S(kh)}{R(kh)} = 1 - \frac{k^2h^2}{2}, \tag{68}$$

that is

$$\tilde{k} = \frac{1}{h}\arccos(1 - \frac{k^2h^2}{2}) = k + \frac{k^3h^2}{24} + O(k^5h^4). \tag{69}$$

2). For the fourth order compact scheme (43)-(45), we have $S(kh) = 1 - \frac{k^2h^2}{2} + \frac{k^2h^2}{12}$ and $R(kh) = -1 - \frac{k^2h^2}{12}$. The resulting numerical wave number is given by:

$$\cos(\tilde{k}h) = -\frac{S(kh)}{R(kh)} = \frac{1 - \frac{k^2h^2}{2} + \frac{k^2h^2}{12}}{1 + \frac{k^2h^2}{12}}, \tag{70}$$

therefore,

$$\tilde{k} = \frac{1}{h}\arccos\Big(\frac{1 - \frac{k^2h^2}{2} + \frac{k^2h^2}{12}}{1 + \frac{k^2h^2}{12}}\Big) = k + \frac{k^5h^4}{480} + O(k^7h^6), \tag{71}$$

by using the Taylor expansion.

3). For the finite element method with P_1 element, it was reported in [25] that $S(kh) = 1 - \frac{k^2h^2}{3}$, $R(kh) = -1 - \frac{k^2h^2}{6}$. The numerical wave number is given by

$$\tilde{k} = \frac{1}{h}\arccos\Big(\frac{1 - \frac{k^2h^2}{3}}{1 + \frac{k^2h^2}{6}}\Big) = k - \frac{k^3h^2}{24} + O(k^5h^4). \tag{72}$$

It is important to note that the numerical wave number is identical to the original wave numbers when the new schemes are used. For other computational schemes, the discrepancy of the wave numbers is obvious.

4. Numerical Examples

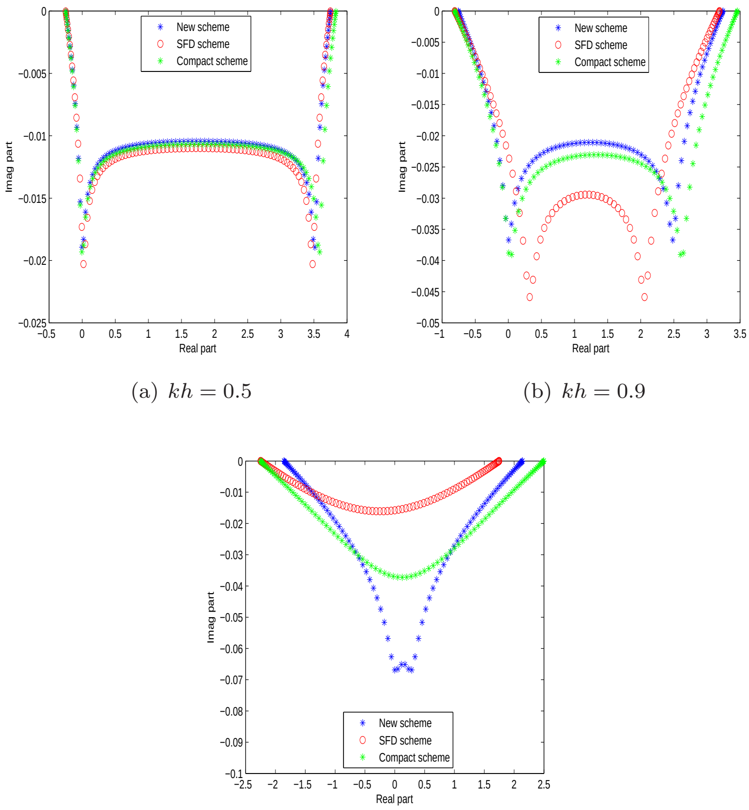
To verify the effectiveness and to compare the performance of the proposed new schemes with other computational methods, numerical simulations are carried out to solve the Helmholtz equation (1)-(3). The test cases include problems with constant and varying wave numbers. Particular attention will be focused on the performance for high wave number problems. Since we are dealing with one dimensional problems, the resulting discrete linear system is given by a tri-diagonal matrix which can be efficiently solved by a direct method using a Matlab software.

4.1. Constant wave number. For the Helmholtz equation (1)-(3), we first consider three test cases by varying the forcing term f and the boundary conditions. Similar examples have been used in the references (see [7, 10, 17, 22, 26, 27, 28, 35, 41]). The boundary condition (3) at $x = 1$ is the Sommerfeld condition in one dimension, which is imposed by considering the problem in free space and postulating no wave are reflected from infinity [25].

Problem 1: The forcing term is given by $f(x) = 40\cos 4x + 80i\sin 3x$ in (1), and the boundary conditions are $u(0) = 0$ and $u_x(1) - iku(1) = 0$.

Table 1. Condition numbers with $h = 0.01$.

k	50	90	150
kh	0.5	0.9	1.5
SFD scheme	503.4	206.6	312.1
Compact scheme	500.1	269.8	184.4
New scheme	499.8	270.7	181.0



(a) $kh = 0.5$

(b) $kh = 0.9$

(c) $kh = 1.5$

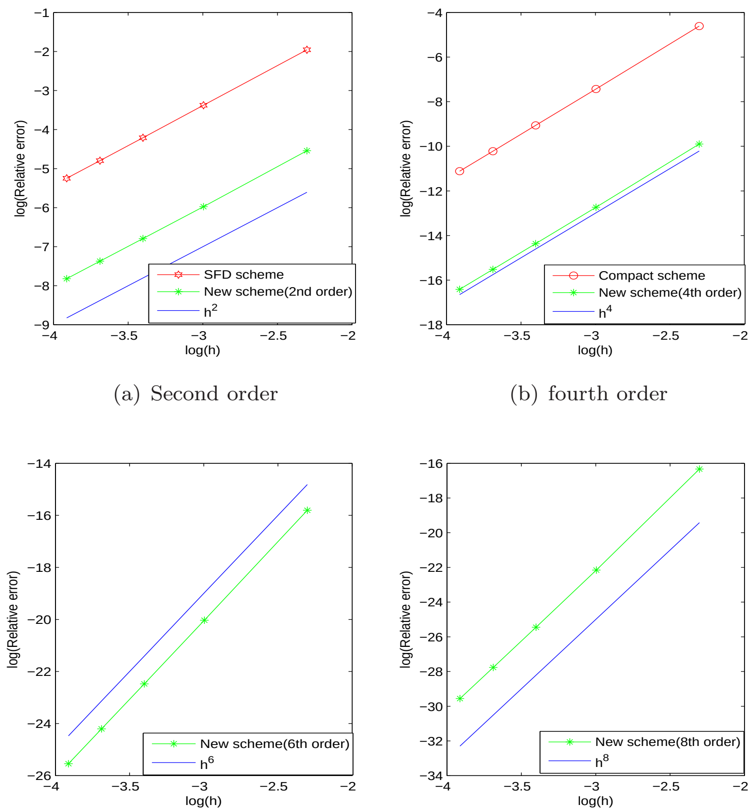
Figure 1. Eigenvalues of different methods with $h = 1/100$.

Problem 2: The forcing term is given by $f(x) = 1$ in (1), and the boundary conditions are $u(0) = 0$ and $u_x(1) - iku(1) = 0$.

It has been shown by Ihlenburg [25] that for a given $f(x)$, the exact solutions of Problems 1 and 2 are determined by $u(x) = \int_0^1 G(x,s)f(s)ds$, where $G(x,s)$ is the Green's function

$$G(x,s) = \frac{1}{k}\begin{cases} \sin(kx)e^{iks}, & 0 \le x \le s, \\ \sin(ks)e^{ikx}, & s \le x \le 1. \end{cases}$$

Problem 3: The forcing term is given by $f(x) = 0$ in (1), and the boundary conditions are $u(0) = 1$ and $u_x(1) - iku(1) = 0$. The exact solution is given by $u(x) = e^{ikx}$.

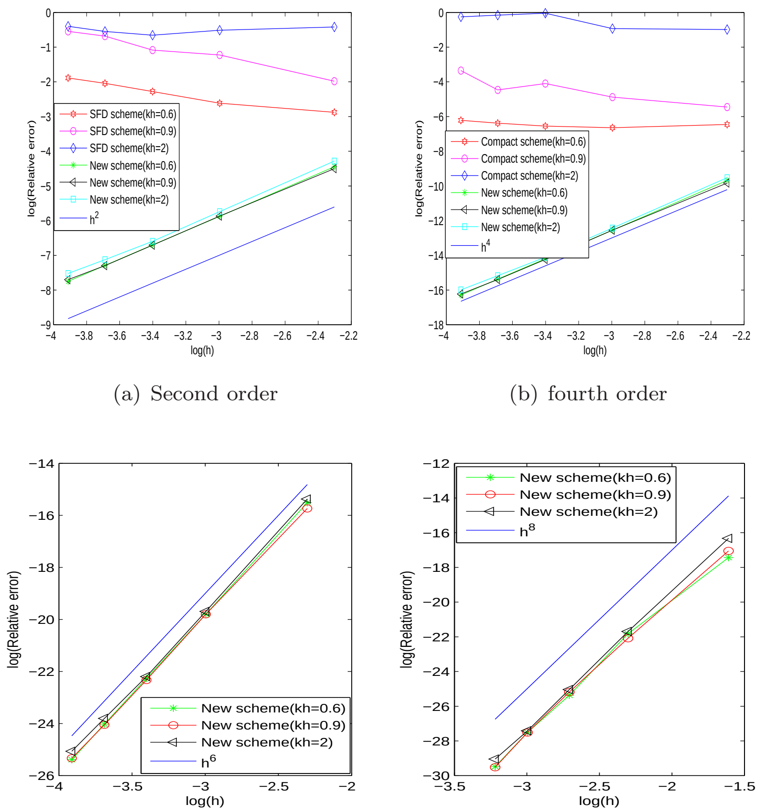


(a) Second order (b) fourth order

(c) Sixth order (d) Eighth order

FIGURE 2. Convergence order.

Problem 1. First, we investigate the condition numbers of the resulting linear system D for various algorithms. Let D^H be the conjugate matrix of D, and define the condition number by $\sqrt{\lambda_{max}(D^H D)/\lambda_{min}(D^H D)}$. Table 1 reports the condition numbers for wave numbers $k = 50, 90, 150$ and $h = 0.01$. It should be recalled that since the resulting linear system does not change with the order of accuracy in the new schemes, the condition number for the new scheme is identical regardless of the order of accuracy. In Table 1, we list the condition numbers for the standard finite difference (SFD), the compact finite difference (CFD) and the new finite difference (NFD) schemes. When kh is small, such as $kh = 0.5$, that condition numbers for the three schemes are very close. It is interesting to note that for the SFD, the condition number decreases when $kh = 0.9$ but then increases when $kh = 1.5$. For the CFD and NFD schemes, the condition numbers keep reducing as kh increases. As we already know that it is more difficult to compute the solution for higher wave numbers, the condition number itself does not reflect the ill-conditioning of the discrete system as k increases. However, more useful information can be revealed by studying the corresponding eigenvalue distribution of D resulting from different schemes as illustrated in Fig. 1. The distributions from the three schemes are similar as kh is small, but the eigenvalue profiles of the SFD clearly show a substantial different compared to that corresponding to the



(a) Second order (b) fourth order

(c) Sixth order (d) Eighth order

FIGURE 3. "Pollution effect" on convergence order.

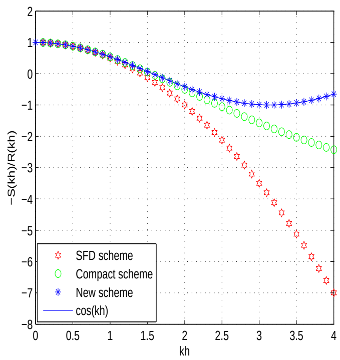


FIGURE 4. Discrete cosine $\cos(\tilde{k}h)$.

CFD and NFD schemes as kh increases. When $kh < 1$ and k is not very large, the distributions for the CFD and NFD are similar.

To confirm the order of convergence derived in Theorem 3.1, we consider Problem 1 with a constant wave number $k = 10$. We investigate computational methods

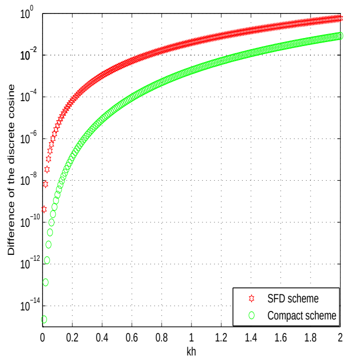


FIGURE 5. Difference of discrete cosine $|\cos(\tilde{k}h) - \cos(kh)|$.

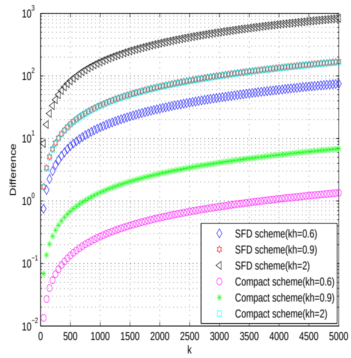
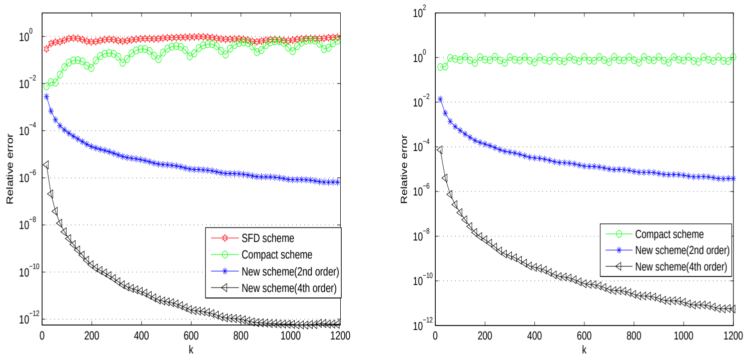
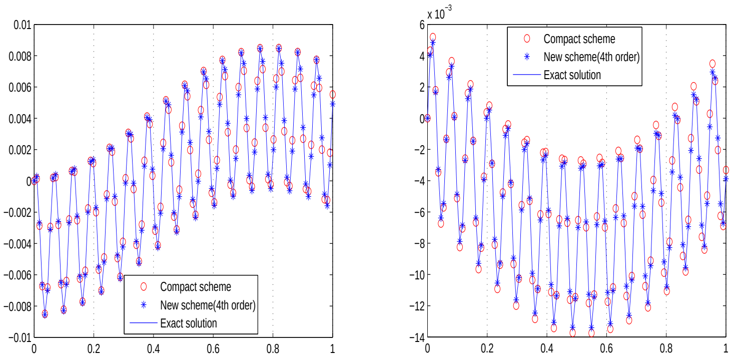


FIGURE 6. Difference between $|k - \tilde{k}|$.



(a) $kh = 0.9$ (b) $kh = 2$

FIGURE 7. Relative error in L^2-norm with respect to k (Problem 1).



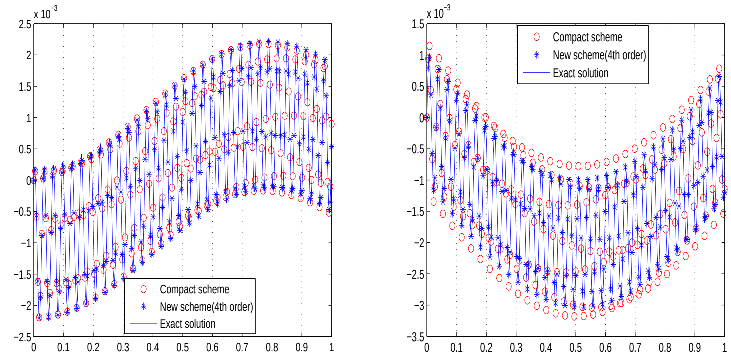
(a) Real part (b) Imaginary part

FIGURE 8. Comparison of various schemes with $k = 100$ and $h = 1/111 (kh \approx 0.9)$.

based on the SFD (40)-(42), CFD (43)-(45) and NFD schemes of second, fourth, sixth and eighth order. The convergence results displayed in Fig. 2 are in good agreement with the theoretical predictions. We observe that even with the same order of convergence, the second and fourth order new schemes produce more accurate numerical solutions than those obtained by the SFD and CFD schemes. Very accurate computed solutions are achieved by the sixth and eight order new schemes.

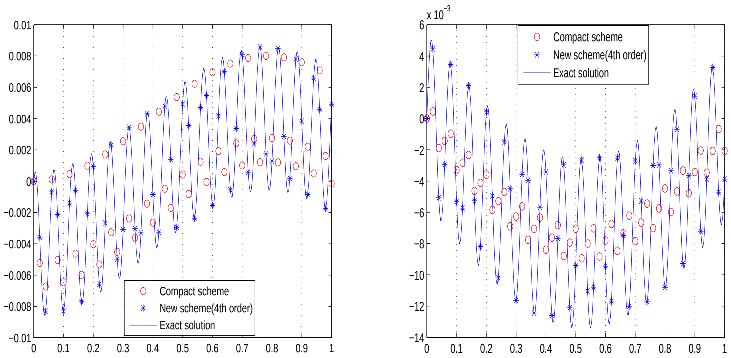
To demonstrate that the new schemes are pollution free, Fig. 3 displays the "pollution effect" on the convergence rates for various numerical schemes. As expected, for the standard difference and compact schemes with a fixed mesh size h, the error is reducing when kh is decreasing. However, for a fixed kh, the error actually is increasing as h is reducing. This clearly indicates the effect due to the pollution error. For the new schemes, we observe that the convergence order is not sensitive with kh, and the error is decreasing as h is reducing. This confirms that the new schemes are pollution free. In Fig. 4, the values of $\cos(\tilde{k}h)$ are plotted for kh in the range from 0 to 4. Only the new scheme agrees with the exact $\cos(kh)$. Although the results using the standard difference and compact schemes seem to produce a good agreement when $kh < 1$, the discrepancy between $\cos(\tilde{k}h) - \cos(kh)$ and $\tilde{k} - k$ are noticeable and cannot be ignored as shown in Figs. 5-6. The errors are increasing as kh or k increases. Fig. 7(a) shows that for $kh = 0.9$, the errors for the standard and compact schemes are raising and reaching to an unacceptable level when the wave number k increases, but the errors for the second and fourth order new schemes are decreasing as k is increasing. Among the two new schemes, the fourth order produces very accurate computed solutions even when kh is 2 as illustrated in Fig. 7(b).

The solutions for Problem 1 using the fourth order new and compact schemes are compared with the exact solutions as presented in Figs. 8-10 for various k and kh. The results obtained by the second order new and standard schemes are less accurate and will not be shown. The accuracy and the effectiveness of the new schemes are clearly demonstrated, the accuracy deteriorates rapidly as kh is increasing for the compact scheme, whereas the new scheme continues to produce very accurate numerical solution when $kh = 2$.



(a) Real part (b) Imaginary part

FIGURE 9. Comparison of various schemes with $k = 200$ and $h = 1/222(kh \approx 0.9)$.

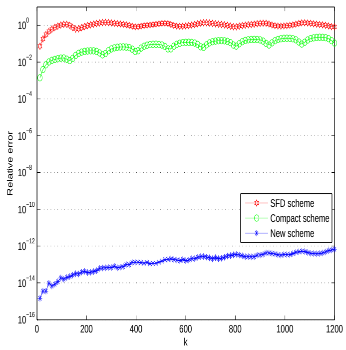


(a) Real part (b) Imaginary part

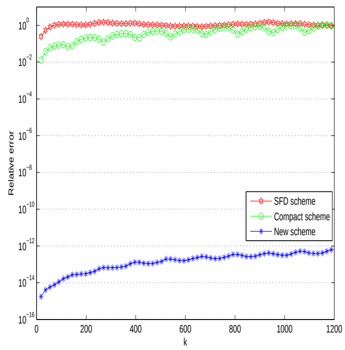
FIGURE 10. Comparison of various schemes with $k = 100$ and $h = 1/50(kh = 2)$.

Problem 2. In Problem 2, we study the case in which the forcing term $f = 1$. This problem had been considered as one of the test cases in [25, 26]. Recall from the derivation of the new schemes, if f does not depend on x, only the first term Y_0 in the summation is not zero and all other terms are zero. Hence, even a simple second order new scheme will not introduce any truncation error and it is capable of producing the exact solution numerically. The remark is confirmed by the results shown in Fig. 11, in which the relative errors for the standard and compact schemes are increasing and reaching to an unacceptable level as k is increasing when kh is fixed. For the new scheme, however, the errors are consistently within the range of 10^{-12} to 10^{-16} (indicating the exact solution is obtained) for all cases regardless the values for k and kh.

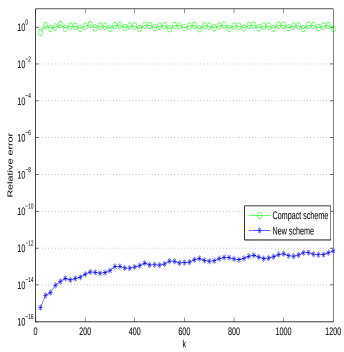
Figs. 12-14 present the numerical solutions for the standard, compact and new schemes for various values of k, kh and h. These results are also compared with the exact solutions. We observe that even for the case $kh \approx 0.6$ and with $k = 100$, the standard difference scheme produces noticeable error in the imaginary part. Moreover, for the case $k = 50$ and $kh \approx 0.9$, the fourth order compact scheme also fails to produce accurate solution for the imaginary part. The new schemes, however, produce accurate computed solutions for all cases.



(a) $kh = 0.6$



(b) $kh = 0.9$



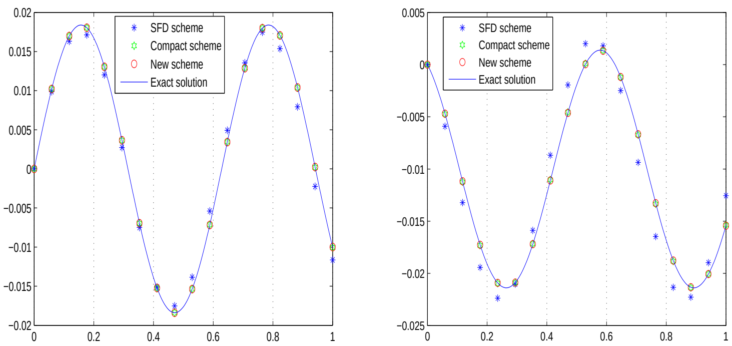
(c) $kh = 2$

FIGURE 11. Relative error in L^2-norm with respect to k (Problem 2).

Problem 3. This problem is similar to Problem 2. Using the NFD scheme, the exact solution is recovered numerically. The plots of the relative errors are similar to those reported in Fig. 11, and the exact numerical value at the discrete grid point can be computed even using $kh = 5$ for a range of k from 100 to 1200. Due to the space limitation, we do not report the detail results.

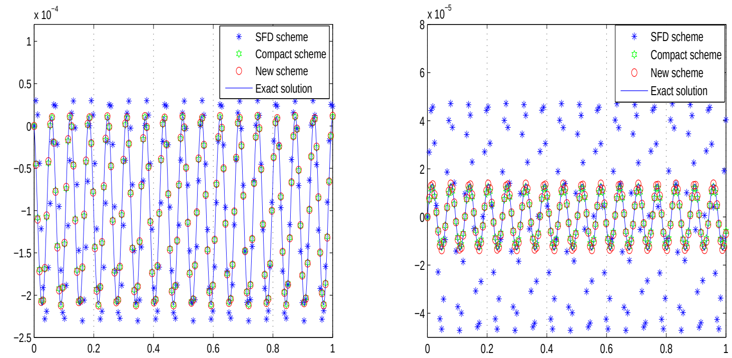
4.2. Varying wave number. The theoretical results presented in this paper are derived for the problems with constant wave numbers. However, to investigate the robustness of the developed new schemes, we now consider the Helmholtz equation with varying wave numbers. It should be pointed out that although the problem has been considered in [8, 11, 18, 13, 31], most of the theoretical or numerical studies in the Helmholtz equation are limited to constant wave numbers.

In the model problem (1)-(3), the constant wave number k suggests that the wave propagates in the homogeneous medium. However, in some cases the medium is



(a) Real part (b) Imaginary part

FIGURE 12. Comparison of various schemes with $k = 10$ and $h = 1/17$ ($kh \approx 0.6$).



(a) Real part (b) Imaginary part

FIGURE 13. Comparison of various schemes with $k = 100$ and $h = 1/167$ ($kh \approx 0.6$).

non-homogeneous, that means that k is not a constant and depends on the position. Hence, the wave number will be replaced by $ka(x)$, where $a(x)$ is known as the inverse of the velocity of the wave. The problem frequently arises in geophysical applications, and the new model equation is now given as follows:

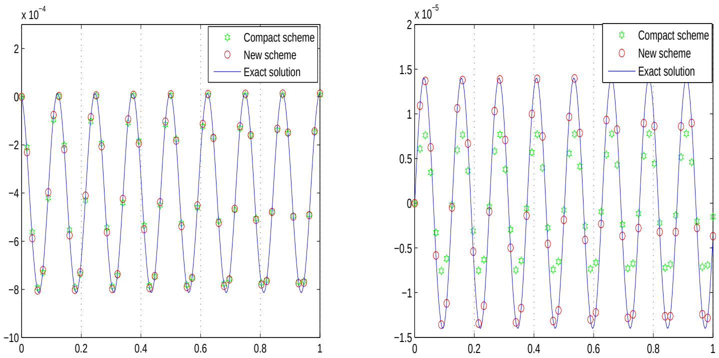
Problem 4:

$$-u_{xx} - (ka(x))^2 u = f(x), \;\; x \in (0,1), \tag{73}$$

$$u(0) = g_1, \tag{74}$$

$$u_x(1) - ika(1)u(1) = g_2, \tag{75}$$

where g_1, g_2 are constant functions. Consider at an interior point x_i, by taking $a(x) = a(x_i)$ and replacing k with $ka(x_i)$, we can easily implement the standard, the compact and the new schemes as before. However, since $a(x_i)$ is only an approximation to $a(x)$ in the neighborhood of $x = x_i$, the original schemes presented in Section 2 may not perform well by simply assuming $ka(x_i)$ is a constant. For



(a) Real part (b) Imaginary part

FIGURE 14. Comparison of various schemes with $k = 50$ and $h = 1/56$ ($kh \approx 0.9$).

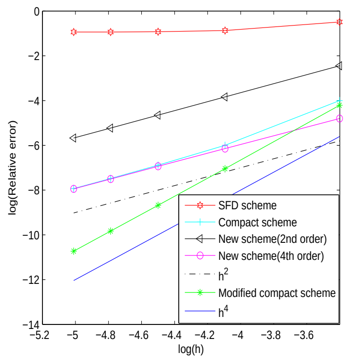
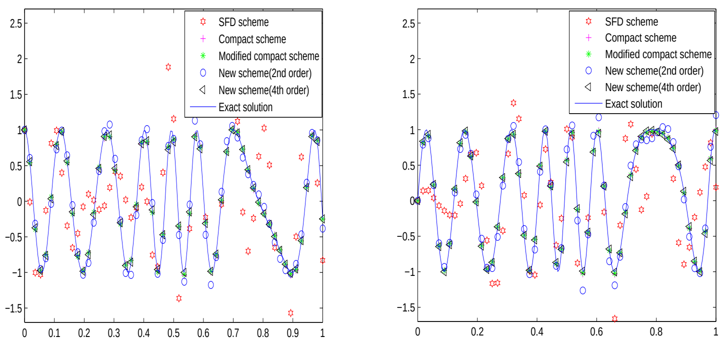
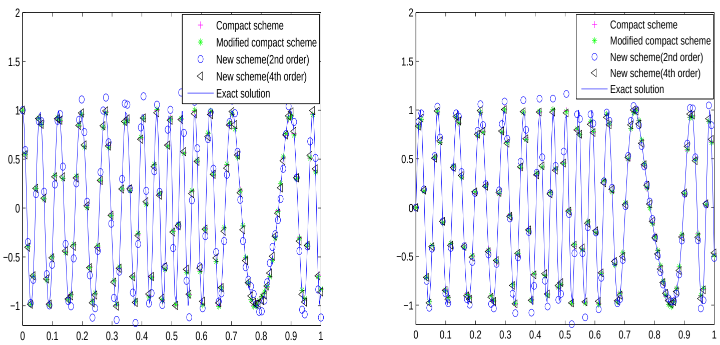


FIGURE 15. Convergence order of various schemes for Problem 4.



(a) Real part (b) Imaginary part

FIGURE 16. Comparison of various schemes with $k = 50$ and $h = 1/56$ ($kh \approx 0.9$).



(a) Real part (b) Imaginary part

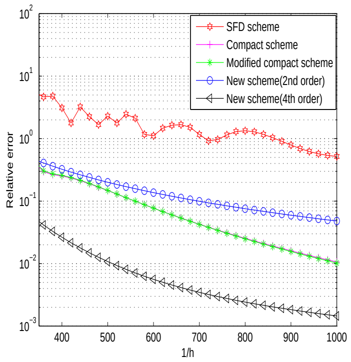
FIGURE 17. Comparison of various schemes with $k = 100$ and $h = 1/111$ ($kh \approx 0.9$).

accurate computational results, we should derive the numerical schemes by taking account of the fact that $ka(x)$ is function of x. For example, following the procedure in [21], we derive a modified compact finite difference scheme (Modified compact scheme) for the varying coefficient problems, and the details are presented in Appendix. The modified compact scheme is more complicated, but we expect it will provide more accurate solutions. It has been found that it is not straightforward to extend the new schemes for varying $ka(x)$. Hence, modified new schemes will not be developed in this work.

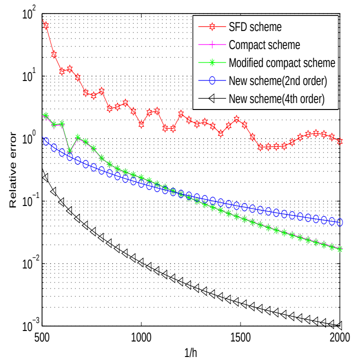
For the test case in Problem 4, we let $a(x) = 1+0.1\cos 10x$, and the exact solution is given by $u(x) = e^{ik(1+0.1\cos 10x)x}$, the right hand side $f(x)$ and g in the boundary condition are determined by (73) and (75). It should be noted that similar forms for $a(x)$ have been considered by other researchers. For example, $a(x) = 1 + c_1 \cos c_2 x$ has been used as a test case in [38], where c_1, c_2 are general constants. Turkel et al. considered a varying coefficient problem with $a(x) = 1 + c_1 \sin c_2 x$ in [11].

To assess the robustness and the performance, we first investigate the convergence order of different schemes for the varying coefficient problem with $k = 20$. From the results presented in Fig. 15, we note that since there exists a error of $O(h^4)$ when using $a(x_i)$ to approximate $a(x)$, the new scheme is only of second order accurate even when the original new scheme is a fourth order scheme for problems with the constant wave numbers. Similarly, the unmodified fourth order compact scheme also reduces to second order convergence for varying wave numbers. The modified compact scheme, however, retains the fourth order convergence.

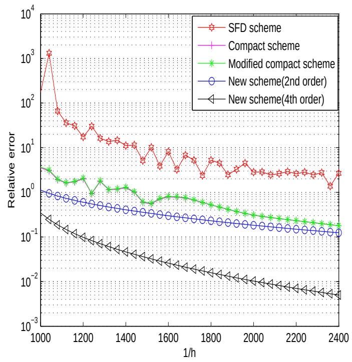
The numerical solutions for $k = 50$ and 100 but keeping $kh \approx 0.9$ are illustrated in Figs. 16 and 17. Among various numerical schemes, the modified compact scheme and the fourth order new scheme produce accurate solutions. To investigate the performance for cases with high wave numbers, we carried out numerical simulations for $k = 500$, 1000 and 2000 (see Fig. 18). It is clear that the unmodified fourth order new scheme produces the best results compared to other schemes considered here. In Fig. 19, we study the pollution effect for varying wave numbers. These results confirm that the standard difference, modified or original compact schemes all suffer from the pollution effect, i.e., the error increases as k increases. However, the errors are consistently bounded for the new schemes even they have



(a) $k = 500$

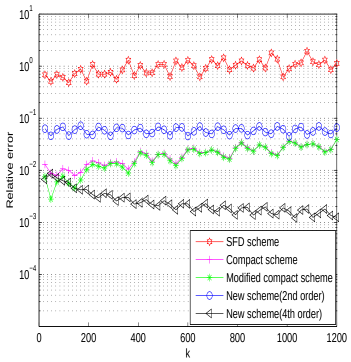


(b) $k = 1000$

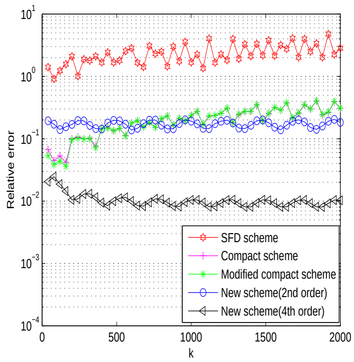


(c) $k = 2000$

FIGURE 18. Relative error with respect to h (Problem 4).



(a) $kh = 0.6$



(b) $kh = 1$

FIGURE 19. Relative error with respect to k (Problem 4).

not been modified to take account of the varying coefficient. The fourth order new scheme produces the best numerical solutions for Problem 4.

5. Conclusions

New finite difference schemes are derived for solving the non-homogeneous one dimensional Helmholtz equation. The new schemes are high order methods, but they have a simple structure as the standard three-point central differences. Convergence and dispersion analysis are presented, and it is proved that the new schemes are pollution free. Numerical simulations are reported for problems with constant and varying wave numbers. The effectiveness and accuracy of the new schemes are validated, and the superior performance compared with the standard and compact difference schemes are clearly demonstrated. The developed new schemes are particularly attractive for problems at high wave numbers. To our knowledge, no other numerical scheme will perform better than the proposed new schemes. Although the new finite difference schemes developed here are only for the one dimensional problem, the idea has been extended to solve the multidimensional Helmholtz equation. Numerical algorithms and simulations for 2D and 3D equations in the polar and spherical coordinates have been reported in [46].

Appendix: Modified compact scheme

To take account of the equation with varying wave numbers, we derive the compact fourth order scheme. First, we consider x_i being the interior point, and let

$$\delta_x^{(1)} u_i = \frac{u_{i+1} - u_{i-1}}{2h},\ \delta_x^{(2)} u_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2},$$

by Taylor expansion, it gives

$$\delta_x^{(2)} u_i = u_i^{(2)} + \frac{h^2}{12} u_i^{(4)} + O(h^4).$$

From the equation with varying coefficients (73), we have

$$\begin{aligned} u_i^{(4)} =& (u_i^{(2)})^{(2)} = (-f_i - k^2 a_i^2 u_i)^{(2)} \\ =& - f_i^{(2)} - k^2 (a_i^2)^{(2)} u_i - 2k^2 (a_i^2)^{(1)} u_i^{(1)} - k^2 a_i^2 u_i^{(2)}. \end{aligned}$$

Using the above two equations, it follows that

$$\begin{aligned} \delta_x^{(2)} u_i =& u_i^{(2)} + \frac{h^2}{12}\big(- f_i^{(2)} - k^2 (a_i^2)^{(2)} u_i - 2k^2 (a_i^2)^{(1)} u_i^{(1)} - k^2 a_i^2 u_i^{(2)}\big) \\ =& - f - k^2 a_i^2 u_i + \frac{h^2}{12}\big(- f_i^{(2)} - k^2 (a_i^2)^{(2)} u_i - 2k^2 (a_i^2)^{(1)} u_i^{(1)} - k^2 a_i^2 \delta_x^{(2)} u_i\big), \end{aligned}$$

which implies that

$$\begin{aligned} &- \big(1 + \frac{k^2h^2}{12} a_i^2 + \frac{k^2h^3}{12} (a_i^2)^{(1)}\big) u_{i+1} + \big(2 - k^2h^2 a_i^2 + \frac{k^2h^2}{6} a_i^2 - \frac{k^2h^4}{12} (a_i^2)^{(2)}\big) u_i \\ &- \big(1 + \frac{k^2h^2}{12} a_i^2 - \frac{k^2h^3}{12} (a_i^2)^{(1)}\big) u_{i-1} = -h^2 (f_i + \frac{h^2}{12} f_i^{(2)}). \end{aligned}$$

Therefore, the modified compact fourth order scheme for the interior point x_i is given by

$$\begin{aligned} &- \big(1 + \frac{k^2h^2}{12} a_i^2 + \frac{k^2h^3}{12} (a_i^2)^{(1)}\big) U_{i+1} + \big(2 - k^2h^2 a_i^2 + \frac{k^2h^2}{6} a_i^2 - \frac{k^2h^4}{12} (a_i^2)^{(2)}\big) U_i \\ &- \big(1 + \frac{k^2h^2}{12} a_i^2 - \frac{k^2h^3}{12} (a_i^2)^{(1)}\big) U_{i-1} = -h^2 (f_i + \frac{h^2}{12} f_i^{(2)}). \end{aligned}$$

Similarly, for the boundary point, we have

$$\delta_x^{(1)} u_i = u_i^{(1)} + \frac{h^2}{6} u_i^{(3)} + O(h^4).$$

Since

$$\begin{aligned} u_i^{(3)} =& (u_i^{(2)})^{(1)} = (-f_i - k^2 a_i^2 u_i)^{(1)} \\ =& - f_i^{(1)} - k^2 (a_i^2)^{(1)} u_i - k^2 a_i^2 u_i^{(1)}, \end{aligned}$$

it follows that

$$\begin{aligned} \delta_x^{(1)} u_i =& u_i^{(1)} + \frac{h^2}{6}\big(- f_i^{(1)} - k^2 (a_i^2)^{(1)} u_i - k^2 a_i^2 u_i^{(1)} \big) \\ =& ika_i u_i + \frac{h^2}{6}\big(- f_i^{(1)} - k^2 (a_i^2)^{(1)} u_i - k^2 a_i^2 \delta_x^{(1)} u_i \big). \end{aligned}$$

After simply calculations, we obtain

$$-u_{i+1} = -u_{i-1} - \frac{ika_i - (h^2 k^2 (a_i^2)^{(1)})/6}{(6 + h^2 k^2 a_i^2)/12h} u_i - \frac{-(h^2 f_i^{(1)})/6}{(6 + h^2 k^2 a_i^2)/12h}.$$

The difference scheme for the boundary condition is then given by

$$-U_{N+1} = -U_{N-1} - \frac{ika_N - (h^2 k^2 (a_N^2)^{(1)})/6}{(6 + h^2 k^2 a_N^2)/12h} U_N - \frac{-(h^2 f_N^{(1)})/6}{(6 + h^2 k^2 a_N^2)/12h}.$$

The modified fourth order compact scheme for varying coefficients is given by:

$$\begin{aligned} &- \big(1 + \frac{k^2h^2}{12} a_j^2 + \frac{k^2h^3}{12} (a_j^2)^{(1)}\big) U_{j+1} + \big(2 - k^2h^2a_j^2 + \frac{k^2h^2}{6} a_j^2 - \frac{k^2h^4}{12} (a_j^2)^{(2)}\big) U_j \\ &- \big(1 + \frac{k^2h^2}{12} a_j^2 - \frac{k^2h^3}{12} (a_j^2)^{(1)}\big) U_{j-1} = -h^2 (f_j + \frac{h^2}{12} f_j^{(2)}), \ 0 < j \le N, \\ &U_0 = 0, \\ &- U_{N+1} + U_{N-1} + \frac{ika_N - (h^2 k^2 (a_N^2)^{(1)})/6}{(6 + h^2 k^2 a_N^2)/12h} U_N = - \frac{-(h^2 f_N^{(1)})/6}{(6 + h^2 k^2 a_N^2)/12h}. \end{aligned}$$

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