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Is Pollution Effect of Finite Difference Schemes Avoidable for Multi-Dimensional Helmholtz Equations with High Wave Numbers?

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Abstract. This paper presents an approach using the method of separation of variables applied to 2D Helmholtz equations in the Cartesian coordinate. The solution is then computed by a series solutions resulted from solving a sequence of 1D problems, in which the 1D solutions are computed using pollution free difference schemes. Moreover, non-polluted numerical integration formulae are constructed to handle the integration due to the forcing term in the inhomogeneous 1D problems. Consequently, the computed solution does not suffer the pollution effect. Another attractive feature of this approach is that a direct method can be effectively applied to solve the tridiagonal matrix resulted from numerical discretization of the 1D Helmholtz equation. The method has been tested to compute 2D Helmholtz solutions simulating electromagnetic scattering from an open large cavity and rectangular waveguide.

AMS subject classifications: 65N06, 65N15, 65N22

Key words: Helmholtz equation, separation of variables, high wave number, pollution free finite difference scheme, large cavity problem, rectangular waveguide.

1 Introduction

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

$$-\Delta u - k^2 u = f, \quad \text{in } \Omega, \tag{1.1}$$

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

The problem arises in many applications related to time harmonic wave propagations, and it has been used to model problems in acoustic, geophysics and electromagnetic wave scattering. There are many difficulties when simulating the Helmholtz equation with high wave numbers, since the solution becomes highly oscillatory when k is very large. The utmost challenge of solving the Helmholtz equation numerically is to eliminate or minimize the pollution error. Due to the pollution effect and in order to ensure the bounded of the relative error [30], conventional numerical algorithms require

$$k^{\gamma_1}(kh)^{\gamma_2}=C_1, \quad \gamma_1>0, \quad \gamma_2\geq 0, \tag{1.2}$$

where h denotes the mesh size and C_1 is a general positive constant. The parameters γ_1 and γ_2 depend on the choice of a specified numerical method. For instance, $\gamma_1=2$, $\gamma_2=2$ and $\gamma_1=1$, $\gamma_2=2$ for the standard finite difference scheme and the finite element method with P_1 element, respectively. Consequently, when the solution is computed by the finite difference and the finite element method, the mesh size $h=\mathcal{O}(1/k^2)$ and $h=\mathcal{O}(1/k^{3/2})$. Therefore, the impact of the pollution effect presents a serious challenge for multi-dimensional problems with high wave number k [5,19,30]. It should be pointed out that the resulting linear system is indefinite and very ill-conditioned, and it is not easy to develop a robust and accurate numerical solver for such systems [6, 9, 16, 17, 22, 36, 43, 59, 60].

Many literatures have been reported devoting to eliminate or minimize the pollution effect, and the reader is referred to [10–12, 14, 15, 24, 25, 27, 34, 37, 41, 42, 44, 45, 48, 51, 53–56] for the finite difference method, and [1, 3, 5, 19, 20, 30–33, 40, 49, 57, 61, 62] for the finite element method. For other numerical techniques, the use of spectral approximation can be found in [46, 47], and the boundary element method in [29, 39]. In these literatures, three common approaches have been considered to overcome the pollution effect, namely, the higher-order method, the parameter method and the combined parameter-higher-order method. For the higher-order finite difference method, we refer to [12, 25, 27, 37, 41, 44, 45, 56]. In [45], Singer and Turkel proposed a fourth order finite difference scheme based on the Pade approximation. Fu [25] proved the error estimate for a compact fourth order method and claimed that the scheme is independent of the wave number. However, the theoretical analysis and numerical results (see [55]) revealed that the error of classical finite difference methods do depend on the wave number in multi-dimensional problems. Higher-order finite element method has been developed to minimize the pollution effect by increasing the order of the polynomial basic functions, and it is usually referred as the p-version FEM (see [1, 30, 32, 40]). In a parameter method, the performance of the finite difference scheme is improved by choosing a suitable parameter [14, 15, 34, 42, 48, 56]. Jo et al. [34] derived a rotated 9-points difference scheme by combining two second derivative operators for the 2D Helmholtz equation. Further investigation is reported in [48] by extending to the rotated 25-points finite difference scheme. Recently, Chen et al. adapted this idea and proposed a new strategy for choosing optimal parameter in [14] and con-

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sidered the three-dimensional problem in [15]. More results on the parameter finite element methods can be found in [3, 5, 30, 31, 40, 57, 61, 62]. Another popular way is the parameter-higher-order method constructed by combining the high-order scheme with the parameter scheme [3, 4, 14, 15, 19, 49, 61].

Although some improvements have been observed, almost all of these methods discussed above can only minimize the pollution effect in some sense. Moreover, the way to determine the global optimal parameter is usually unknown. Based on the current literatures on solving the Helmholtz equation by numerical methods, the error estimates can be summarized as follows: under suitable conditions, we have

$$\frac{||u-U||}{||u||} \leq C_1 k^2 (kh)^2, \tag{1.3}$$

for the standard second order finite difference method;

$$\frac{||u-U||}{||u||} \leq C_1 k^2 (kh)^4, \tag{1.4}$$

for the fourth order compact difference scheme;

$$\frac{||(u-U)'||}{||u'||} \leq C_1 \Big(\Big(\frac{kh}{2p}\Big)^p + k \Big(\frac{kh}{2p}\Big)^{2p} \Big), \tag{1.5}$$

for the p-version finite element method (see [30,32]). Here, $||\cdot||$ is the L^2-norm, u' denotes the first derivative of u, u and U are the solution of the Helmholtz equation and the corresponding numerical approximation. By assuming $p > C_1 \ln k$, Melenk and Sauter [40] improved the error estimate for the p-version finite element method and show that

$$\frac{||u-U||_{\mathcal{H}}}{||u||_{\mathcal{H}}} \leq C_1 \Big(\frac{h}{p} + \Big(\frac{kh}{\sigma p}\Big)^p \Big), \tag{1.6}$$

where σ is a positive constant, and $||u||_{\mathcal{H}} = \big(||u'||^2 + k^2 ||u||^2\big)^{1/2}$.

These results clearly indicate that due to the pollution effect, the error is closely related to the wave number k. In spite of the conventional rule of thumb requiring about 8 to 10 grid points per wavelength in order to ensure a reliable solution for wave propagation problems (i.e. $kh \approx 0.6$ to 0.8), the mesh size h must be much finer and

$$kh \ll 1, \tag{1.7}$$

in order to obtain a reasonable accurate numerical solution for the Helmholtz equation at high wave numbers by applying these methods. It has generally been accepted that the pollution effect is unavoidable for the finite element method (FEM) in simulating multi-dimensional Helmholtz equation at high wave number [5].

The present study aims to demonstrate that pollution free numerical schemes can be developed for certain multi-dimensional problems, and the error is not depended upon

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the wave number k. Hence, to obtain a reliable accurate numerical solution, we only need the condition

$$kh = C_1. \tag{1.8}$$

The idea is firstly suggested in [37], in which the authors constructed a new finite difference scheme with optimal weights determined by symbolic computation and the new scheme is exact for the 1D homogeneous Helmholtz equation with the Dirichlet boundary condition. Motivated by this work, Wong and Li [56] and Wang and Wong [54] developed a global difference scheme for 1D Helmholtz problem. In stead of using a truncated series approach, the new scheme is derived by satisfying the original Helmholtz equation and utilizing all terms in the Taylor series expansion. For a 1D inhomogeneous model with the radiation boundary condition, it has been proven that the numerical solution is pollution free and the error is independent of the wave number k. The new scheme produces exact numerical solution even when $kh > 1$ provided the forcing term is constant, and it has also been tested for problems with varying wave numbers. Using the method of separation of variables, Wang et al. [55] recently extended the new scheme for multi-dimensional Helmholtz equations, and demonstrated that pollution free numerical solution can be computed for problems in 2D annulus domain in the polar coordinate and in 3D hollow sphere domain in the spherical coordinate. The results of our previous study confirm that the relative error is independent of k and can be estimated by

$$\frac{||u-U||}{||u||} \leq C_1 h^{n-1}, \tag{1.9}$$

where n is the convergence order.

In this study, we demonstrate that it is possible to extend the pollution free numerical scheme to the 2D Helmholtz equation in Cartesian coordinates. However, different from the 2D problems in polar coordinates, the formulation produces integration terms due to the forcing and the boundary condition and they may be effected by the wave number k. Special numerical integration formulae are derived in order to eliminate the pollution error. The remaining article is organized as follows. In Section 2, we introduce two models in Cartesian coordinates. Section 3 devotes to the method for the numerical solutions, and the derivation of the pollution free difference schemes for the Helmholtz equation and the non-polluted numerical integration are presented. To validate the performance of the numerical algorithms, simulation results for two test cases are reported in Section 4. Finally, conclusions and future works are given in Section 5.

2 Problems in Cartesian coordinates

Assuming the domain in (1.1) is defined by $\Omega := (0,a) \times (0,b)$, we consider two real problems which are used to model by this equation and arise in science and engineering applications.

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Case 1: Electromagnetic scattering from an open large cavity

The problem has been studied in [6, 8, 13, 20, 38, 59, 60] for a rectangular domain with boundary conditions given by

$$u=0, \quad \text{on } \{0\}\times(0,b)\cup(0,a)\times\{0\}\cup\{a\}\times(0,b), \tag{2.1}$$

$$\frac{\partial u}{\partial \nu}=T(u)+g_1, \quad \text{on } (0,a)\times\{b\}, \tag{2.2}$$

where

$$T(u)=\frac{jk}{2}\oint_0^a \frac{1}{|x-x'|}H_1^{(1)}(k|x-x'|)u(x',b)dx'$$

with $\oint$ denoting a Hadamard finite-part integral (see [50,58]), $j^2=-1$ and $H_1^{(1)}$ being the first order Hankel function of the first kind, $g_1(x)$ is a given function and ν is the outward normal vector.

One of the difficulties in the present formulation is due to the nonlocal operator $T(u)$ in (2.2) which will destroy the sparsity of the linear system. Another challenge is that higher smoothness of the solution is required to handle the singularity of the kernel function in the integral operator, and more seriously "pollution effect" in approximation of the numerical integration will be resulted. Many works are developed to address these problems (see [21,26,30,50,58]). A popular procedure is to approximate the nonlocal operator by a local one. Here, by applying the second order approximation (see [21,26,30]), a local operator $\hat{T}(u)$ is constructed to replace $T(u)$ in (2.2), where

$$\hat{T}(u):=\Big(jk+\frac{3j}{4k}\frac{\partial^2}{\partial x^2}-\frac{1}{4k^2}\frac{\partial^3}{\partial y\partial x^2}\Big)u. \tag{2.3}$$

Now, applying the classical mathematical technique as described in [28], it is not hard to verify that the eigenfunction in the x-direction is given by $\sin(m\pi x/a)$ with m being a positive integer. Thus the solution of (1.1), (2.1)-(2.2) can be expressed as a series solution defined as follows:

$$u=\sum_{m=1}^{\infty}\tilde{u}_m(y)\sin\Big(\frac{m\pi}{a}x\Big). \tag{2.4}$$

Consequently, by using (2.3) and (2.4), the solution of the cavity problem (1.1), (2.1)-(2.2) can now be computed by solving a sequence of the following one-dimensional Helmholtz equations in the y-direction:

$$-\tilde{u}_m''(y)-\tilde{k}^2\tilde{u}_m(y)=\tilde{f}_m(y), \quad y\in(0,b), \tag{2.5}$$

$$\tilde{u}_m(0)=0, \tag{2.6}$$

$$\Big(1-\frac{1}{4k^2}\Big(\frac{m\pi}{a}\Big)^2\Big)\tilde{u}_m'(b)=\Big(jk-\frac{3j}{4k}\Big(\frac{m\pi}{a}\Big)^2\Big)\tilde{u}_m(b)+\tilde{g}_{1,m}(b), \tag{2.7}$$

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where

$$\tilde{k}^2 = k^2 - \left(\frac{m\pi}{a}\right)^2, \tag{2.8}$$

$$\tilde{f}_m(y) = \frac{2}{a}\int_0^a f(x,y)\sin\left(\frac{m\pi}{a}x\right)dx, \tag{2.9}$$

$$\tilde{g}_{1,m}(b) = \frac{2}{a}\int_0^a g_1(x,b)\sin\left(\frac{m\pi}{a}x\right)dx. \tag{2.10}$$

Here, the boundary condition (2.6)-(2.7) are derived by multiplying (2.1)-(2.2) with the eigenfunction $\sin(m\pi x/a)$ and then integrating from 0 to a in the x-direction. Obviously, when $(1-\frac{(m\pi/a)^2}{4k^2})=0$, the boundary condition (2.7) reduces to the Dirichlet condition which is a trivial case. In this study, we focus on cases in which $(1-\frac{(m\pi/a)^2}{4k^2})\neq 0$.

Case 2: Rectangular waveguide

The solution of this problem satisfies the 2D Helmholtz equation with the boundary conditions given by

$$\frac{\partial u}{\partial \nu} = 0, \quad \text{on } (0,a)\times\{b\}\cup(0,a)\times\{0\}, \tag{2.11}$$

$$\frac{\partial u}{\partial \nu} = g_2, \quad \text{on } \{0\}\times(0,b), \tag{2.12}$$

$$\frac{\partial u}{\partial \nu} = -jku, \quad \text{on } \{a\}\times(0,b), \tag{2.13}$$

where g_2 is a given function. Here, solid wall conditions are imposed at two ends in the y-direction, and a source term is placed on the left and a radiation condition is specified at the right in the x-direction. The problem has been investigated in [9, 35, 36].

Due to the homogeneous Neumann boundary condition imposed on the boundary $y=0$ and $y=b$, it is easy to verify that the eigenfunction in the y-direction is given by $\cos(m\pi y/b)$. By multiplying (1.1), (2.11)-(2.13) with $\cos(m\pi y/b)$, respectively and integrating from 0 to b, the solution can be expressed as

$$u = \sum_{m=1}^{\infty} \hat{u}_m(x)\cos\left(\frac{m\pi}{b}y\right). \tag{2.14}$$

Here, $\hat{u}_m(x)$ is the solution of the following one-dimensional Helmholtz equation in the x-direction:

$$-\hat{u}_m''(x) - \hat{k}^2\hat{u}_m(x) = \hat{f}_m(x), \quad x\in(0,a), \tag{2.15}$$

$$\hat{u}_m'(0) = \hat{g}_{2,m}, \tag{2.16}$$

$$\hat{u}_m'(a) = -jk\hat{u}_m(a), \tag{2.17}$$

where $\hat{k}^2 = k^2 - (m\pi/b)^2$,

$$\hat{f}_m = \frac{2}{b}\int_0^b f(x,y)\cos(m\pi y/b)dy \quad \text{and} \quad \hat{g}_{2,m} = \frac{2}{b}\int_0^b g_2(a,y)\cos(m\pi y/b)dy.$$

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3 Method for solutions

Using the method of separation of variables, the solution of the 2D Helmholtz equation is obtained by solving a sequence of 1D problems given in (2.5)-(2.7) for Case 1 and (2.15)-(2.17) for Case 2. The main contribution of this work is to present pollution free numerical schemes to discretize the differential equation and the boundary condition. Since the formulations for Case 1 and Case 2 are similar, we will focus on the implementation for Case 1.

3.1 Pollution free difference schemes

The Helmholtz equation given in Eq. (2.5) is inhomogeneous with a constant wave number, since k is constant for a fixed value of m. Pollution free numerical algorithms have already been developed, and the detailed derivation is given in [54]. For completeness, we will briefly describe the numerical scheme.

Let $h=\frac{b}{N}(N\in Z^+)$ satisfy $0<h<1$, denote the grid point as $y_i=ih$ $(i\in Z,\ 0<i\leq N)$. By applying the Taylor expansion, we have

$$\begin{aligned}\tilde{u}_m(y_i+h)=&\tilde{u}_m(y_i)+h\tilde{u}_m^{(1)}(y_i)+\frac{h^2}{2!}\tilde{u}_m^{(2)}(y_i)+\frac{h^3}{3!}\tilde{u}_m^{(3)}(y_i)+\cdots\\&+\frac{h^n}{n!}\tilde{u}_m^{(n)}(y_i)+\cdots,\end{aligned}\tag{3.1}$$

$$\begin{aligned}\tilde{u}_m(y_i-h)=&\tilde{u}_m(y_i)-h\tilde{u}_m^{(1)}(y_i)+\frac{h^2}{2!}\tilde{u}_m^{(2)}(y_i)-\frac{h^3}{3!}\tilde{u}_m^{(3)}(y_i)+\cdots\\&+(-1)^n\frac{h^n}{n!}\tilde{u}_m^{(n)}(y_i)+\cdots,\end{aligned}\tag{3.2}$$

where $\tilde{u}_m^{(n)}(y_i)$ denotes the n-th derivative of $\tilde{u}_m(y)$ at y_i. By adding (3.1) and (3.2), it gives

$$\begin{aligned}\tilde{u}_m(y_i+h)+\tilde{u}_m(y_i-h)=2\Big[&\tilde{u}_m(y_i)+\frac{h^2}{2!}\tilde{u}_m^{(2)}(y_i)+\frac{h^4}{4!}\tilde{u}_m^{(4)}(y_i)+\frac{h^6}{6!}\tilde{u}_m^{(6)}(y_i)+\cdots\\&+\frac{h^{2n}}{(2n)!}\tilde{u}_m^{(2n)}(y_i)+\cdots\Big].\end{aligned}\tag{3.3}$$

From Eq. (2.5), we have

$$\begin{aligned}\tilde{u}_m^{(2n)}(y_i)=&(-1)^n\tilde{k}^{2n}\tilde{u}_m(y_i)+(-1)\tilde{f}_m^{(2n-2)}(y_i)+\cdots\\&+(-1)^{n-1}\tilde{k}^{2n-4}\tilde{f}_m^{(2)}(y_i)+(-1)^n\tilde{k}^{2n-2}\tilde{f}_m(y_i).\end{aligned}$$

Under the assumption

$$\tilde{k}h=constant\quad\text{and}\quad||\tilde{f}_m^{(n)}||\leq M_1,\tag{3.4}$$

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with M_1 being a general constant independent of k, using the above equations and the series expansion for trigonometric function, Eq. (3.3) can be rewritten as

$$\tilde{u}_m(y_i+h)+\tilde{u}_m(y_i-h)=2\big[\cos(\tilde{k}h)\tilde{u}_m(y_i)+F(\tilde{f}_m(y_i))\big], \tag{3.5}$$

where

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

and

$$\begin{aligned}
&Y_0=\frac{[\cos(\tilde{k}h)-1]}{\tilde{k}^2}\tilde{f}_m(y_i)\sim\mathcal{O}(h^2),\\
&Y_1=(-1)\frac{[\cos(\tilde{k}h)-1+\frac{(\tilde{k}h)^2}{2!}]}{\tilde{k}^4}\tilde{f}_m^{(2)}(y_i)\sim\mathcal{O}(h^4),\\
&\quad\vdots\\
&Y_{n-1}=(-1)^{n-1}\frac{\big[\cos(\tilde{k}h)-1+\frac{(\tilde{k}h)^2}{2!}-\cdots+(-1)^n\frac{(\tilde{k}h)^{2n-2}}{(2n-2)!}\big]}{\tilde{k}^{2n}}\tilde{f}_m^{(2n-2)}(y_i)\sim\mathcal{O}(h^{2n}),\\
&\quad\vdots
\end{aligned}$$

in L^2-norm.

For simplicity, we let $\tilde{u}_{m,i}=\tilde{u}_m(y_i)$, $\tilde{u}_{m,i+1}=\tilde{u}_m(y_i+h)$, $\tilde{u}_{m,i-1}=\tilde{u}_m(y_i-h)$. Hence, for any interior grid point y_i, assuming that $\tilde{f}_m$,$\tilde{g}_{1,m}$ are independent of the wave number, a pollution free discretization scheme for (2.5) can be constructed from (3.5), such that

$$-\tilde{U}_{m,i+1}+2\cos(\tilde{k}h)\tilde{U}_{m,i}-\tilde{U}_{m,i-1}=-2F_n(\tilde{f}_{m,i}), \tag{3.6}$$

where $\tilde{U}_{m,i}$ is the approximation of $\tilde{u}_{m,i}$ and

$$F_n(\tilde{f}_{m,i})=\sum_{m=0}^{n-1}Y_m=Y_0+Y_1+\cdots+Y_{n-1}.$$

It is important to note that the error terms are independent of the wave number k under the assumption of (3.4). Moreover, the numerical scheme is exact (i.e., no error) by taking only Y_0 if $\tilde{f}_m(y_i)$ is zero or a constant. However, to obtain an accurate numerical solution for (2.5)-(2.7), a pollution free scheme must be constructed for the boundary condition (2.7). Using a similar procedure for the interior point, from the Taylor series expansion and the original equation (2.5), we have

$$\begin{aligned}
\tilde{u}_m(y_i+h)-\tilde{u}_m(y_i-h)=2\Big[&h\tilde{u}_m^{(1)}(y_i)+\frac{h^3}{3!}\tilde{u}_m^{(3)}(y_i)+\frac{h^5}{5!}\tilde{u}_m^{(5)}(y_i)+\cdots\\
&+\frac{h^{2n+1}}{(2n+1)!}\tilde{u}_m^{(2n+1)}(y_i)+\cdots\Big],
\end{aligned} \tag{3.7}$$

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and

$$\tilde{u}_m^{(2n+1)}(y_i)=(-1)^n\tilde{k}^{2n}\tilde{u}_m^{(1)}(y_i)+(-1)\tilde{f}_m^{(2n-1)}(y_i)+\cdots+(-1)^n\tilde{k}^{2n-2}\tilde{f}_m^{(1)}(y_i).$$

Therefore, it follows that

$$\tilde{k}[\tilde{u}_m(y_i+h)-\tilde{u}_m(y_i-h)]=2\left[\sin(\tilde{k}h)\tilde{u}_m^{(1)}(y_i)+B(\tilde{f}_m(y_i))\right], \tag{3.8}$$

where

$$B(\tilde{f}_m(y_i))=\sum_{m=1}^{+\infty}Z_m=Z_1+Z_2+\cdots+Z_n+\cdots,$$

and

$$\begin{aligned}
Z_1&=\frac{\sin(\tilde{k}h)-\tilde{k}h}{\tilde{k}^2}\tilde{f}_m^{(1)}(y_i)\sim\mathcal{O}(h^2),\\
Z_2&=(-1)\frac{\sin(\tilde{k}h)-\tilde{k}h+\frac{(\tilde{k}h)^3}{3!}}{\tilde{k}^4}\tilde{f}_m^{(3)}(y_i)\sim\mathcal{O}(h^4),\\
&\vdots\\
Z_n&=(-1)^{n-1}\frac{\sin(\tilde{k}h)-\tilde{k}h+\frac{(\tilde{k}h)^3}{3!}+\cdots+\frac{(\tilde{k}h)^{2n-1}}{(2n-1)!}}{\tilde{k}^{2n}}\tilde{f}_m^{(2n-1)}(y_i)\sim\mathcal{O}(h^{2n}),\\
&\vdots
\end{aligned}$$

in L^2-norm. Finally, a pollution free difference scheme for the boundary condition (2.7) is given by

$$-\tilde{U}_{m,N+1}+\frac{2c_1\sin(\tilde{k}h)\tilde{U}_{m,N}}{\tilde{k}}+\tilde{U}_{m,N-1}=-\frac{2c_2\sin(\tilde{k}h)\tilde{g}_{1,m}+B_n(\tilde{f}_{m,N})}{\tilde{k}}, \tag{3.9}$$

where

$$\begin{aligned}
c_1&=\left(jk-\frac{3j}{4k}\left(\frac{m\pi}{a}\right)^2\right)/\left(1-\frac{1}{4k^2}\left(\frac{m\pi}{a}\right)^2\right),\\
c_2&=1/\left(1-\frac{1}{4k^2}\left(\frac{m\pi}{a}\right)^2\right),\\
B_n(\tilde{f}_{m,N})&=\sum_{m=1}^{n}Z_m=Z_1+Z_2+\cdots+Z_n.
\end{aligned}$$

Hence, by combining (3.6), (2.1) and (3.9), pollution free difference schemes of $2n$-order accurate for (2.5)-(2.7) can be expressed as follows:

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NFD:

$$\begin{aligned}
&-\tilde{U}_{m,i+1}+2\cos(\tilde{k}h)\tilde{U}_{m,i}-\tilde{U}_{m,i-1}=-2F_n(\tilde{f}_{m,i}), \quad 0<i\leq N,\\
&\tilde{U}_{m,0}=0,\\
&-\tilde{U}_{m,N+1}+\frac{2c_1\sin(\tilde{k}h)\tilde{U}_{m,N}}{\tilde{k}}+\tilde{U}_{m,N-1}=-\frac{2c_2\sin(\tilde{k}h)\tilde{g}_{1,m}+B_n(\tilde{f}_{m,N})}{\tilde{k}}.
\end{aligned}$$

It has been proven in [54] that the NFD scheme is pollution free under the assumption that the L^2-norms of $\tilde{f}_m$ and $\tilde{f}_m^{(n)}$ are independent of the wave number k.

3.2 Pollution free numerical integration formula

In the present formulation, $\tilde{f}_m$ and $\tilde{g}_{1,m}$ are expressed as integral forms defined in (2.9)-(2.10). Not only they depend on f and g_1 from the original problem (1.1) and (2.2), but they are also affected by the eigenfunction $\sin(\frac{m\pi}{a}x)$ in the x-direction. On the other hand, in a practical computation, the solution is obtained by a truncated series summing from $m=1$ to M in (2.4), where M is a constant. However, to ensure that the error $||u-\sum_{m=1}^{M}\tilde{u}_m(y)\sin(m\pi x/a)||$ is sufficiently small, we require

$$\frac{m\pi}{a}=\mathcal{O}(kb). \tag{3.10}$$

Hence, $\tilde{f}_m$ and $\tilde{g}_{1,m}$ may indeed depend on the wave number k, and the "pollution effect" will be admitted in the computed solution. In fact applying a classical composite numerical integration rule (such as the Newton-Cotes rule or Gauss rule), a typical remainder term can be estimated as

$$O(\bar{f}^{(n)}h^n),$$

where $\bar{f}=f\sin(m\pi y/a)$ or $g_1\sin(m\pi y/a)$. Therefore, considering (3.10), it holds, under the assumption of (3.4), that

$$||\bar{f}^{(n)}h^n||=\mathcal{O}(k^{\alpha(n)})$$

with $\alpha(n)\geq 0$ being a function of n. This will deteriorate the convergence order of the discrete scheme. Worse more, the presence of the "pollution effect" may appear. Now, to obtain a pollution free computed solution, we develop new numerical integration formulae for $\tilde{f}_m$ and $\tilde{g}_{1,m}$, so that the error is independent of the wave number k under the assumption of (3.4).

Consider a given function $v(x)$, and f_μ is determined such that $v(x)$ satisfies the one-dimensional Helmholtz equation

$$-v''(x)-k_\mu^2 v(x)=f_\mu(x), \quad x\in(0,a), \tag{3.11}$$

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where $k_\mu = \mathcal{O}(k) > 0$ will take different values at different occurrences. Obviously, $\sin(m\pi x/a)$ satisfies (3.11) when $k_\mu = m\pi/a$ and $f_\mu(x) = 0$. Hence, let $f_\mu(x) = 0$ in (3.11), and note that the following derivation can be modified if $f_\mu(x) \neq 0$. Now, consider new definition for the difference quotient which will be frequently used in the following. To construct new difference formulae for the first derivative, we use the Taylor expansion (3.1) and Eq. (3.11), then apply a similar derivation reported for (3.5) and (3.8). Hence,

$$\begin{aligned} v(x_i+h) =& v(x_i)+hv^{(1)}(x_i)+\frac{h^2}{2!}v^{(2)}(x_i)+\frac{h^3}{3!}v^{(3)}(x_i)+\cdots+\frac{h^n}{n!}v^{(n)}(x_i)+\cdots \\ =& hv^{(1)}(x_i)+\frac{h^3}{3!}v^{(3)}(x_i)+\cdots+\frac{h^{(2n+1)}}{(2n+1)!}v^{(2n+1)}(x_i)+\cdots \\ &+v(x_i)+\frac{h^2}{2!}v^{(2)}(x_i)+\cdots+\frac{h^{(2n)}}{(2n)!}v^{(2n)}(x_i)+\cdots \\ =& \frac{\sin(k_\mu h)v^{(1)}(x_i)}{k_\mu}+\cos(k_\mu h)v(x_i). \end{aligned} \tag{3.12}$$

Thus, the new forward numerical difference quotient is given by

$$\textbf{NFNDQ1:} \quad v_i^{(1)} = \frac{k_\mu[v_{i+1}-\cos(k_\mu h)v_i]}{\sin k_\mu h}. \tag{3.13}$$

Similarly, the new backward numerical difference quotient is:

$$\textbf{NBNDQ1:} \quad v_i^{(1)} = \frac{k_\mu[\cos(k_\mu h)v_i-v_{i-1}]}{\sin k_\mu h}. \tag{3.14}$$

Thanks to (3.8), we have the new central numerical difference quotient

$$\textbf{NCNDQ1:} \quad v_i^{(1)} = \frac{k_\mu[v_{i+1}-v_{i-1}]}{2\sin k_\mu h}. \tag{3.15}$$

To extend for the second derivative, we derive the new forward numerical difference quotient using the definition of (3.13) and (3.14),

$$\textbf{NFNDQ2:} \quad v_i^{(2)} = \frac{k_\mu^2[v_{i+2}-2\cos(k_\mu h)v_{i+1}+\cos^2(k_\mu h)v_i]}{\sin^2 k_\mu h}, \tag{3.16}$$

and the new backward numerical difference quotient

$$\textbf{NBNDQ2:} \quad v_i^{(2)} = \frac{k_\mu^2[\cos^2(k_\mu h)v_i-2\cos(k_\mu h)v_{i-1}+v_{i-2}]}{\sin^2 k_\mu h}. \tag{3.17}$$

Due to (3.3), it holds

$$\textbf{NCNDQ2:} \quad v_i^{(2)} = \frac{k_\mu^2[v_{i+1}-2v_i+v_{i-1}]}{4\sin^2(k_\mu h/2)}. \tag{3.18}$$

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Remark 3.1. Different from the classical numerical difference quotient, the derived new formulae are exact and without any truncation error. Furthermore, when $k_\mu h \to 0$, the new formulae (3.13)-(3.15) convert back to the classical forward (FNDQ1), backward (FNBQ1) and central (CNDQ1) numerical difference quotients for the first derivative; and (3.18) converts to the standard central numerical difference quotient (CNDQ2) for the second derivative.

Remark 3.2. Similar procedure can be applied to construct new difference quotients for higher order derivatives $v^{(n)}$.

Next, we construct new numerical integration rules related to (3.11) in which the error is not affected by the wave number. Consider two cases with the integration has the form given by

$$\int_0^a v\tilde{v}dx. \tag{3.19}$$

For Case I, consider $v^{(n)}$ or $\tilde{v}^{(n)}$ depending on k. Without loss of generality, let $v^{(n)}$ be independent of k and $\tilde{v}^{(n)}$ depend on k. Assuming that $x\in[x_i,x_{i+1}]$, (3.12) suggests that

$$\tilde{v}(x)=\frac{\sin(k_\mu(x-x_i))\tilde{v}^{(1)}(x_i)}{k_\mu}+\cos(k_\mu(x-x_i))\tilde{v}(x_i). \tag{3.20}$$

Applying (3.20) and using the piecewise linear Lagrange interpolation $\Pi_1 v$ to approximate v, we have

$$\begin{aligned}\int_0^a v\tilde{v}dx&=\sum_{i=0}^{N-1}\int_{x_i}^{x_{i+1}}\Pi_1 v\tilde{v}dx+\mathcal{O}(\tilde{v}h^2+\tilde{v}^{(1)}h^3)\\&=\sum_{i=0}^{N-1}\int_{x_i}^{x_{i+1}}\Pi_1 v\Big(\frac{\sin(\tilde{k}_\mu(x-x_i))\tilde{v}^{(1)}(x_i)}{\tilde{k}_\mu}\\&\quad+\cos(\tilde{k}_\mu(x-x_i))\tilde{v}(x_i)\Big)dx+\mathcal{O}(\tilde{v}h^2+\tilde{v}^{(1)}h^3).\end{aligned}$$

After simple calculations, the new numerical integration rule corresponding to the composite Trapezoidal rule is followed

$$\begin{aligned}\textbf{NNIR1:}\quad\int_0^a v\tilde{v}dx\approx\sum_{i=0}^{N-1}\big(&A_1v(x_i)\tilde{v}^{(1)}(x_i)+A_2v(x_i)\tilde{v}(x_i)\\&+A_3v(x_{i+1})\tilde{v}^{(1)}(x_i)+A_4v(x_{i+1})\tilde{v}(x_i)\big),\end{aligned} \tag{3.21}$$

with $\tilde{v}^{(1)}$ defined in (3.13), and the coefficients given by

$$\begin{aligned}A_1&=-\frac{\sin(\tilde{k}_\mu h)-\tilde{k}_\mu h}{\tilde{k}_\mu^3 h}, & A_2&=-\frac{\cos(\tilde{k}_\mu h)-1}{\tilde{k}_\mu^2 h},\\A_3&=\frac{\sin(\tilde{k}_\mu h)-\tilde{k}_\mu h\cos(\tilde{k}_\mu h)}{\tilde{k}_\mu^3 h}, & A_4&=\frac{\cos(\tilde{k}_\mu h)+\tilde{k}_\mu h\sin(\tilde{k}_\mu h)-1}{\tilde{k}_\mu^2 h}.\end{aligned}$$

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By applying the piecewise second order Lagrange interpolation $\Pi_2 v$ to v, we obtain

$$\begin{aligned}\int_0^a v\tilde{v}dx &= \sum_{i=0}^{N/2-1}\int_{x_{2i}}^{x_{2(i+1)}} \Pi_2 v\tilde{v}dx+\mathcal{O}(\tilde{v}h^4+\tilde{v}^{(1)}h^5),\\ &= \sum_{i=0}^{N/2-1}\int_{x_{2i}}^{x_{2(i+1)}} \Pi_2 v\Big(\frac{\sin(\tilde{k}_\mu(x-x_{i+1}))\tilde{v}^{(1)}(x_{i+1})}{\tilde{k}_\mu}\\ &\quad +\cos(\tilde{k}_\mu(x-x_{i+1}))\tilde{v}(x_{i+1})\Big)dx+\mathcal{O}(\tilde{v}h^4+\tilde{v}^{(1)}h^5).\end{aligned}$$

The new numerical integration rule corresponding to the composite Simpson's rule is written as

$$\begin{aligned}\textbf{NNIR2:}\quad \int_0^a v\tilde{v}dx \approx &\sum_{i=0}^{N/2-1}\big(\tilde{A}_1 v(x_{2i})\tilde{v}^{(1)}(x_{2i+1})+\tilde{A}_2 v(x_{2i})\tilde{v}(x_{2i+1})\\ &+\tilde{A}_3 v(x_{2i+1})\tilde{v}(x_{2i+1})+\tilde{A}_4 v(x_{2i+2})\tilde{v}^{(1)}(x_{2i+1})\\ &+\tilde{A}_5 v(x_{2i+2})\tilde{v}(x_{2i+1})\big),\end{aligned}\tag{3.22}$$

with $\tilde{v}^{(1)}$ defined in (3.13), and

$$\begin{aligned}\tilde{A}_1 &= -\frac{\sin(\tilde{k}_\mu h)-\tilde{k}_\mu h\cos(\tilde{k}_\mu h)}{\tilde{k}_\mu^3 h},\\ \tilde{A}_2 &= \frac{\tilde{k}_\mu^2 h^2\sin(\tilde{k}_\mu h)+2\tilde{k}_\mu h\cos(\tilde{k}_\mu h)-2\sin(\tilde{k}_\mu h)}{\tilde{k}_\mu^3 h^2},\\ \tilde{A}_3 &= -\frac{4(\tilde{k}_\mu h\cos(\tilde{k}_\mu h)-\sin(\tilde{k}_\mu h))}{\tilde{k}_\mu^3 h^2},\\ \tilde{A}_4 &= \frac{\sin(\tilde{k}_\mu h)-\tilde{k}_\mu h\cos(\tilde{k}_\mu h)}{\tilde{k}_\mu^3 h},\\ \tilde{A}_5 &= \tilde{A}_2.\end{aligned}$$

Now, let v and $\tilde{v}$ both depend on k as in Case II, namely

$$\begin{aligned}\int_0^a v\tilde{v}dx = \sum_{i=0}^{N-1}\int_{x_i}^{x_{i+1}} &\Big(\frac{\sin(k_\mu(x-x_{i+1}))v^{(1)}(x_{i+1})}{k_\mu}+\cos(k_\mu(x-x_{i+1}))v(x_{i+1})\Big)\\ &\times\Big(\frac{\sin(\tilde{k}_\mu(x-x_{i+1}))\tilde{v}^{(1)}(x_{i+1})}{\tilde{k}_\mu}+\cos(\tilde{k}_\mu(x-x_{i+1}))\tilde{v}(x_{i+1})\Big)dx.\end{aligned}$$

The new numerical integration rule NNIR3 can be expressed by

$$\begin{aligned}\textbf{NNIR3:}\quad \int_0^a v\tilde{v}dx = &\sum_{i=0}^{N-1}(\tilde{\tilde{A}}_1 v^{(1)}(x_i)\tilde{v}^{(1)}(x_i)+\tilde{\tilde{A}}_2 v^{(1)}(x_i)\tilde{v}(x_i)\\ &+\tilde{\tilde{A}}_3 v(x_i)\tilde{v}^{(1)}(x_i)+\tilde{\tilde{A}}_4 v(x_i)\tilde{v}(x_i)),\end{aligned}\tag{3.23}$$

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where

$$\tilde{\tilde{A}}_1=\frac{1}{2}\Big[\frac{\sin((k_\mu-\tilde{k}_\mu)h)}{k_\mu-\tilde{k}_\mu}-\frac{\sin((k_\mu+\tilde{k}_\mu)h)}{k_\mu+\tilde{k}_\mu}\Big],$$
$$\tilde{\tilde{A}}_2=-\frac{1}{2}\Big[\frac{\cos((k_\mu+\tilde{k}_\mu)h)}{k_\mu+\tilde{k}_\mu}+\frac{\cos((k_\mu-\tilde{k}_\mu)h)}{k_\mu-\tilde{k}_\mu}\Big],$$
$$\tilde{\tilde{A}}_3=-\frac{1}{2}\Big[\frac{\cos((k_\mu+\tilde{k}_\mu)h)}{k_\mu+\tilde{k}_\mu}-\frac{\cos((k_\mu-\tilde{k}_\mu)h)}{k_\mu-\tilde{k}_\mu}\Big],$$
$$\tilde{\tilde{A}}_4=\frac{1}{2}\Big[\frac{\sin((k_\mu-\tilde{k}_\mu)h)}{k_\mu-\tilde{k}_\mu}+\frac{\sin((k_\mu+\tilde{k}_\mu)h)}{k_\mu+\tilde{k}_\mu}\Big],$$

if $k_\mu\neq\tilde{k}_\mu$; and

$$\tilde{\tilde{A}}_1=\frac{1}{2}\Big[h-\frac{\sin(2k_\mu h)}{2k_\mu}\Big],$$
$$\tilde{\tilde{A}}_2=\tilde{\tilde{A}}_3=\frac{\sin^2(k_\mu h)}{2k_\mu},$$
$$\tilde{\tilde{A}}_4=\frac{1}{2}\Big[h+\frac{\sin(2k_\mu h)}{2k_\mu}\Big],$$

if $k_\mu=\tilde{k}_\mu$.

Remark 3.3. Higher order approximations can be derived for Case I by using higher order interpolation formulae to approximate v. However, NNIR3 will produce exact numerical solution for Case II.

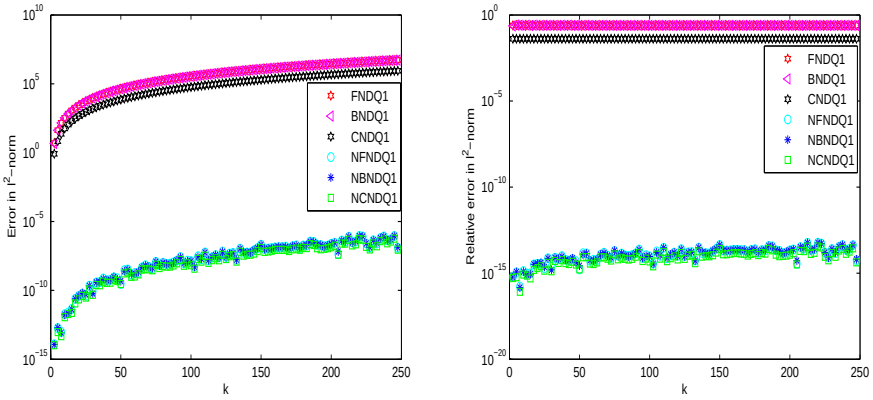
4 Numerical experiments

To validate the effectiveness of the developed algorithms, we present the following numerical simulations.

4.1 Numerical differentiation and integration

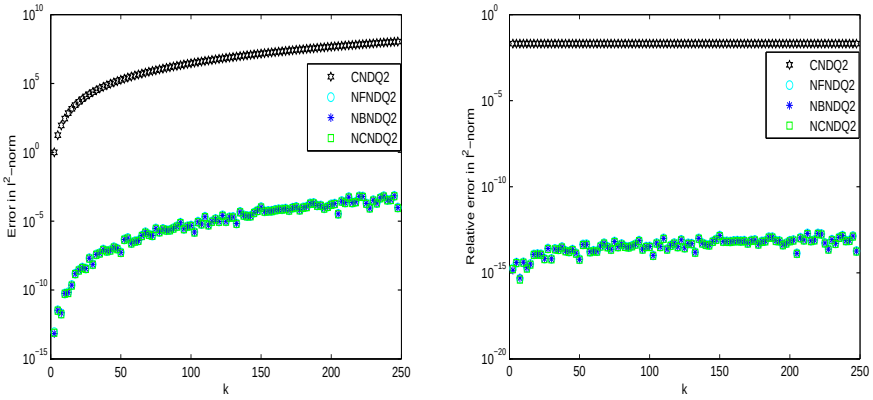
First, we present computational results to verify that the proposed new difference quotients are not affected by the wave number k. Let $v(y)=k^{3/2}\sin(ky)$, $y\in(0,2)$, the error and relative error for computing the first derivative using the proposed new schemes NFNDQ1, NBNDQ1, NCNDQ1 and the classical forward (FNDQ1), backward (BNDQ1) and central (CNDQ1) numerical difference quotients are compared in Fig. 1. Fig. 2 illustrates the corresponding results for the second derivative using NFNDQ2, NBNDQ2, NCNDQ2 and the standard central difference scheme (CNDQ2). The results displayed

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(a) Error (b) Relative error

Figure 1: Comparison of numerical difference quotients for first derivative.



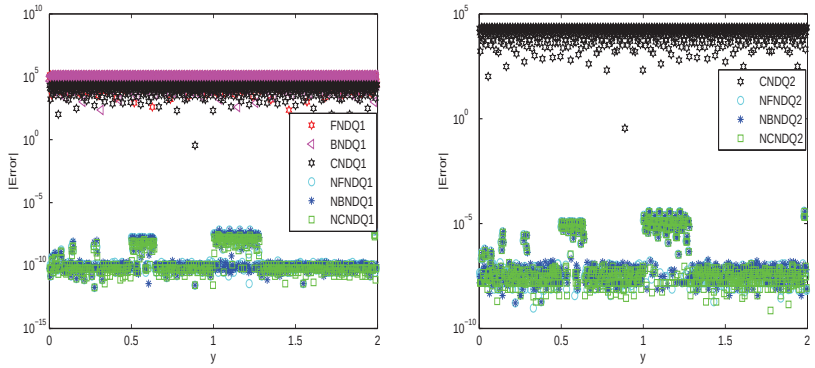
(a) Error (b) Relative error

Figure 2: Comparison of numerical difference quotients for second derivative.

in Figs. 1-2 speak for itself, and the relative errors from the proposed new schemes are very accurate and also independent of k. Let $k=200$, the absolute errors for the first and second order derivatives using various schemes for y from 0 to 2 are plotted in Fig. 3.

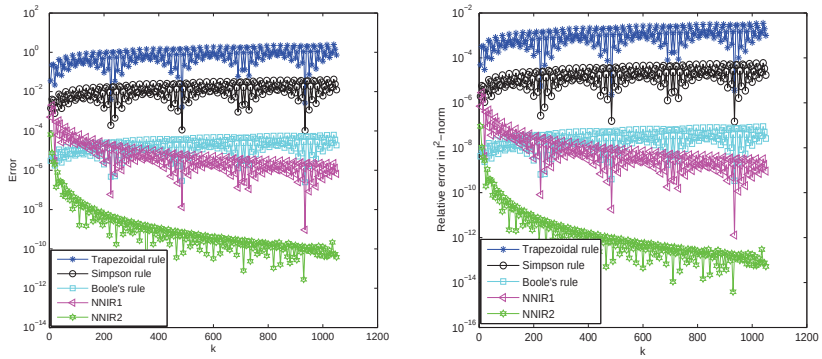
To evaluate the performance of the developed pollution free numerical formulae, we consider two test cases: Case I $v=e^y$, $\tilde{v}=k^{3/2}\sin(ky)$; and Case II $v=\cos(ky)$, $\tilde{v}=k^{3/2}\sin(ky)$. Applying the new numerical integration rules NNIR1, NNIR2 and NNIR3 and the classical composite formulae based on the composite Trapezoidal, Simpson and Boole's rules for y from 0 to 1, the errors and relative errors for various integration formulae are shown in Figs. 4-5. As expected, the relative error of the classical schemes increases as the wave number k increasing. However, the relative errors for the

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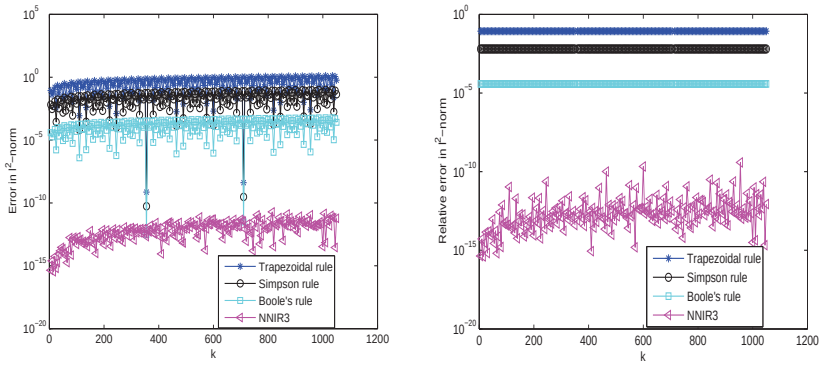
(a) First order derivative (b) Second order derivative

Figure 3: Errors of different numerical difference quotients for $k=200$.



(a) Error (b) Relative error

Figure 4: Comparison of different schemes for Case I.



(a) Error (b) Relative error

Figure 5: Comparison of different schemes for Case II.

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new schemes are actually decreasing as k increases for Case I and almost exact numerical solution is obtained (as indicates by the relative errors reaching the level of machine error) in Case II. Thus, the numerical accuracy of the pollution free difference schemes for the 2D Helmholtz equation will not be deteriorated by the application of the new proposed numerical integration schemes.

4.2 Large cavity problem

In order to demonstrate that the proposed method for solution presented in Section 3 does not suffer a pollution effect, we consider solving the 2D Helmholtz equation modelling the electromagnetic scattering from an open large cavity.

Following the study reported in [20], we consider an artificial example with a known solution defined by (1.1), (2.1)-(2.2) on a unit square $a=b=1$. The functions f and g_1 are chosen such that the exact solution is given by $u(x,y)=\sin(m\pi x)\sin(\pi y)$ and $m=\lfloor k/\pi \rfloor$. The new finite difference scheme (NFD) is used to compute the 1D numerical solution $\tilde{U}_m=\{U_{m,i}\}_{i=0}^{N}$ of $\tilde{u}_m$. Then, the overall 2D numerical solution is achieved by summing the series given in (2.4). The errors in l^2-norm for the wave number k in the range of 97 to 105 are plotted in Fig. 6. The error profile shown in Fig. 6 is in good agreement with that reported in [20], and the error jumps located at the three eigenvalues are clearly observed. Notice that a much higher accuracy of 10^{-10} is achieved by the present method compared to a 10^{-5} obtained using the finite element method with P_4 element.

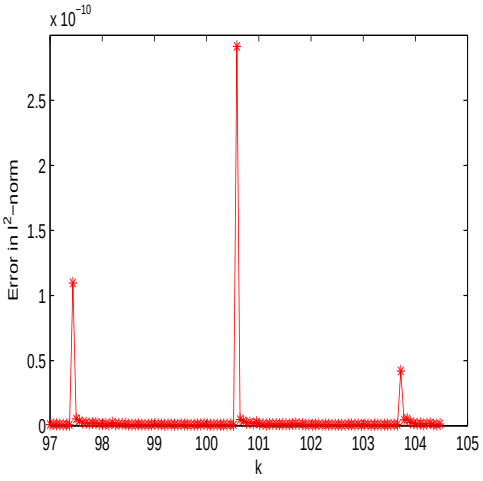
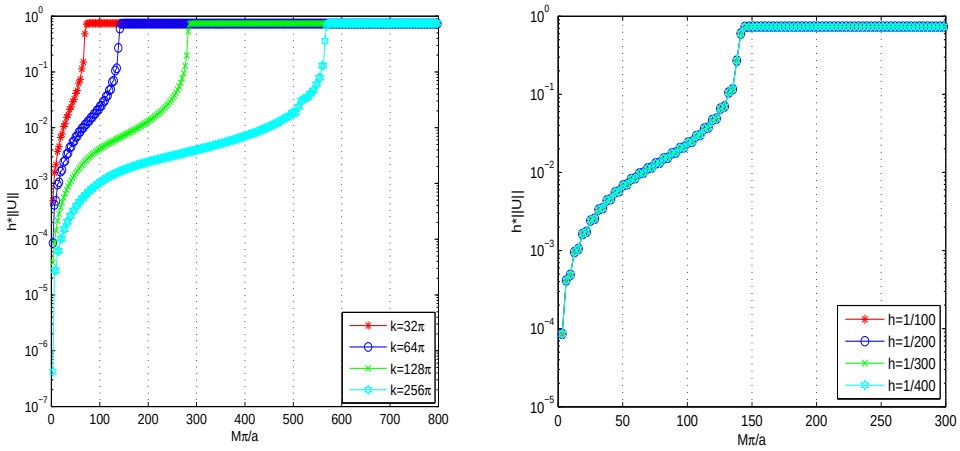


Figure 6: Error in l^2-norm with $h=1/128$.

Next, we consider a test case which has been investigated in [38, 60]. Here, $a=1$, $b=1/4$, $f=0$, $g_1=-2j\beta e^{j\alpha x}$, $\alpha=k\sin\theta$, $\beta=k\cos\theta$ and $\theta=\pi/4$. We first verify that there exists a value M for the summation in (2.4) so that the computed solution will reach a steady solution when $M\pi/a=\mathcal{O}(kb)$ as shown in Fig. 7. Hence the numerical solutions

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(a) $h=200$ (b) $k=64\pi$

Figure 7: Convergence of series solution.

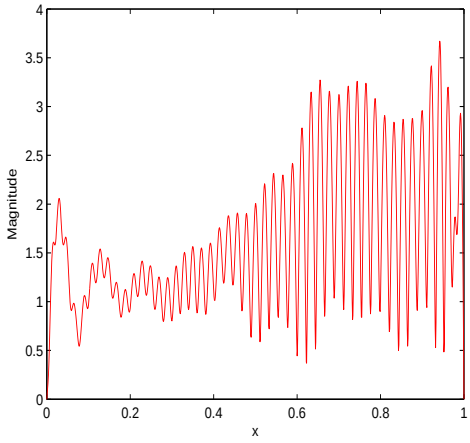
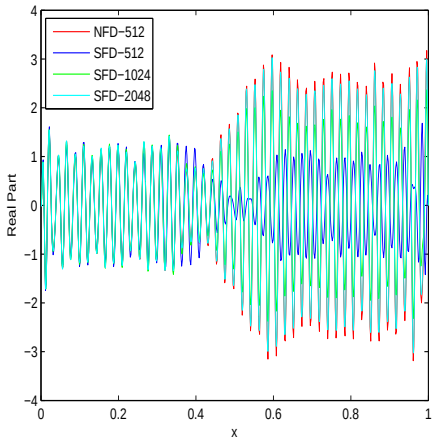


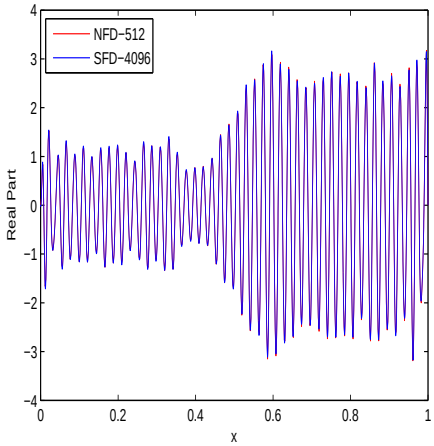
Figure 8: Magnitude with $k=64\pi$ at $y=1/4$.

presented in this work will base on the steady solutions resulted when $M\pi/a=\mathcal{O}(kb)$ is satisfied. The magnitude of the solution for k=64π and h=$1/320$ is shown in Fig. 8. It is in good agreement with that illustrated in [60] computed by a compact fourth order scheme and used the nonlocal Hadamard finite-part integral operator $T(u)$ in (2.2). Consider the case $k=128\pi$, we compare the numerical solutions using the NFD scheme and standard finite difference (SFD) method (also based on solving (2.5)-(2.7)) with $h=1/512$, $1/1024$, $1/2048$, $1/4096$. The results are shown in Fig. 9. It is found that the solution of NFD with $h=1/512$ ($kh\approx 0.785$) is almost as accurate to that resulted by the standard finite

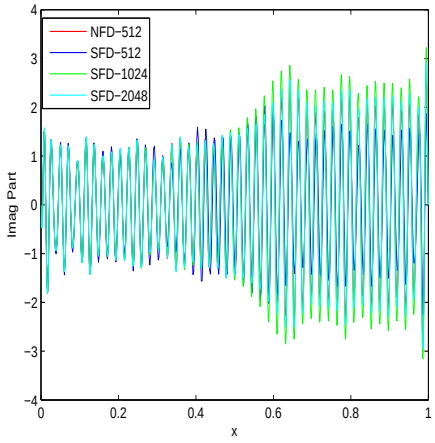
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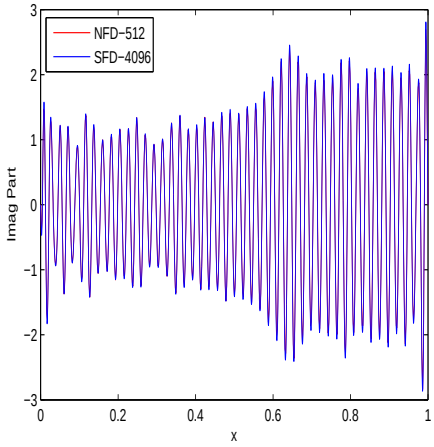
(a) Real part



(b) Real Part



(c) Imag part



(d) Imag part

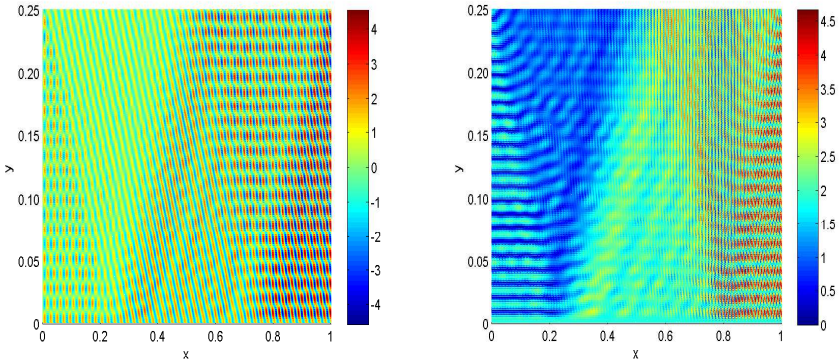
Figure 9: Solution with $k=128\pi$ at $y=1/4$.

difference scheme with $h=1/4096$ ($kh\approx 0.098$). Additional simulation results for the real part and magnitude for $k=128\pi$, 256π, 512π are shown in Figs. 10-12. The computed solutions are pollution free and nonphysical oscillation is not observed.

4.3 Rectangular waveguide

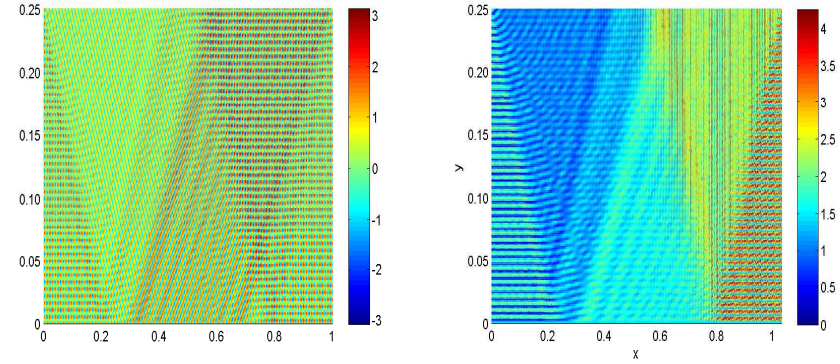
The same approach is now applied to compute the Helmholtz equation modelling a rectangular waveguide. The test case is constructed by setting $f=0$ in (1.1) and $g_2=e^{-\frac{1}{2}(y-\frac{1}{2})^2}$ in (2.12). This example has also been studied in [9, 36]. Using the series solutions and

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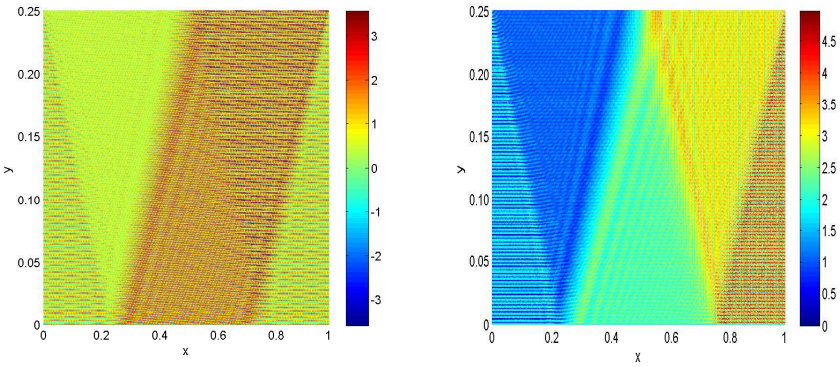
(a) Real part (b) Magnitude

Figure 10: Real part and magnitude with $k=128\pi$ and $h=1/680$.



(a) Real part (b) Magnitude

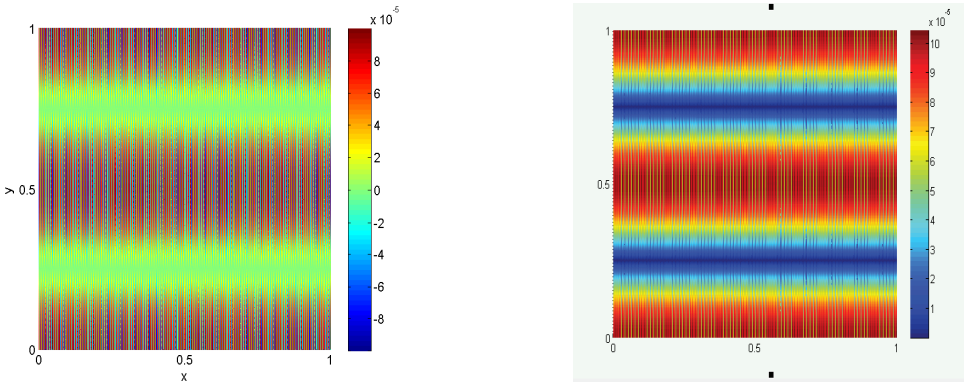
Figure 11: Real part and magnitude with $k=256\pi$ and $h=1/1360$.



(a) Real part (b) Magnitude

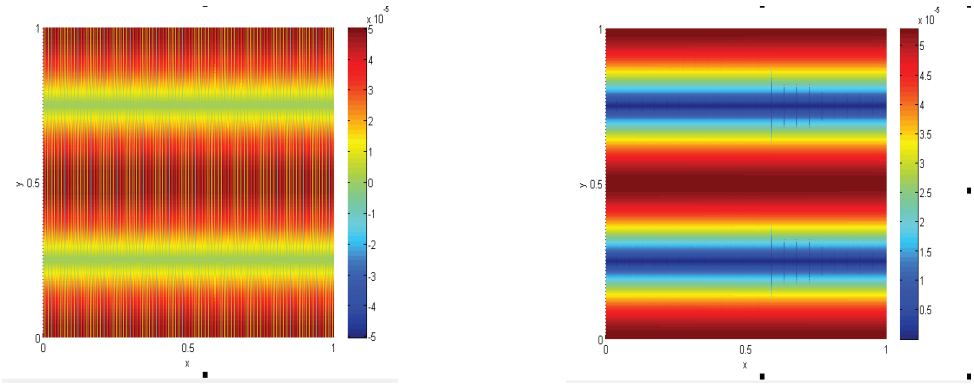
Figure 12: Real part and magnitude with $k=512\pi$ and $h=1/2720$.

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(a) Real part (b) Magnitude

Figure 13: Real part and magnitude with $k=256\pi$ and $h=1/1024$.



(a) Real part (b) Magnitude

Figure 14: Real part and magnitude with $k=512\pi$ and $h=1/2048$.

the pollution free NFD algorithm with $kh\approx 0.8$, we display the computed waveguide solutions in Figs. 13-14. The real part of the solution and the magnitude for $k=256\pi$ and $k=512\pi$ are computed using $h=1/1024$ and $1/2048$, respectively.

5 Conclusions

In this study, the solution of 2D Helmholtz equations in Cartesian coordinates is obtained by solving a sequence of 1D problems. A new pollution free difference schemes is developed which is capable of producing accurate numerical solutions with $kh\approx 0.6-0.8$ for

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2D problems at high wave numbers. In order to ensure the computed solution does not suffer the pollution effect and achieve the predicted convergence order, a pollution free numerical integration formula is constructed to handle the integration resulting from an inhomogeneous forcing term. The proposed method has been tested for problems arising from a rectangular waveguide and electromagnetic scattering from an open large cavity. Together with our early work on pollution free difference schemes for 2D/3D Helmholtz equations in polar/spherical coordinates, we can now remark that the pollution effect can be avoided for certain multi-dimensional Helmholtz equations if the problem can be solved by the method of separation of variables. This approach has another attractive feature, namely the resulting indefinite linear system is given by a tridigonal matrix and can be solved efficiently by a direct method. Although many work has been devoted to develop efficient numerical algorithms for indefinite and ill-conditioned linear system resulting from discretization of a multi-dimensional Helmholtz equation at high wave number, robust and accurate iterative solver has yet to be constructed for this problem. It should be noted that the method of separation of variables cannot be guaranteed for all applications. In addition to the limitation for a regular computational domain, the success of the present approach also depends on the type of boundary condition imposed for a specific problem. In conclusion, more study is needed to extend the pollution free numerical algorithms for multi-dimensional Helmholtz equations on a general domain. Moreover, it is of great interest to develop non-polluted schemes for applications with varying wave numbers, problems with discontinuous coefficients and non-standard boundary conditions.

Acknowledgments

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