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ANALYSIS OF POLLUTION-FREE APPROACHES FOR MULTI-DIMENSIONAL HELMHOLTZ EQUATIONS

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Abstract. Motivated by our recent work about pollution-free difference schemes for solving Helmholtz equation with high wave numbers, this paper presents an analysis of error estimate for the numerical solution on the annulus and hollow sphere domains. By applying the weighted-test-function method and defining two special interpolation operators, we first derive the existence, uniqueness, stability and the pollution-free error estimate for the one-dimensional problems generated from a method based on separation of variables. Utilizing the spherical harmonics and approximations results, we then prove the pollution-free error estimate in L^2 -norm for multi-dimensional Helmholtz problems.

Key words. Helmholtz equation, error estimate, finite difference method, polar and spherical coordinates, pollution-free scheme.

1. Introduction

This paper is focused on the Helmholtz equation defined as follows:

(1)
$$-\Delta \tilde{u} - k^2 \tilde{u} = 0, \text{ in } \mathbb{R}^d \backslash \mathbb{B}_1,$$

(2)
$$(\partial_r \tilde{u} + jk\tilde{u})|_{\partial \mathbb{B}_1} = \tilde{g}_1,$$

(3)
$$\partial_r \tilde{u} - jk\tilde{u} = o\left(||\mathbf{x}||^{\frac{1-d}{2}}\right), \text{ as } ||\mathbf{x}|| \to \infty,$$

where k is the wave number, \mathbb{B}_1 is a bounded domain in \mathbb{R}^d , $\mathbf{x} = (x_1, \dots, x_d)$ (d = 1, 2, 3), \tilde{g}_1 is a given function, ∂_r denotes the radial derivative and $j^2 = -1$. Applying an absorbing boundary condition method, or the perfectly matched layers (PML) method, the problem (1)-(3) may be reduced to the following equation (see [7, 15, 16, 23, 26, 43, 44, 57]):

(4)
$$-\Delta \tilde{u} - k^2 \tilde{u} = 0, \text{ in } \Omega := \mathbb{B}_2 \setminus \mathbb{B}_1,$$

(5)
$$(\partial_r \tilde{u} + jk\tilde{u})|_{\partial \mathbb{B}_1} = \tilde{g}_1,$$

(6)
$$(\partial_r \tilde{u} - jk\tilde{u})|_{\partial \mathbb{B}_2} = \tilde{g}_2,$$

where $\mathbb{B}_2 \in \mathbb{R}^d$ (d = 1, 2, 3) is a sufficiently large ball containing \mathbb{B}_1 and \tilde{g}_2 is a given function.

It is well-known that solving the Helmholtz equation with high wave numbers numerically is very difficult and challenging due to the high oscillation solutions. Moreover, the resulted linear system is indefinite and ill-conditioned (see [1, 12, 13, 14, 22, 28, 29, 30, 31, 32, 33, 34, 50]). Another difficulty is that the "pollution effect" exists in almost all computational schemes applied to multi-dimensional Helmholtz equation such that the accuracy of the numerical solution becomes totally unacceptable for the cases with high wave numbers unless very fine meshes are used in the computation. In the past several decades, many studies have been reported to eliminate or reduce the "pollution effect". For example,

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Babuška et al. [4, 47] considered the generalized finite element method to minimize the "pollution effect". Another popular technique is based on the *h-p* finite element method (see [19, 32, 33, 54]), in which the "pollution effect" is reduced by increasing the order of the polynomial basis function or decreasing the mesh size *h*. For the finite difference methods, many higher order compact schemes were developed [21, 42, 45, 46, 49]. Recently, Chen et al. [15, 16] proposed two methods, in which the numerical dispersion is minimized by choosing optimal parameters. Other computational techniques based on the spectral methods were investigated, and the reader is referred to [6, 8, 17, 20, 27, 37, 39, 43, 44, 59]. However, it is important to note that although pollution-free numerical schemes have been reported in [24, 52, 53], there does not exist any analysis results about pollution-free methods for solving the multi-dimensional problems.

To ensure the bound of the relative error for the numerical solution of the problem (4)-(6), it is usually necessary to impose the following condition

(7)
$$k^{\beta}(kh)^{\gamma} = constant.$$

Here, h denotes the mesh size, and two constants $\beta > 0, \gamma > 0$ are real numbers. For example, $\beta = 2$, and $\gamma = 2$ and 4, when the solution is computed by the standard central finite difference scheme and the compact fourth order difference scheme, respectively. Considering that the Helmholtz problem is numerically solved with a fixed value of kh, and due to the relation given in (7), the numerical error will not decrease even when the mesh size is reduced. This adverse behaviour is the direct consequence of the "pollution effect", and more detailed discussion is reported in [31]. It has been cited by Babuška and Sauter [5] that the "pollution effect" can not be avoided on a general bounded domain for the finite element approximation of two- (2D) and three-dimensional (3D) Helmholtz equations.

In this study, we focus on the pollution-free difference method. It should be noted that the standard finite difference and the higher order compact methods are constructed based on a truncated Taylor series expansion, and the truncation errors depend on the wave numbers and thus causing the "pollution effect" unavoidable. To eliminate the pollution, pollution-free difference schemes for the one-dimensional Helmholtz equation have been proposed in [25, 36, 50, 53, 56], in which the derivation takes account of all terms in the Taylor series expansion. Compared with the standard finite difference methods, the numerical error of the pollution-free scheme depends only on the mesh size h but independent of the wave number k. Therefore, the numerical error is decreasing as the mesh size is reduced [50, 56]. Consequently, the condition (7) can be relaxed to the common "rule of thumb" (i.e., 8 to 10 discrete mesh points for each wavelength), that is

(8)
$$kh = \mathcal{C}_1 \le \frac{\pi}{4}.$$

Compared to (7), relatively large value of kh could be employed even when the wave number is very high. Numerical simulations reported in [52] also verify that the pollution-free difference scheme can produce a stable numerical solution even when kh > 1. According to the condition (7), the mesh size of the standard finite difference or compact difference schemes must satisfy the condition

for problems with high wave numbers. Therefore, a pollution-free scheme is much more efficient than the standard and compact finite difference schemes. A detailed development for 1D problems has been reported in [50, 56]. However, this approach can not be extended directly to problems on a general domain in 2D and 3D.

The main difficulty is due to the mixed-term u_{xxyy} appearing in the Taylor series which can not be eliminated. By using a method of separation of variables, we extended the pollution-free approach to problems on annulus and hollow sphere domains [52], circular cylindrical domains [24] and rectangle domains [51]. The developed pollution-free difference schemes have been shown numerically to have first-, second- and third-order accurate. The effectiveness for multi-dimensional problems has been demonstrated by numerical simulations, and the goal of this paper is to fill in the analysis of the error estimate which has not been reported before.

We now focus on the theoretical analysis for the first-order pollution-free algorithm proposed in [52] for the annulus and hollow sphere domains. Under the assumption of (8), the main contribution of this study is to prove the following error estimate

(10)
$$||\tilde{u} - U||_{L^2(\Omega)} \le \mathcal{C}h,$$

where \widetilde{U} is the approximation solution obtained by the pollution-free scheme and \mathcal{C} is a positive constant independent of h and k. Although only special domain is considered here, to our best knowledge, this is the first attempt to derive the pollution-free error for the finite difference method of multi-dimensional Helmholtz equations. The numerical experiments in Section 4 confirm the correction of the estimate (10).

The paper is organized as follows: In Section 2, we first transform the problem (4)-(6) into a series of 1D problems, and some theoretical results for 2D and 3D problems are presented. The proofs of the separated 1D problems are reported in detail in Section 3, and the theoretical prediction is numerical confirmed in Section 4. Finally, conclusions are made in Section 5.

2. Error estimates in 2D and 3D

This section is divided into three parts: a multi-dimensional problem will be transformed into a series of one-dimensional equations in Section 2.1; then we recall the finite difference method proposed in [52] and state the existence, uniqueness, stability and error estimates for the separated problems in Section 2.2; finally, the detailed deduction of the pollution-free error estimates for 2D and 3D Helmholtz equations with high wave numbers are shown in Section 2.3.

2.1. Transformation of the equation. Now consider the Helmholtz equation in the polar and spherical coordinates. For more details on this topic, the reader is referred to [11, 31, 41, 43, 44, 52, 55].

Assume that a and b are two real numbers satisfying b > a > 0, \mathbb{B}_1 and \mathbb{B}_2 are defined as $\mathbb{B}_1 := \{\mathbf{x} \in \mathbb{R}^1 | 0 \le \mathbf{x} < a\}$ and $\mathbb{B}_2 := \{\mathbf{x} \in \mathbb{R}^1 | 0 \le \mathbf{x} < b\}$, and $\mathbb{B}_1 = \{\mathbf{x} \in \mathbb{R}^d | |\mathbf{x}| < a\}$ and $\mathbb{B}_2 = \{\mathbf{x} \in \mathbb{R}^d | |\mathbf{x}| < b\}$ with d = 2 or 3, respectively. Then, by applying a separation of variables, the solution of the Helmholtz equation (4)-(6) can be expressed as a series solution given by (see [3, 31, 41])

(11)
$$\tilde{u}(\mathbf{x}) = \tilde{u}(r,\theta) = \sum_{m=0}^{\infty} u^m(r) e^{jm\theta}$$

and

(12)
$$\tilde{u}(\mathbf{x}) = \tilde{u}(r,\theta,\phi) = \sum_{m=0}^{\infty} \sum_{l=1}^{2m+1} u^{ml}(r) Y_{m,l}(\theta,\phi),$$

in the polar and spherical coordinates, respectively. Here,

$$u^{m}(r) = (\tilde{u}, e^{jm\theta}) = \int_{0}^{2\pi} \tilde{u}(r, \theta) e^{-jm\theta} d\theta,$$
$$u^{lm}(r) = (\tilde{u}, Y_{m,l}(\theta, \phi)) = \int_{0}^{2\pi} \int_{0}^{\pi} \tilde{u}(r, \theta, \phi) \overline{Y}_{m,l}(\theta, \phi) d\phi d\theta,$$

with $\overline{Y}_{m,l}(\theta,\phi)$ being the conjugate of $Y_{m,l}(\theta,\phi)$ and

$$Y_{m,1}(\theta,\phi) = C_m P_1(\cos\theta),$$

$$Y_{m,2l}(\theta,\phi) = C_{m,l} P_m^l(\cos\theta) \cos(l\phi), \ l = 1, \cdots, m,$$

$$Y_{m,2l+1}(\theta,\phi) = C_{m,l} P_m^l(\cos\theta) \sin(l\phi), \ l = 1, \cdots, m,$$

and $P_m(t)$ is the Legerdre polynomial of degree m with

$$P_m(t) = \frac{1}{2^m m!} \frac{d^m}{dt^m} [(t^2 - 1)^m],$$

and

$$P_m^l(t) = (-1)^l (1-t^2)^{\frac{1}{2}l} \frac{d^l}{dt^l} P_m(t) \ (1 \le l \le m),$$
$$C_m = \sqrt{\frac{2m+1}{4\pi}}, \ C_{m,l} = \sqrt{\frac{2m+1}{2\pi} \frac{(m-l)!}{(m+l)!}}.$$

With this approach, the solution of the original problem (4)-(6) can be computed by solving a sequence (for each m in 2D and (m, l) in 3D) of the following onedimensional equations in the radial r direction:

(13)
$$-\frac{1}{r^{d-1}}\frac{\partial}{\partial r}\left(r^{d-1}\frac{\partial u}{\partial r}\right) + d_m\frac{u}{r^2} - k^2u = 0, \ r \in \mathbb{I} := (a,b), \ d = 1,2,3,$$

(14) $(u^{(1)} + jku)|_{r=a} = g_1,$

(15)
$$(u^{(1)} - jku)|_{r=b} = g_2,$$

where $d_m = 0, m^2, m(m+1)$ in 1D, 2D and 3D, respectively. For the reason of simplicity, we let u denote u^m or u^{ml} here, and g_1, g_2 are two constants resulted from coordinate transforms, and $u^{(n)} = \frac{\partial^n u}{\partial r^n}$. Since it is much simpler for the case d = 1, we mainly focus on problems for d = 2, 3.

Recall that we are particularly interested in the Helmholtz equation with large wave numbers, and under the assumption that k is sufficiently large, we have the following lemma:

Lemma 2.1. Suppose that u is the solution of the problem (13)-(15), and g_1, g_2 are two bounded numbers, then we have the following stability estimates

(16)
$$k^{1-s} || u^{(s)} ||_{L^2(\mathbb{I})} \leq \mathcal{C}_0, \ s = 0, \ 1, \ 2,$$

where C_0 is a positive constant independent of $k, u, u^{(n)}$, but depends on g_1, g_2 and the domain.

Proof. The lemma can be easily obtained by applying a similar process reported in [10, 43], and the detail is omitted here.

By setting (see [52, 58])

(17)
$$u = r^{-\frac{d-1}{2}}v,$$

equations (13)-(15) can be rewritten as

(18)
$$-v^{(2)} - k^2(r)v = 0, \ r \in \mathbb{I},$$

(19)
$$\left(v^{(1)} + (jk + \frac{d-1}{2r})v\right)|_{r=a} = a^{\frac{d-1}{2}}g_1,$$

(20)
$$\left(v^{(1)} - (jk + \frac{d-1}{2r})v\right)|_{r=b} = b^{\frac{d-1}{2}}g_2,$$

with

(21)
$$k^{2}(r) = k^{2} - \frac{4d_{m} + d^{2} - 4d + 3}{4r^{2}}.$$

When $k^2(r) \leq 0$, the equation (18) reduces to a classical reaction-diffusion problem, which has been widely investigated and can be efficiently solved under the assumption of (8) (see, e.g., [38]). In the following, we will only consider the case that $k^2 \ge k^2(r) > 0$, which is indeed a Helmholtz equation.

2.2. Finite difference scheme. For the problem (18)-(20), pollution-free finite difference methods have been proposed in [52]. For completeness, we briefly report here. Let the domain I be covered by a uniform mesh with mesh size $h = \frac{b-a}{N}$ ($N \in$ \mathbb{Z}^+), and the grid points in the computational domain be defined as $r_i = a + ih \ (i \in \mathbb{Z}, 0 \le i \le N)$, $\mathbb{I}_i = (r_{i-1}, r_{i+1})$. For the reason of simplicity, we let $k_i^{(n)} = [k(r)]^{(n)}|_{r=r_i}, v_i^{(n)} = [v(r)]^{(n)}|_{r=r_i}$. Thanks to (17), (18) and Lemma 2.1, it is valid that

(22)
$$||v^{(n)}||_{L^2(\mathbb{I})} = \mathcal{O}(k^{n-1}), \ n \in \mathbb{Z}$$

In a practical computation, a good numerical solution of $\tilde{u}(\mathbf{x})$ in (11) or (12) can be achieved by replacing the infinity in the summation with M such that $M = \mathcal{O}(k)$. Assuming

$$(23) h \ll a,$$

it holds

(24)
$$d_m = \mathcal{O}(k^2) \text{ and } |(k_i^2)^{(n)}| = \mathcal{O}(k^2), \ n \in \mathbb{Z}.$$

Considering the Taylor's expansion, it follows

(25)
$$v_{i+1} + v_{i-1} = 2 \left[v_i + \frac{h^2}{2!} v_i^{(2)} + \frac{h^4}{4!} v_i^{(4)} + \frac{h^6}{6!} v_i^{(6)} + \dots + \frac{h^{2n}}{(2n)!} v_i^{(2n)} + \dots \right].$$

By using (22), we have

(26)
$$||h^{2n}v^{(2n)}||_{L^2(\mathbb{I}_i)} = \mathcal{O}(h)$$

which means that all terms $h^{2n}v^{(2n)}$ have the same order with respect to h under the assumption (8). On the other hand, due to (18), we have

(27)
$$h^{2n}v_i^{(2n)} = h^{2n}\sum_{m=0}^{2n-2} \left(\begin{array}{c} 2n-2\\ 2n-2-m \end{array}\right) (k_i^2)^{(m)}v_i^{(2n-2-m)}$$

where $\binom{n}{m} = \frac{n!}{m!(n-m)!}$. By applying (22) and (24), there holds

(28)
$$||h^{2n}(k^2)^{(m)}v^{(2n-2-m)}||_{L^2(\mathbb{I}_i)} = \mathcal{O}(h^{m+1})$$

which implies that the norm of $h^{2n} v_i^{(2n)}$ can be decomposed to a summation as follows

$$\left\| \frac{1}{(2n)!} h^{2n} v^{(2n)} \right\|_{L^{2}(\mathbb{I}_{i})} = \left\| \frac{h^{2n}}{(2n)!} \sum_{m=0}^{2n-2} \binom{2n-2}{2n-2-m} (k^{2})^{(m)} v^{(2n-2-m)} \right\|_{L^{2}(\mathbb{I}_{i})}$$

$$(29) \qquad \qquad = \frac{\mathcal{O}(h)}{(2n)!} + \frac{\mathcal{O}(h^{2})}{(2n)!} + \dots + \frac{\mathcal{O}(h^{2n-1})}{(2n)!}, \ \forall n \in \mathbb{Z}.$$

By combining (29) and collecting the term equivalent to $\mathcal{O}(h^m)$, $m = 1, 2, \cdots$, on the right hand side of (25), we can rearrange it as

(30)
$$v_{i+1} + v_{i-1} = 2[D_i^1 v_i + D_i^2 v_i^{(1)} + D_i^3 v_i + \cdots]$$

where the grouping of $D_i^m = D^m(r)|_{r=r_i}, m = 1, 2, \cdots$, are determined functions satisfying

(31)
$$||D^{2m-1}v||_{L^2(\mathbb{I}_i)} = \mathcal{O}(h^{2m-1}), ||D^{2m}v^{(1)}||_{L^2(\mathbb{I}_i)} = \mathcal{O}(h^{2m}).$$

By taking account of only the term equivalent to $\mathcal{O}(h)$ on the right hand side of (30), we have

(32)
$$v_{i+1} + v_{i-1} = 2D_i^1 v_i + RD_i^1,$$

with $RD_i^1 = RD^1(r)|_{r=r_i}$ being the remainder term and

(33)
$$D_i^1 = \cos(k_i h)$$
, satisfying $0 < D_i^1 < 1$.

On the other hand, there holds that

(34)
$$v_{i+1} = v_i + \frac{h^2}{2!} v_i^{(2)} + \dots + \frac{h^{(2n)}}{(2n)!} v_i^{(2n)} + \dots + \frac{h^{(2n+1)}}{(2n+1)!} v_i^{(2n+1)} + \dots$$

Similar to (30), we can rewrite the above equation as

$$v_{i+1} = D_i^1 v_i + D_i^2 v_i^{(1)} + D_i^3 v_i + \cdots + B_i^1 v_i^{(1)} + B_i^2 v_i + B_i^3 v_i^{(1)} + \cdots$$

where $B_i^m = B^m(r)|_{r=r_i}, m = 1, 2, \cdots$ are determined functions with

(36)
$$||B^{2m-1}v^{(1)}||_{L^2(\mathbb{I}_i)} = \mathcal{O}(h^{2m-1}), ||B^{2m}v||_{L^2(\mathbb{I}_i)} = \mathcal{O}(h^{2m})$$

By collecting all terms equivalent to $\mathcal{O}(h)$ on the right hand side of (34), there yields

(37)
$$v_{i+1} = D_i^1 v_i + B_i^1 v_i^{(1)} + RL_i^1,$$

with $RL_i^1 = RL^1(r)|_{r=r_i}$ being the remainder term and

(38)
$$B_i^1 = \frac{\sin(k_i h)}{k_i} > 0, \text{ satisfying } |B_i^1| = \mathcal{O}(h).$$

Setting i = 0 in (37) and using (19), we obtain

(39)
$$v_1 = D_0^1 v_0 + B_0^1 \left[-\left(jk + \frac{d-1}{2a}\right) v_0 + a^{\frac{d-1}{2}} g_1 \right] + RL_0^1.$$

Similarly, it holds

(35)

(40)
$$v_{N-1} = D_N^1 v_N - B_N^1 \left[\left(jk + \frac{d-1}{2b} \right) v_N + b^{\frac{d-1}{2}} g_1 \right] + RR_N^1,$$

where $RR_N^1 = RR^1(r)|_{r=b}$ is the remainder term. Let V_i denote the numerical solution of the finite difference method, omitting the remainder terms in (32), (39) and (40), respectively, we derive the following algorithm:

Algorithm 1:

(41)
$$-V_{i+1} - V_{i-1} + 2D_i^1 V_i = 0, \ 0 < i < N,$$

(42)
$$V_1 = D_0^1 V_0 + B_0^1 \Big[- \Big(jk + \frac{d-1}{2a} \Big) V_0 + a^{\frac{d-1}{2}} g_1 \Big],$$

(43)
$$V_{N-1} = D_N^1 V_N - B_N^1 \left[\left(jk + \frac{d-1}{2b} \right) V_N + b^{\frac{d-1}{2}} g_2 \right].$$

Let the vector space $S_h = \{ \mathbf{V} | \mathbf{V} = \{ V_i \}_{i=0}^N \}$. For any mesh function $\mathcal{V} = \{ V_i | 0 \le i \le N \}$, define that

$$\begin{split} \delta_{r}V_{i-\frac{1}{2}} &= \frac{V_{i} - V_{i-1}}{h}, \ V_{i} \in \mathcal{V}, 1 \leq i \leq N, \\ \delta_{r}^{2}V_{i} &= \frac{\delta_{r}V_{i+1/2} - \delta_{r}V_{i-1/2}}{h}, \ V_{i} \in \mathcal{V}, 1 \leq i \leq N-1, \\ (\mathbf{U}, \mathbf{V}) &= h\left[\frac{1}{2}U_{0}\overline{V}_{0} + \sum_{i=1}^{N-1}U_{i}\overline{V}_{i} + \frac{1}{2}U_{N}\overline{V}_{N}\right], \ \mathbf{U}, \mathbf{V} \in \mathcal{S}_{h}, \\ ||\mathbf{V}||_{\mathcal{L}^{2}} &= \sqrt{(\mathbf{V}, \mathbf{V})}, \ \mathbf{V} \in \mathcal{S}_{h}, \\ ||\delta_{r}\mathbf{V}||_{\mathcal{L}^{2}} &= \sqrt{h\sum_{i=1}^{N}(\delta_{r}V_{i-\frac{1}{2}})(\delta_{r}\overline{V}_{i-\frac{1}{2}})} = \sqrt{h\sum_{i=1}^{N}|\delta_{r}V_{i-\frac{1}{2}}|^{2}}, \ \mathbf{V} \in \mathcal{S}_{h}, \\ ||\delta_{r}^{2}\mathbf{V}||_{\mathcal{L}^{2}} &= \sqrt{h\sum_{i=1}^{N-1}(\delta_{r}^{2}V_{i})(\delta_{r}^{2}\overline{V}_{i})} = \sqrt{h\sum_{i=1}^{N-1}|\delta_{r}^{2}V_{i}|^{2}}, \ \mathbf{V} \in \mathcal{S}_{h}. \end{split}$$

For the continuous function v(r), we define $\Pi_i v(r) = v(r)|_{r=r_i} = v_i$, $\Pi v(r) = \{\Pi_i v(r)\}_{i=0}^N \in \mathcal{S}_h$ and

$$||v||_{\mathcal{L}^2} = \sqrt{(\Pi v(r), \Pi v(r))}.$$

For **Algorithm** 1, we have the following results, which will be proved in Section 3.

Theorem 2.1 (Existence and Uniqueness). Let g_1, g_2 be two bounded numbers. Under the assumption of (8) and (23), Algorithm 1 generates a unique discretized solution $\mathbf{V} = \{V_i\}_{i=0}^N \in \mathcal{S}_h$.

Theorem 2.2 (Stability). Let g_1, g_2 be two bounded numbers. Under the assumption of (8) and (23), the discretized solution $\mathbf{V} = \{V_i\}_{i=0}^N \in \mathcal{S}_h$ generated by **Algorithm 1** satisfies that

(44)
$$||\delta_r \mathbf{V}||_{\mathcal{L}^2} + k||\mathbf{V}||_{\mathcal{L}^2} \leq \mathcal{C},$$

(45) $||\delta_r^2 \mathbf{V}||_{\mathcal{L}^2} \leq \mathcal{C}k.$

For any $\mathbf{V} = \{V_i\}_{i=0}^N \in S_h$, let us define new interpolation operators $\mathcal{P}^{\tilde{i}}$ $(\tilde{i} = 1, 2)$ as

$$\mathcal{P}^{1}\mathbf{V} = \frac{V_{i+1} - \cos(k_{i}h)V_{i}}{\sin(k_{i}h)} \sin[k_{i}(r - r_{i})] + V_{i}\cos[k_{i}(r - r_{i})], \ r \in [r_{i}, r_{i+1}],$$
$$\mathcal{P}^{2}\mathbf{V} = k_{i}\frac{V_{i+1} - \cos(k_{i}h)V_{i}}{\cos(k_{i}h)}\cos[k_{i}(r - r_{i})] - k_{i}V_{i}\sin[k_{i}(r - r_{i})], \ r \in [r_{i}, r_{i+1}],$$

and the continuous functions $\widetilde{\mathbf{V}}(r), \widetilde{\mathbf{V}}^{(1)}(r)$ by

$$\widetilde{\mathbf{V}}(r) = \mathcal{P}^{1}\mathbf{V}, \ r \in [a, b],$$
$$\widetilde{\mathbf{V}}^{(1)}(r) = \mathcal{P}^{2}\mathbf{V}, \ r \in [a, b].$$

The error estimates for Algorithm 1 is then given by the following Theorem.

Theorem 2.3 (Error estimate). Let g_1, g_2 be two bounded numbers, v and \mathbf{V} be the solution of the problem (18)-(20) and **Algorithm 1**, respectively. Setting $e(r) = v(r) - \widetilde{\mathbf{V}}(r)$, under the assumption of (8) and (23), there holds that

(46)
$$h||e^{(1)}||_{L^{2}(\mathbb{I})} + ||e||_{L^{2}(\mathbb{I})} \leq \mathcal{C}(h||v^{(1)}||_{L^{2}(\mathbb{I})} + ||v||_{L^{2}(\mathbb{I})}).$$

2.3. New error estimates in 2D and 3D. Next, we will derive the error estimate in 2D and 3D. Firstly, we recall the regularity of the solution for the problem in multi-dimensions.

Lemma 2.2. [40] Suppose $\Omega \in \mathbb{R}^d$ (d = 2,3) be contained by a ball with the radius $R \geq R_0 > 0$ with R_0 being a constant. Then the solution of the problem (4)-(6) satisfies

(47)
$$||\tilde{u}||_{H^1(\Omega)} + k||\tilde{u}||_{L^2(\Omega)} \le \mathcal{C},$$

where $H^{\tilde{i}}(\Omega), \tilde{i} = 0, 1$ is the classical Hilbert space, and $H^0(\Omega) = L^2(\Omega)$.

Setting $\mathbb{S}^1 = [0, 2\pi)$ and $\mathbb{S}^2 = [0, 2\pi) \times [0, \pi)$, the equation (4)-(6) can be rewritten as follows (see [43, 44])

(48)
$$-\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Delta_{\mathbb{S}^{d-1}}\right)\tilde{u} - k^2\tilde{u} = 0, \text{ in } \Omega := \mathbb{I} \times \mathbb{S}^{d-1},$$

(49)
$$\partial_r \tilde{u} + jk\tilde{u} = \tilde{g}_1, \text{ on } \mathbb{S}_a^{a-1},$$

(50)
$$\partial_r \tilde{u} - jk\tilde{u} = \tilde{g}_2, \text{ on } \mathbb{S}_b^{a-1}$$

where $\Delta_{\mathbb{S}^1} = \frac{\partial^2}{\partial^2 \theta}$ and $\Delta_{\mathbb{S}^2} = \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \theta} + \frac{\partial^2}{\partial \theta^2}$.

For a function \tilde{v} on \mathbb{S}^2 , defining the gradient operator $\vec{\nabla}$ on the unit sphere by $\vec{\nabla}_{\mathbb{S}^2} = \left(\frac{1}{\sin\theta}\partial_{\phi}\tilde{v}, \partial_{\phi}\tilde{v}\right)_{\mathbb{S}^2}$, there holds

$$-(\Delta_{\mathbb{S}^2}\tilde{u},\tilde{v})_{\mathbb{S}^2} = (\vec{\nabla}_{\mathbb{S}^2}\tilde{u},\vec{\nabla}_{\mathbb{S}^2}\tilde{v})_{\mathbb{S}^2}.$$

Since $\vec{\nabla}_{\mathbb{S}^1}$ is a standard gradient operator, it is valid that

$$(\vec{\nabla}_{\mathbb{S}^{d-1}}\widetilde{Y},\vec{\nabla}_{\mathbb{S}^{d-1}}\widetilde{Y})_{\mathbb{S}^{d-1}} = d_m,$$

where $\widetilde{Y} = e^{jm\theta}$ or $Y_{m,l}(\theta, \phi)$. In order to describe the error estimate, considering (11) and (12), we define a nonisotropic space $\widetilde{H}^s(\mathbb{I}; H^t(\mathbb{S}^{d-1}))$ as follows:

$$\begin{split} \widetilde{H}^s(\mathbb{I}; H^t(\mathbb{S}^1)) &= \Big\{ \widetilde{u} \in L^2(\Omega) \Big| \sum_{m=0}^{\infty} d_m^t ||u^m(r)||_{H^s(\mathbb{I})}^2 < +\infty \Big\}, \\ \widetilde{H}^s(\mathbb{I}; H^t(\mathbb{S}^2)) &= \Big\{ \widetilde{u} \in L^2(\Omega) \Big| \sum_{m=0}^{\infty} \sum_{l=1}^{2m+1} d_m^t ||u^{ml}(r)||_{H^s(\mathbb{I})}^2 < +\infty \Big\}, \end{split}$$

and the norm on $\widetilde{H}^{s}(\mathbb{I}; H^{t}(\mathbb{S}^{d-1}))$ by

$$\begin{split} ||\tilde{u}||_{\tilde{H}^{s}(\mathbb{I};H^{t}(\mathbb{S}^{1}))} &= \Big(\sum_{m=0}^{\infty} d_{m}^{t} ||u^{m}(r)||_{H^{s}(\mathbb{I})}^{2}\Big)^{\frac{1}{2}}, \\ ||\tilde{u}||_{\tilde{H}^{s}(\mathbb{I};H^{t}(\mathbb{S}^{2}))} &= \Big(\sum_{m=0}^{\infty} \sum_{l=1}^{2m+1} d_{m}^{t} ||u^{ml}(r)||_{H^{s}(\mathbb{I})}^{2}\Big)^{\frac{1}{2}}, \end{split}$$

in 2D and 3D, respectively. Obviously, it holds

(51)
$$||\tilde{u}||_{\widetilde{H}^{s}(\mathbb{I};H^{t}(\mathbb{S}^{d-1}))} \leq \mathcal{C}||\tilde{u}||_{H^{s+t}(\Omega)}.$$

In order to understand the analysis well in the following, we also need to introduce some other spaces. For the detail, the reader is referred to [3, 18]. Define the Sobolev space $\mathcal{W}_p^s(\mathbb{S}^{d-1})$ to be the space of functions $f \in L^p(\mathbb{S}^{d-1})$ whose distributional derivatives $D_{\tilde{i},\tilde{j}}^s f \in L^p(\mathbb{S}^{d-1}), 1 \leq \tilde{i} < \tilde{j} \leq d$, i.e.,

$$\mathcal{W}_p^s = \{ f \in L^2(\mathbb{S}^{d-1}) \Big| ||f||_{L^p(\mathbb{S}^{d-1})} + \sum_{1 \leq \tilde{i} < \tilde{j} \leq d} ||D^s_{\tilde{i},\tilde{j}}f||_{L^p(\mathbb{S}^{d-1})} < +\infty \}.$$

 $\mathcal{W}_2^s(\mathbb{S}^{d-1}) = H^s(\mathbb{S}^{d-1}).$ Let SO(d) denote the group of rotations on \mathbb{R}^d . For $1 \leq \tilde{i} < \tilde{j} \leq d$ and $\tilde{t} \in [-\pi, \pi]$, we denote $Q_{\tilde{i}, \tilde{j}, \tilde{t}}$ as a rotation with the angle \tilde{t} in the $(x_{\tilde{i}}, x_{\tilde{j}})$ -plane, and define the *s*th difference operator $\Delta_{\tilde{i}, \tilde{j}, \tilde{t}}^s$ by

$$\Delta^s_{\tilde{i},\tilde{j},\tilde{t}} = (I - T_{Q_{\tilde{i},\tilde{j},\tilde{t}}})^s = \sum_{k=0}^s (-1)^k \binom{s}{k} T_{Q_{\tilde{i},\tilde{j},\tilde{t}}}$$

where $T_Q f(x) = f(Qx)$ for $Q \in SO(d)$. For $s \in \mathbb{Z}$, $1 \le p \le +\infty$ and $\alpha \in [0, 1)$, the Lipschitz space $\mathcal{W}_p^{s,\alpha}(\mathbb{S}^{d-1})$ is defined as

$$\begin{split} \mathcal{W}_p^{s,\alpha}(\mathbb{S}^{d-1}) &:= \left\{ f \in \mathcal{W}_p^s(\mathbb{S}^{d-1}) \middle| \ ||f||_{L^p(\mathbb{S}^{d-1})} \\ &+ \max_{1 \leq \tilde{i} < \tilde{j} \leq d} \sup_{0 < |\tilde{t}| \leq 1} \frac{||\Delta_{\tilde{i},\tilde{j},\tilde{t}}(D^s_{\tilde{i},\tilde{j}}f)||_{L^p(\mathbb{S}^{d-1})}}{|\tilde{t}|^\alpha} < +\infty \right\}. \end{split}$$

Denote by Π_n^d the space of polynomials of total degree n in d variables, and by $\Pi_n(\mathbb{S}^{d-1}) = \Pi_n^d|_{\mathbb{S}^{d-1}}$ the space of all polynomials in Π_n^d restricted on \mathbb{S}^{d-1} . And define the approximation

$$E_{n,p}(f) = \inf_{g \in \Pi_n^d} ||f - g||_{L^p(\mathbb{S}^{d-1})}, \ 1 \le p \le +\infty.$$

Let

(52)
$$\mathcal{Q}_M^2 \tilde{u}(r,\theta) = \sum_{m=0}^M u^m(r) e^{jm\theta},$$

(53)
$$\mathcal{Q}_{M}^{3}\tilde{u}(r,\theta,\phi) = \sum_{m=0}^{M} \sum_{l=1}^{2m+1} u^{ml}(r) Y_{m,l}(\theta,\phi),$$

the following approximation propositions hold:

Lemma 2.3 [18]. If $s \in \mathbb{N}, \alpha \in [0, 1), f \in \mathcal{W}_p^{s, \alpha}(\mathbb{S}^{d-1})$, and $1 \le p \le \infty$, then

(54)
$$E_{M,p}(f) \le \frac{\mathcal{C}||f||_{\mathcal{W}_p^{s,\alpha}(\mathbb{S}^{d-1})}}{M^{s+\alpha}}.$$

Lemma 2.4 [2, 3]. Assume $f \in \mathcal{W}_2^s(\mathbb{S}^1)$, $\mathcal{Q}_M^2 f$ is defined in (52), it holds

(55)
$$||f - \mathcal{Q}_M^2 f||_{L^2(\mathbb{S}^1)} \le \mathcal{C}M^{-s} ||f||_{\mathcal{W}_2^s(\mathbb{S}^1)}.$$

Assume $f \in \mathcal{W}_p^{s,\alpha}(\mathbb{S}^2)$, $\mathcal{Q}_M^3 f$ is defined in (53), it holds

(56)
$$||f - \mathcal{Q}_M^3 f||_{L^2(\mathbb{S}^2)} \le \mathcal{C}E_{M,p}(f)$$

Let

(57)
$$\widetilde{\mathbf{U}}(r) = \sum_{m=0}^{M} r^{-\frac{1}{2}} \widetilde{\mathbf{V}}^{m} e^{jm\theta},$$

(58)
$$\widetilde{\mathbf{U}}(r) = \sum_{m=0}^{M} \sum_{l=1}^{2m+1} r^{-1} \widetilde{\mathbf{V}}^{ml} Y_{m,l}(\theta, \phi).$$

From (17) and the definition of $\widetilde{\mathbf{V}}$, we know that (57)-(58) are the solutions generated by **Algorithm** 1. Then, we have the following results:

Theorem 2.4. Suppose that Ω is an annulus or hollow sphere domain, $\tilde{g}_1, \tilde{g}_2 \in L^2(\partial\Omega)$, $\tilde{u} \in H^s(\Omega)$ is the solution of the problem (4)-(6) and \tilde{U} is defined in (57)-(58). Under the assumption of (8) and (23), it holds

(59)
$$\|\tilde{u} - \widetilde{\mathbf{U}}\|_{H^{\tilde{i}}(\Omega)} \le \mathcal{C}\left(h^{1-\tilde{i}} + \frac{k^{s-1+\tilde{i}}}{M^s}\right), \ \tilde{i} = 0, 1.$$

Proof. We only prove the case of d = 3 here. The case of d = 2 is similar.

When $\tilde{i} = 0$, using Lemmas 2.3 and 2.4 with $\alpha = 0$ and p = 2, Theorem 2.3, (51) and the definitions above, we have

$$\begin{split} ||\tilde{u} - \mathbf{U}||_{L^{2}(\Omega)}^{2} &= ||\tilde{u} - \mathbf{U}||_{L^{2}(\mathbb{I};L^{2}(\mathbb{S}^{2}))}^{2} \\ &= ||\tilde{u} - \mathcal{Q}_{M}^{3}\tilde{u} + \mathcal{Q}_{M}^{3}\tilde{u} - \widetilde{\mathbf{U}}||_{L^{2}(\mathbb{I};L^{2}(\mathbb{S}^{2}))}^{2} \\ &\leq ||\tilde{u} - \mathcal{Q}_{M}^{3}\tilde{u}||_{L^{2}(\mathbb{I};L^{2}(\mathbb{S}^{2}))}^{2} + ||\mathcal{Q}_{M}^{3}\tilde{u} - \widetilde{\mathbf{U}}||_{L^{2}(\mathbb{I};L^{2}(\mathbb{S}^{2}))}^{2} \\ &\leq \frac{\mathcal{C}||\tilde{u}||_{L^{2}(\mathbb{I};W_{2}^{s}(\mathbb{S}^{2}))}}{M^{2s}} + \mathcal{C}\sum_{m=0}^{M}\sum_{l=1}^{2m+1} ||e^{ml}||_{L^{2}(\mathbb{I})}^{2} \\ &\leq \frac{\mathcal{C}||\tilde{u}||_{L^{2}(\mathbb{I};H^{s}(\mathbb{S}^{2}))}^{2}}{M^{2s}} + \mathcal{C}\sum_{m=0}^{M}\sum_{l=1}^{2m+1} \left(h^{2}\Big|\Big|\frac{\partial u^{ml}}{\partial r}\Big|\Big|_{L^{2}(\mathbb{I})}^{2} + ||u^{ml}||_{L^{2}(\mathbb{I})}^{2}\Big) \\ &\leq \frac{\mathcal{C}||\tilde{u}||_{H^{s}(\Omega)}^{2}}{M^{2s}} + \mathcal{C}(h^{2}||\tilde{u}||_{\tilde{H}^{1}(\mathbb{I};L^{2}(\mathbb{S}^{2}))}^{2} + ||\tilde{u}||_{L^{2}(\mathbb{I};L^{2}(\mathbb{S}^{2}))}^{2}\Big), \end{split}$$

which implies the desired results by applying Lemma 2.2, (4) and (8).

When $\tilde{i} = 1$, due to $||\tilde{u} - \widetilde{\mathbf{U}}||^2_{H^{\tilde{i}}(\Omega)} = ||\tilde{u} - \widetilde{\mathbf{U}}||^2_{L^2(\mathbb{I}; H^1(\mathbb{S}^2))} + |\tilde{u} - \widetilde{\mathbf{U}}|^2_{H^1(\mathbb{I}; L^2(\mathbb{S}^2))}$, applying the similar process as above, we can get the desired result too. The proof is completed.

Remark 1. Theorem 2.4 suggests that the error in L^2 -norm is first-order convergence when the summation number M in (57) and (58) is larger than the wave number k. And it also holds by using Lemma 2.2 that

$$\frac{||\tilde{u} - \mathbf{U}||_{H^{\tilde{i}}(\Omega)}}{||\tilde{u}||_{H^{\tilde{i}}(\Omega)}} \le \mathcal{C}, \ \tilde{i} = 0, 1,$$

which are confirmed by numerical experiments in [52].

3. Proof of the results for Algorithm 1

In this section, we will investigate the existence, uniqueness, stability and error estimates of **Algorithm** 1, which have not been reported for the pollution-free finite difference method before.

3.1. Existence and uniqueness. Firstly, we recall the following lemma which will be frequently used.

Lemma 3.1 [48]. For any $V_i, \overline{U}_i \in \mathcal{V}$, there holds that

$$-h\sum_{i=1}^{N-1} (\delta_r^2 V_i) \overline{U}_i = h\sum_{i=1}^N (\delta_r V_{i-\frac{1}{2}}) (\delta_r \overline{U}_{i-\frac{1}{2}}) + (\delta_r V_{\frac{1}{2}}) \overline{U}_0 - (\delta_r V_{N-\frac{1}{2}}) \overline{U}_{N-1}.$$

Proof of Theorem 2.1. We now prove the uniqueness of the algorithm. Assuming **Algorithm** 1 generalizes two solution sequences $\widehat{\mathbf{V}}, \ \widehat{\widehat{\mathbf{V}}} \in \mathcal{S}_h$, setting $\mathbf{V} = \widehat{\mathbf{V}} - \widehat{\widehat{\mathbf{V}}} \in \mathcal{S}_h$, then \mathbf{V} satisfies

(60)
$$-V_{i+1} - V_{i-1} + 2D_i^1 V_i = 0, \ 0 < i < N,$$

(61)
$$V_1 = -B_0^1 \left(jk + \frac{d-1}{2a} \right) V_0 + D_0^1 V_0,$$

(62)
$$V_{N-1} = -B_N^1 \left(jk + \frac{d-1}{2b} \right) V_N + D_N^1 V_N.$$

Note that (60) can be written as

(63)
$$-\delta_r^2 V_i - \omega_i^1 V_i = 0,$$

where

(64)
$$\omega_i^1 = \frac{2(1-D_i^1)}{h^2} := \frac{\bar{\omega}_i^1}{h^2}$$

satisfying $\omega_i^1 > 0$ based on the assumption of (8). By multiplying (63) with $h\overline{V}_i$, then summing-up the equation for *i* from 1 to N-1 and applying Lemma 3.1, we get

$$h\sum_{i=1}^{N} |\delta_r V_{i-\frac{1}{2}}|^2 + (\delta_r V_{\frac{1}{2}})\overline{V}_0 - (\delta_r V_{N-\frac{1}{2}})\overline{V}_N - h\sum_{i=1}^{N-1} \omega_i^1 |V_i|^2 = 0.$$

Using (61)-(62), we have

$$0 = ||\delta_r \mathbf{V}||_{\mathcal{L}^2}^2 - h \sum_{i=1}^{N-1} \omega_i^1 |V_i|^2 + \frac{D_0^1 - \frac{B_0^1(d-1)}{2a} - 1}{h} |V_0|^2 + \frac{D_N^1 - \frac{B_N^1(d-1)}{2b} - 1}{h} |V_N|^2 - j \left(\frac{B_0^1 k}{h} |V_0|^2 + \frac{B_N^1 k}{h} |V_N|^2\right)$$

Considering (38), the imaginary part equaling 0 in the above equation implies

(65)
$$V_0 = V_N = 0.$$

Using (65), it follows from (60) that

$$\begin{pmatrix} 2D_1^1 & -1 & & & \\ -1 & 2D_2^1 & -1 & & & \\ & & \ddots & & & \\ & & & -1 & 2D_{N-2}^1 & -1 \\ & & & & & -1 & 2D_{N-1}^1 \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ \vdots \\ V_{N-2} \\ V_{N-1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}.$$

Due to (33), the matrix is nonsingular and the system has an unique solution, i.e., $V_i = 0, i = 1, ..., N - 1$. The uniqueness is proved.

To prove the existence, noting that the following Gärding-type inequality holds:

$$Re\left(-h\sum_{i=1}^{N-1}((\delta_r^2 V_i)\overline{V}_i - h\omega_i^1 V_i\overline{V}_i)\right) + 5\mathcal{C}_1 k^2 ||\mathbf{V}||_{\mathcal{L}^2}^2 \ge ||\delta_r \mathbf{V}||_{\mathcal{L}^2}^2,$$

and by the classical Fredholm alternative argument see [35], **Algorithm** 1 has a nontrivial solution or it has at least one solution. Since the uniqueness is proved, existence follows from the above argument.

3.2. Stability analysis. In this subsection, we will analyze the stability of the algorithm.

Lemma 3.2. Let g_1, g_2 be two bounded numbers. Under the assumption of (8) and (23), the discretized solutions at i = 0 and N satisfy that

$$(66) |V_0| + |V_N| \le \frac{\mathcal{C}}{k},$$

$$(67) \qquad \qquad |\delta_r V_{\frac{1}{2}}| + |\delta_r V_{N-\frac{1}{2}}| \le \mathcal{C}.$$

Proof. Firstly, multiplying (41) by $h\overline{V}_i$, then taking the summation for *i* from 1 to N-1 and using Lemma 3.1, it holds

$$||\delta_r \mathbf{V}||_{\mathcal{L}^2}^2 + (\delta_r V_{\frac{1}{2}})\overline{V}_0 - (\delta_r V_{N-\frac{1}{2}})\overline{V}_N - h\sum_{i=1}^{N-1} \omega_i^1 |V_i|^2 = 0.$$

Applying (42)-(43), we have

$$\begin{aligned} ||\delta_{r}\mathbf{V}||_{\mathcal{L}^{2}}^{2} - h\sum_{i=1}^{N-1} \omega_{i}^{1}|V_{i}|^{2} + \frac{D_{0}^{1} - \frac{B_{0}^{1}(d-1)}{2a} - 1}{h}|V_{0}|^{2} + \frac{D_{N}^{1} - \frac{B_{N}^{1}(d-1)}{2b} - 1}{h}|V_{N}|^{2} \\ &- j\left(\frac{B_{0}^{1}k}{h}|V_{0}|^{2} + \frac{B_{N}^{1}k}{h}|V_{N}|^{2}\right) \\ (68) \qquad = -\frac{B_{0}^{1}a^{\frac{d-1}{2}}g_{1}}{h}\overline{V}_{0} - \frac{B_{N}^{1}b^{\frac{d-1}{2}}g_{2}}{h}\overline{V}_{N}. \end{aligned}$$

The real and imaginary parts of the above equation satisfy, respectively, that

$$\frac{B_0^1 k}{h} |V_0|^2 + \frac{B_N^1 k}{h} |V_N|^2$$
(69)
$$= Im \left(\frac{B_0^1 a^{\frac{d-1}{2}} g_1}{h} \overline{V}_0 \right) + Im \left(\frac{B_N^1 b^{\frac{d-1}{2}} g_2}{h} \overline{V}_N \right),$$

$$||\delta_r \mathbf{V}||_{\mathcal{L}^2}^2 - h \sum_{i=1}^{N-1} \omega_i^1 |V_i|^2 + \frac{D_0^1 - \frac{B_0^1 (d-1)}{2a} - 1}{h} |V_0|^2 + \frac{D_N^1 - \frac{B_N^1 (d-1)}{2b} - 1}{h} |V_N|^2$$
(70)

$$= Re\left(-\frac{B_0^1 a^{\frac{d-1}{2}}g_1}{h}\overline{V}_0\right) + Re\left(-\frac{B_N^1 b^{\frac{d-1}{2}}g_2}{h}\overline{V}_N\right).$$

Since

$$\left| Im \left(-\frac{B_0^1 a^{\frac{d-1}{2}} g_1}{h} \overline{V}_0 \right) \right| \le \frac{B_0^1 k}{2h} |V_0|^2 + \frac{\mathcal{C}B_0^1 |g_1|^2}{kh},$$
$$\left| Im \left(-\frac{B_N^1 b^{\frac{d-1}{2}} g_2}{h} \overline{V}_N \right) \right| \le \frac{B_N^1 k}{2h} |V_N|^2 + \frac{\mathcal{C}B_N^1 |g_2|^2}{kh},$$

putting above two estimates into (69), and noting (8) and (38), it follows

$$k(|V_0|^2 + |V_N|^2) \le \frac{\mathcal{C}(|g_1|^2 + |g_2|^2)}{k},$$

which implies (66). Applying (38), (42), (43) and (66), there holds that

$$|\delta_r V_{\frac{1}{2}}|^2 \leq \frac{[2a(D_0^1-1)+B_0^1(d-1)]^2+[\sqrt{2}aB_0^1k]^2}{a^2h^2}|V_0|^2 + \frac{(B_0^1a^{d-1})^2}{h^2}|g_1|^2 \leq \mathcal{C}.$$

Similarly, we can prove $|\delta_r V_{N-\frac{1}{2}}| \leq C$, which combining with the above inequality implies (67). The proof is completed.

Proof of Theorem 2.2. Using (70), Lemma 3.2 and the Cauchy inequality, we obtain

(71)
$$||\delta_r \mathbf{V}||_{\mathcal{L}^2}^2 \le h \sum_{i=0}^N \omega_i^1 |V_i|^2 + \mathcal{C}.$$

Multiplying (41) by $hr_i^{\alpha}(\delta_r \overline{V}_{i-\frac{1}{2}})$ (where $\alpha \in \mathbb{R}$ is a parameter which will be determined in the following), it follows

(72)
$$-hr_i^{\alpha}(\delta_r^2 V_i)(\delta_r \overline{V}_{i-\frac{1}{2}}) - h\omega_i^1 r_i^{\alpha} V_i(\delta_r \overline{V}_{i-\frac{1}{2}}) = 0.$$

It is easily to verify that

$$2Re\left(-hr_{i}^{\alpha}(\delta_{r}^{2}V_{i})(\delta_{r}\overline{V}_{i-\frac{1}{2}})\right) = -hr_{i}^{\alpha}(\delta_{r}^{2}V_{i})(\delta_{r}\overline{V}_{i-\frac{1}{2}}) - hr_{i}^{\alpha}(\delta_{r}^{2}\overline{V}_{i})(\delta_{r}V_{i-\frac{1}{2}}) \\ = h^{2}r_{i}^{\alpha}|\delta_{r}^{2}V_{i}|^{2} + r_{i}^{\alpha}|\delta_{r}V_{i-\frac{1}{2}}|^{2} - r_{i}^{\alpha}|\delta_{r}V_{i+\frac{1}{2}}|^{2},$$

thus, it holds that

$$Re\left(-h\sum_{i=1}^{N-1}r_{i}^{\alpha}(\delta_{r}^{2}V_{i})(\delta_{r}\overline{V}_{i-\frac{1}{2}})\right) = \frac{h^{2}}{2}\sum_{i=1}^{N-1}r_{i}^{\alpha}|\delta_{r}^{2}V_{i}|^{2} + \frac{h}{2}\sum_{i=1}^{N-1}\frac{r_{i}^{\alpha}-r_{i-1}^{\alpha}}{h}|\delta_{r}V_{i-\frac{1}{2}}|^{2} + \frac{r_{0}^{\alpha}}{2}|\delta_{r}V_{\frac{1}{2}}|^{2} - \frac{r_{N}^{\alpha}}{2}|\delta_{r}V_{N-\frac{1}{2}}|^{2}.$$

$$(73)$$

Similarly, we have

(74)

$$Re\left(-h\sum_{i=1}^{N-1}\omega_{i}^{1}r_{i}^{\alpha}V_{i}(\delta_{r}\overline{V}_{i-\frac{1}{2}})\right)$$

$$=-\frac{h^{2}}{2}\sum_{i=1}^{N-1}\omega_{i}^{1}r_{i}^{\alpha}|\delta_{r}V_{i-\frac{1}{2}}|^{2}+\frac{h}{2}\sum_{i=1}^{N-1}\frac{\omega_{i+1}^{1}r_{i+1}^{\alpha}-\omega_{i}^{1}r_{i}^{\alpha}}{h}|V_{i}|^{2}$$

$$-\frac{\omega_{N}^{1}r_{N}^{\alpha}}{2}|V_{N-1}|^{2}+\frac{\omega_{1}^{1}r_{1}^{\alpha}}{2}|V_{0}|^{2}.$$

Then, multiplying (41) by $hr_i^\alpha \delta_r \overline{V}_{i+\frac{1}{2}},$ it follows

(75)
$$-hr_i^{\alpha}(\delta_r^2 V_i)(\delta_r \overline{V}_{i+\frac{1}{2}}) - h\omega_i^1 r_i^{\alpha} V_i(\delta_r \overline{V}_{i+\frac{1}{2}}) = 0.$$

By a similar process in (73)-(74), we have

(76)

$$Re\left(\sum_{i=1}^{N-1} -hr_{i}^{\alpha}(\delta_{r}^{2}V_{i})(\delta_{r}\overline{V}_{i-\frac{1}{2}})\right)$$

$$= -\frac{h^{2}}{2}\sum_{i=1}^{N-1}r_{i}^{\alpha}|\delta_{r}^{2}V_{i}|^{2} + \frac{h}{2}\sum_{i=1}^{N-1}\frac{r_{i}^{\alpha} - r_{i-1}^{\alpha}}{h}|\delta_{r}V_{i-\frac{1}{2}}|^{2}$$

$$+ \frac{r_{0}^{\alpha}}{2}|\delta_{r}V_{\frac{1}{2}}|^{2} - \frac{r_{N}^{\alpha}}{2}|\delta_{r}V_{N-\frac{1}{2}}|^{2},$$

and

$$Re\left(-h\sum_{i=1}^{N-1}\omega_{i}^{1}r_{i}^{\alpha}V_{i}(\delta_{r}\overline{V}_{i+\frac{1}{2}})\right)$$

$$=\frac{h^{2}}{2}\sum_{i=1}^{N-1}\omega_{i-1}^{1}r_{i-1}^{\alpha}|\delta_{r}V_{i-\frac{1}{2}}|^{2}+\frac{h}{2}\sum_{i=1}^{N-1}\frac{\omega_{i}^{1}r_{i}^{\alpha}-\omega_{i-1}^{1}r_{i-1}^{\alpha}}{h}|V_{i}|^{2}-\frac{\omega_{N-1}^{1}r_{N-1}^{\alpha}}{2}|V_{N}|^{2}$$

$$(77) +\frac{\omega_{0}^{1}r_{0}^{\alpha}}{2}|V_{1}|^{2}-\frac{h^{2}}{2}w_{0}^{1}r_{0}^{\alpha}|\delta_{r}V_{\frac{1}{2}}|^{2}+\frac{h^{2}}{2}w_{N-1}r_{N-1}^{\alpha}|\delta_{r}V_{N-\frac{1}{2}}|^{2}.$$

Adding (72) and (75), taking the summation for i from 1 to N-1 in the resulted equation, using (64), (73), (74), (76), (77) and Lemma 3.2, we get

$$(78) \\ h \sum_{i=1}^{N-1} \frac{D_i^1 r_i^{\alpha} - D_{i-1}^1 r_{i-1}^{\alpha}}{h} |\delta_r V_{i-\frac{1}{2}}|^2 + \frac{1}{h^2} \left(h \sum_{i=1}^{N-1} \frac{\bar{\omega}_{i+1}^1 r_{i+1}^{\alpha} - \bar{\omega}_{i-1}^1 r_{i-1}^{\alpha}}{h} |V_i|^2 \right) \le \mathcal{C}.$$

In order to ensure that the first term on the left hand side is nonnegative, it is necessary to impose that the function $D^1(r)r^{\alpha}$ is a non-decreasing function, that is

$$[\cos[k(r)h]r^{\alpha}]^{(1)} = \alpha r^{\alpha-1} \cos[k(r)h] - r^{\alpha-3} \sin[k(r)h]h \frac{4d_m + d^2 - 4d + 3}{2k(r)} \ge 0.$$

Under the assumption of (8), we can check that $C_2 := h \frac{4d_m + d^2 - 4d + 3}{2k(r)} = \mathcal{O}(1)$, therefore,

$$[\cos(k(r)h)r^{\alpha}]^{(1)} = r^{\alpha-3} \{\alpha r^2 \cos[k(r)h] - \mathcal{C}_2 \sin[k(r)h] \}.$$

By taking $\alpha \geq \max_{a \leq r \leq b} \{ \frac{C_2 \sin[k(r)h]}{r^2 \cos[k(r)h]} \}$, $[\cos(k(r)h)r^{\alpha}]^{(1)}$ is nonnegative which suggests that the first term on the left hand side is nonnegative.

Noting (64), it is easily to check that $\bar{w}^1(r)r^{\alpha}$ and $(\bar{w}^1(r)r^{\alpha})^{(1)}$ are both smooth and increasing. Thus $\exists \xi_i \in [r_{i-1}, r_{i+1}]$ such that $\frac{\bar{w}^1(r_{i-1})r_{i-1}^{\alpha}-\bar{w}^1(r_{i+1})r_{i+1}^{\alpha}}{h}$ $= (\bar{w}^1(r)r^{\alpha})^{(1)}|_{r=\xi_i} \ge (\bar{w}^1(r)r^{\alpha})^{(1)}|_{r=a} := \mathcal{C}_3 > 0$. Thus, after using (8), we get

$$\frac{1}{h^2} \left(h \sum_{i=1}^{N-1} \frac{\bar{\omega}_{i+1}^1 r_{i+1}^\alpha - \bar{\omega}_{i-1}^1 r_{i-1}^\alpha}{h} |V_i|^2 \right) \ge \mathcal{C}k^2 \left(h \sum_{i=1}^{N-1} |V_i|^2 \right)$$
$$= \mathcal{C}k^2 ||\mathbf{V}||_{\mathcal{L}^2}^2 - \frac{1}{2h} (|V_0|^2 + |V_N|^2).$$

Putting the above estimate into (78), and using Lemma 3.2, we have

$$||\mathbf{V}||_{\mathcal{L}^2}^2 \le \frac{\mathcal{C}}{k^2},$$

which combining with (71) implies (44).

Finally, dividing (8) by ω_i^1 , multiplying the resulted equation by $-h\delta_r^2 \overline{V}_i$ and using Lemma 3.1 and (44), we can derive (45). The proof is completed.

3.3. Error estimates. This subsection is devoted to the error estimates for Algorithm 1. It follows form (8) and (27) that

$$\begin{split} & \left| \left| \frac{1}{(2n)!} h^{2n} \binom{2n-2}{2n-2-m} (k^2)^{(m)} v^{(2n-2-m)} \right| \right|_{L^2(\mathbb{I}_i)} \\ & \leq \begin{cases} \frac{C h^{m+1} ||v^{(1)}||_{L^2(\mathbb{I}_i)}}{(2n)(2n-1)(2n-2-m)!(m)!}, \ m \text{ is odd} \\ \frac{C h^m ||v||_{L^2(\mathbb{I}_i)}}{(2n)(2n-1)(2n-2-m)!(m)!}, \ m \text{ is even} \end{cases} . \end{split}$$

Thus, for any fixed m, we have

$$\begin{split} & \Big\| \sum_{n=1}^{+\infty} \frac{1}{(2n)!} h^{2n} \Big(\frac{2n-2}{2n-2-m} \Big) (k^2)^{(m)} v^{(2n-2-m)} \Big\|_{L^2(\mathbb{I}_i)} \\ & \leq \begin{cases} \sum_{n=1}^{+\infty} \frac{Ch^{m+1} ||v^{(1)}||_{L^2(\mathbb{I}_i)}}{n^2}, \ m \text{ is odd} \\ \sum_{n=1}^{+\infty} \frac{Ch^m ||v||_{L^2(\mathbb{I}_i)}}{n^2}, \ m \text{ is even} \end{cases} \\ & \leq \begin{cases} \mathcal{C}h^{m+1} ||v^{(1)}||_{L^2(\mathbb{I}_i)}, \ m \text{ is odd} \\ \mathcal{C}h^m ||v||_{L^2(\mathbb{I}_i)}, \ m \text{ is even} \end{cases}, \end{split}$$

which combining Lemma 2.1 implies (31). Similarly, we can derive (36). Therefore, the following Lemma holds:

Lemma 3.3. Under the assumption of (8) and (23), there hold that

(79)
$$||RD^{1}||_{L^{2}(\mathbb{I}_{i})} \leq Ch(h||v^{(1)}||_{L^{2}(\mathbb{I}_{i})} + ||v||_{L^{2}(\mathbb{I}_{i})}),$$

(80)
$$||RL^{1}||_{L^{2}(\mathbb{I}_{i})} \leq Ch(h||v^{(1)}||_{L^{2}(\mathbb{I}_{i})} + ||v||_{L^{2}(\mathbb{I}_{i})}),$$

(81)
$$||RR^{1}||_{L^{2}(\mathbb{I}_{i})} \leq Ch(h||v^{(1)}||_{L^{2}(\mathbb{I}_{i})} + ||v||_{L^{2}(\mathbb{I}_{i})}).$$

Lemma 3.4. For any smooth function v(r), there holds that

(82)
$$||v||_{\mathcal{L}^2}^2 \le \mathcal{C}(h||v^{(1)}||_{L^2(\mathbb{I})}^2 + ||v||_{L^2(\mathbb{I})}^2).$$

Proof. For any smooth function f(r), because it satisfies

$$(r_{i+1} - r_i)f(r_i) = \int_{r_i}^{r_{i+1}} f(r)dr + \int_{r_i}^{r_{i+1}} (r - r_i)f^{(1)}(r)dr,$$

$$(r_{i+1} - r_i)f(r_{i+1}) = \int_{r_i}^{r_{i+1}} f(r)dr - \int_{r_i}^{r_{i+1}} (r_{i+1} - r)f^{(1)}(r)dr.$$

Setting $f(r) = v(r)\overline{v}(r)$, and summing for *i* from 0 to N-1 in the above two equalities, it yields the results of Lemma 3.4.

Lemma 3.5. Suppose that g_1, g_2 are two bounded numbers. v is the solution of the problem (18)-(20) and $\mathbf{V} = \{V_i\}_{i=0}^N \in S_h$ is the discretized solution generated by **Algorithm** 1. Set $E_i = \prod_i v(r) - V_i, i = 0, \dots, N$. Under the assumption of (8) and (23), the errors at i = 0 and N satisfy

(83)
$$|E_0|^2 + |E_N|^2 \le h \left[\frac{\mathcal{C}}{\epsilon_1} (h || v^{(1)} ||_{L^2(\mathbb{I})}^2 + || v ||_{L^2(\mathbb{I})}^2) + h \sum_{i=1}^{N-1} \epsilon_1 \omega_{i-1}^1 r_{i-1}^{\alpha} |E_i|^2 \right],$$
(84)

$$|\delta_r E_{\frac{1}{2}}|^2 + |\delta_r E_{N-\frac{1}{2}}|^2 \leq \frac{\mathcal{C}}{h} \left[\frac{\mathcal{C}}{\epsilon_2} (h||v^{(1)}||^2_{L^2(\mathbb{I})} + ||v||^2_{L^2(\mathbb{I})}) + h \sum_{i=1}^{N-1} \epsilon_2 \omega_{i-1}^1 r_{i-1}^{\alpha} |E_i|^2 \right],$$

where $\epsilon_{\tilde{i}}, \tilde{i} = 1, 2$ are two parameters generated from the Young inequality and independent on h and k.

Proof. Subtracting (41), (42) and (43) from (32), (39) and (40) respectively, we

K. WANG, Y.S. WONG, AND J. HUANG

have

(85)
$$-E_{i+1} - E_{i-1} + 2D_i^1 E_i = RD_i^1, \ 0 < i < N,$$

(86)
$$E_1 = -B_0^1 \left(jk + \frac{a-1}{2a} \right) E_0 + D_0^1 E_0 + RL_0^1,$$

(87)
$$E_{N-1} = -B_N^1 \left(jk + \frac{d-1}{2b} \right) E_N + D_N^1 E_N + RR_N^1.$$

Multiplying (85) by $h\overline{E}_i$, then taking the summation for *i* from 1 to N-1 and using Lemma 3.1, (86) and (87), we have

$$||\delta_{r}\mathbf{E}||_{\mathcal{L}^{2}}^{2} - h\sum_{i=1}^{N-1}\omega_{i}^{1}|E_{i}|^{2} + \frac{D_{0}^{1} - \frac{B_{0}^{1}(d-1)}{2a} - 1}{h}|E_{0}|^{2} + \frac{D_{N}^{1} - \frac{B_{N}^{1}(d-1)}{2b} - 1}{h}|E_{N}|^{2}$$
$$- j\left(\frac{B_{0}^{1}k}{h}|E_{0}|^{2} + \frac{B_{N}^{1}k}{h}|E_{N}|^{2}\right)$$
$$(88) \qquad = \sum_{i=1}^{N-1}\frac{RD_{i}^{1}}{h}\overline{E}_{i} - \frac{RL_{0}^{1}}{h}\overline{E}_{0} - \frac{RR_{N}^{1}}{h}\overline{E}_{N}.$$

The real and imaginary parts of the above equation satisfy, respectively, that

$$=Re\Big(\sum_{i=1}^{N-1}\frac{RD_i^1}{h}\overline{E}_i\Big)+Re\Big(-\frac{RL_0^1}{h}\overline{E}_0\Big)+Re\Big(-\frac{RR_n^1}{h}\overline{E}_N\Big).$$

It is easily to check by using (64) that

$$\begin{split} \left| Im \left(\frac{RL_0^1}{h} \overline{E}_0 \right) \right| &\leq \frac{B_0^1 k}{2h} |E_0|^2 + \frac{\mathcal{C}}{B_0^1 k h} |RL_0^1|^2, \\ \left| Im \left(\frac{RR_N^1}{h} \overline{E}_N \right) \right| &\leq \frac{B_N^1 k}{2h} |E_N|^2 + \frac{\mathcal{C}}{B_N^1 k h} |RR_N^1|^2, \\ Im \left(-\sum_{i=1}^{N-1} \frac{RD_i^1}{h} \overline{E}_i \right) \right| &\leq h \sum_{i=1}^{N-1} \epsilon_1 \omega_{i-1}^1 r_{i-1}^\alpha |E_i|^2 + \frac{\mathcal{C}}{\epsilon_1 h^2} ||RD^1||_{\mathcal{L}^2}^2, \end{split}$$

with ϵ_1 being a parameter. Putting the above estimates into (89), and using (38), it follows

$$\begin{aligned} &\frac{1}{h}(|E_0|^2 + |E_N|^2) \\ \leq &\frac{\mathcal{C}(|RL_0^1|^2 + |RR_N^1|^2)}{h} + \frac{\mathcal{C}}{\epsilon_1 h^2} ||RD^1||_{\mathcal{L}^2}^2 + h \sum_{i=1}^{N-1} \epsilon_1 \omega_{i-1}^1 r_{i-1}^{\alpha} |E_i|^2. \end{aligned}$$

Therefore, using Lemma 3.4 and (79)-(81), we have

(91)
$$|E_0|^2 + |E_N|^2 \le h\left[\frac{\mathcal{C}}{\epsilon_1}(h||v^{(1)}||^2_{L^2(\mathbb{I})} + ||v||^2_{L^2(\mathbb{I})}) + h\sum_{i=1}^{N-1} \epsilon_1 \omega_{i-1}^1 r_{i-1}^{\alpha} |E_i|^2\right].$$

Using (79)-(81) and (91), it is valid that

$$\begin{split} |\delta_{r}E_{\frac{1}{2}}|^{2} &\leq \!\!\frac{[2a(D_{0}^{1}-1)+B_{0}^{1}(d-1)]^{2}+[\sqrt{2}aB_{0}^{1}k]^{2}}{a^{2}h^{2}}|E_{0}|^{2}+\frac{(B_{0}^{1}a^{d-1})^{2}}{h^{2}}|RL_{0}^{1}|^{2} \\ &\leq \!\!\frac{\mathcal{C}}{h}\left[\frac{\mathcal{C}}{\epsilon_{2}}(h||v^{(1)}||_{L^{2}(\mathbb{I})}^{2}+||v||_{L^{2}(\mathbb{I})}^{2})+h\sum_{i=1}^{N-1}\epsilon_{2}\omega_{i-1}^{1}r_{i-1}^{\alpha}|E_{i}|^{2}\right]. \end{split}$$

Following the similar process, we can get (84). The proof is completed.

Lemma 3.6. Suppose that g_1, g_2 are two bounded numbers. v is the solution of the problem (18)-(20) and $\mathbf{V} = \{V_i\}_{i=0}^N \in S_h$ is the discretized solution generated by **Algorithm 1**. Set $E_i = \prod_i v(r) - V_i, i = 0, \dots, N$. Under the assumption of (8) and (23), the error $\mathbf{E} = \{E_i\}_{i=0}^N \in S_h$ satisfies

(92)
$$h||\delta_{r}\mathbf{E}||_{\mathcal{L}^{2}} + ||\mathbf{E}||_{\mathcal{L}^{2}} \leq \mathcal{C}(h||v^{(1)}||_{L^{2}(\mathbb{I})} + ||v||_{L^{2}(\mathbb{I})}).$$

Proof. Using Lemma 3.5 in (90), we obtain

(93)
$$||\delta_{r}\mathbf{E}||_{\mathcal{L}^{2}}^{2} \leq h \sum_{i=0}^{N-1} (1+5\epsilon_{1})\omega_{i-1}^{1}r_{i-1}^{\alpha}|E_{i}|^{2} + \frac{\mathcal{C}}{\epsilon_{1}}(h||v^{(1)}||_{L^{2}(\mathbb{I})}^{2} + ||v||_{L^{2}(\mathbb{I})}^{2}).$$

Multiplying (85) by $hr_i^{\alpha}\delta_r\overline{E}_{i-\frac{1}{2}}$ and $hr_i^{\alpha}\delta_r\overline{E}_{i+\frac{1}{2}}$ respectively, similarly to the process of analyzing the stability, we have

$$\begin{split} h\sum_{i=1}^{N-1} \frac{D_{i}^{1}r_{i}^{\alpha} - D_{i-1}^{1}r_{i-1}^{\alpha}}{h} |\delta_{r}E_{i-\frac{1}{2}}|^{2} + \frac{1}{h^{2}} \left(h\sum_{i=1}^{N} \frac{\omega_{i+1}^{1}r_{i+1}^{\alpha} - \omega_{i-1}^{1}r_{i-1}^{\alpha}}{h} |E_{i}|^{2}\right) \\ &= -r_{0}^{\alpha} |\delta_{r}E_{\frac{1}{2}}|^{2} + r_{N}^{\alpha} |\delta_{r}E_{N-\frac{1}{2}}|^{2} + \frac{\omega_{N}^{1}r_{N}^{\alpha}}{2} |E_{N}|^{2} - \frac{\omega_{1}^{1}r_{1}^{\alpha}}{2} |E_{0}|^{2} \\ &+ \frac{\omega_{N-1}^{1}r_{N-1}^{\alpha}}{2} |E_{N}|^{2} - \frac{\omega_{0}^{1}r^{\alpha}}{2} |E_{1}|^{2} + \frac{h^{2}}{2} \omega_{0}^{1}r^{\alpha} |\delta_{r}E_{\frac{1}{2}}|^{2} - \frac{h^{2}}{2} \omega_{N-1}^{1}r_{N-1}^{\alpha} |\delta_{r}E_{N-\frac{1}{2}}|^{2} \end{split}$$

$$(94) \\ &- \sum_{i=1}^{N-1} \frac{r_{i}^{\alpha}}{h} RD_{i}^{1} (\delta_{r}\overline{E}_{i-\frac{1}{2}}) - \sum_{i=1}^{N-1} \frac{r_{i}^{\alpha}}{h} RD_{i}^{1} (\delta_{r}\overline{E}_{i+\frac{1}{2}}). \end{split}$$

It is easily to check that

$$\begin{split} & \Big| - \sum_{i=1}^{N-1} \frac{r_i^{\alpha}}{h} RD_i^1(\delta_r \overline{E}_{i-\frac{1}{2}}) \Big| \\ \leq & h \sum_{i=1}^{N-1} \frac{\epsilon_3 D_{i-1}^1 r_{i-1}^{\alpha}}{h} |\delta_r E_{i-\frac{1}{2}}|^2 + \frac{\mathcal{C}}{\epsilon_3 h} (h||v^{(1)}||_{L^2(\mathbb{I})}^2 + ||v||_{L^2(\mathbb{I})}^2), \\ & \Big| - \sum_{i=1}^{N-1} \frac{r_i^{\alpha}}{h} RD_i^1(\delta_r \overline{E}_{i+\frac{1}{2}}) \Big| \\ \leq & h \sum_{i=1}^{N-1} \frac{\epsilon_4 D_i^1 r_i^{\alpha}}{h} |\delta_r E_{i+\frac{1}{2}}|^2 + \frac{\mathcal{C}}{\epsilon_4 h} (h||v^{(1)}||_{L^2(\mathbb{I})}^2 + ||v||_{L^2(\mathbb{I})}^2)) \\ = & h \sum_{i=1}^{N-1} \frac{\epsilon_4 D_{i-1}^1 r_{i-1}^{\alpha}}{h} |\delta_r E_{i-\frac{1}{2}}|^2 + \frac{\mathcal{C}}{\epsilon_4 h} (h||v^{(1)}||_{L^2(\mathbb{I})}^2 + ||v||_{L^2(\mathbb{I})}^2)) \\ & - \epsilon_4 D_0^1 r_0^{\alpha} |\delta_r E_{\frac{1}{2}}|^2 + \epsilon_4 D_{N-1}^1 r_{N-1}^{\alpha} |\delta_r E_{N-\frac{1}{2}}|^2 \\ \leq & h \sum_{i=1}^{N-1} \frac{\epsilon_4 D_{i-1}^1 r_{i-1}^{\alpha}}{h} |\delta_r E_{i-\frac{1}{2}}|^2 + \frac{\mathcal{C}}{\epsilon_4 h} \left[(h||v^{(1)}||_{L^2(\mathbb{I})}^2 + ||v||_{L^2(\mathbb{I})}^2) \right] \\ & + h \sum_{i=1}^{N-1} \epsilon_4 \omega_{i-1}^1 r_{i-1}^{\alpha} |E_i|^2 \right]. \end{split}$$

Similarly,

$$\begin{split} & \left| \frac{\omega_{N+1}^{1}r_{N+1}^{\alpha}}{2} |E_{N}|^{2} - \frac{\omega_{1}^{1}r_{1}^{\alpha}}{2} |E_{0}|^{2} + \frac{\omega_{N}^{1}r_{N}^{\alpha}}{2} |E_{N}|^{2} - \frac{\omega_{0}^{1}a^{\alpha}}{2} |E_{1}|^{2} \right| \\ \leq & \mathcal{C}h\left[\frac{\mathcal{C}}{\epsilon_{5}}(h||v^{(1)}||_{L^{2}(\mathbb{I})}^{2} + ||v||_{L^{2}(\mathbb{I})}^{2}) + h\sum_{i=1}^{N-1} \epsilon_{5}\omega_{i-1}^{1}r_{i-1}^{\alpha}|E_{i}|^{2} \right], \\ & \left| \frac{h^{2}}{2}\omega_{0}^{1}r_{0}^{\alpha}|\delta_{r}E_{\frac{1}{2}}|^{2} - \frac{h^{2}}{2}\omega_{N-1}^{1}r_{N-1}^{\alpha}|\delta_{r}E_{N-\frac{1}{2}}|^{2} - r_{0}^{\alpha}|\delta_{r}E_{\frac{1}{2}}|^{2} + r_{N-1}^{\alpha}|\delta_{r}E_{N-\frac{1}{2}}|^{2} \right| \\ \leq & \frac{\mathcal{C}}{h}\left[\frac{\mathcal{C}}{\epsilon_{6}}(h||v^{(1)}||_{L^{2}(\mathbb{I})}^{2} + ||v||_{L^{2}(\mathbb{I})}^{2}) + h\sum_{i=1}^{N-1} \epsilon_{6}\omega_{i-1}^{1}r_{i-1}^{\alpha}|E_{i}|^{2} \right]. \end{split}$$

Substituting the above estimates into (94), we obtain

$$\begin{split} &h\sum_{i=1}^{N-1} \frac{D_{i}^{1}r_{i}^{\alpha} - (1+\epsilon_{3}+\epsilon_{4})D_{i-1}^{1}r_{i-1}^{\alpha}}{h} |\delta_{r}E_{i-\frac{1}{2}}|^{2} \\ &+ \frac{1}{h^{2}} \left\{ h\sum_{i=1}^{N} \Big[\frac{\bar{\omega}_{i+1}^{1}r_{i+1}^{\alpha} - (1+h^{2}(\epsilon_{4}+\epsilon_{5})+\epsilon_{6})\bar{\omega}_{i-1}^{1}r_{i-1}^{\alpha}}{h} \Big] |E_{i}|^{2} \right\} \\ &\leq & \frac{\mathcal{C}}{h^{2}} \Big(\sum_{\tilde{i}=3}^{6} \frac{1}{\epsilon_{\tilde{i}}} \Big) (h^{2}||v^{(1)}||_{L^{2}(\mathbb{I})}^{2} + ||v||_{L^{2}(\mathbb{I})}^{2}). \end{split}$$

Consider the second term on the left hand side in the above inequality. Since $\frac{\bar{\omega}_{i+1}^1 r_{i+1}^{\alpha} - \bar{\omega}_{i-1}^1 r_{i-1}^{\alpha}}{h} = (\bar{\omega}^1(r)r^{\alpha})^{(1)}|_{r=\xi_i \in \mathbb{I}_i} > (\bar{\omega}^1(r)r^{\alpha})^{(1)}|_{r=a} > 0$, we can choose $\epsilon_4, \epsilon_5, \epsilon_6$ small enough such that $\frac{\bar{\omega}_{i+1}^1 r_{i+1}^{\alpha} - (1+h^2(\epsilon_4+\epsilon_5)+\epsilon_6)\bar{\omega}_{i-1}^1 r_{i-1}^{\alpha}}{h} > \frac{1}{2}(\bar{\omega}^1(r)r^{\alpha})^{(1)}|_{r=a} = \frac{C_3}{2} > 0$. Similarly, we can

ensure that the first term is nonnegative. Combining with (93), we have (92). The proof is completed.

Proof of Theorem 2.3. Since

$$\begin{aligned} ||e||_{L^{2}(\mathbb{I})}^{2} \leq ||v - \mathcal{P}^{1}v||_{L^{2}(\mathbb{I})}^{2} + ||\mathcal{P}^{1}v - \widetilde{\mathbf{V}}||_{L^{2}(\mathbb{I})}^{2} \\ \leq \mathcal{C} \sum_{i=1}^{N-1} (||v - \mathcal{P}^{1}v||_{L^{2}(\mathbb{I}_{i})}^{2} + ||\mathcal{P}^{1}v - \widetilde{\mathbf{V}}||_{L^{2}(\mathbb{I}_{i})}^{2}). \end{aligned}$$

from (34), we have

$$v(r) = \frac{v_{i+1} - \cos(k_i h)v_i}{\sin(k_i h)} \sin[k_i (r - r_i)] + v_i \cos[k_i (r - r_i)] + \left[1 + \frac{\sin[k_i (r - r_i)]}{\sin(k_i h)}\right] RL^1, \ r \in \mathbb{I}_i,$$

which implies, by using (80), that

$$||v - \mathcal{P}^{1}v||_{L^{2}(\mathbb{I}_{i})}^{2} = \mathcal{C}||RL^{1}||_{L^{2}(\mathbb{I}_{i})}^{2} \leq \mathcal{C}h^{2}(h^{2}||v^{(1)}||_{L^{2}(\mathbb{I}_{i})}^{2} + ||v||_{L^{2}(\mathbb{I}_{i})}^{2}).$$

By the definition of \mathcal{P}^1 , obviously it is continuous, which follows, by using Lemma 3.6, that

$$\begin{aligned} ||\mathcal{P}^{1}v - \tilde{\mathbf{V}}||_{L^{2}(\mathbb{I}_{i})}^{2} = ||\mathcal{P}^{1}v - \mathcal{P}^{1}\mathbf{V}||_{L^{2}(\mathbb{I}_{i})}^{2} \leq \mathcal{C}||\mathbf{E}||_{\mathcal{L}^{2}}^{2} \\ \leq \mathcal{C}(h^{2}||v^{(1)}||_{L^{2}(\mathbb{I}_{i})}^{2} + ||v||_{L^{2}(\mathbb{I}_{i})}^{2}). \end{aligned}$$

Therefore

$$||e||_{L^{2}(\mathbb{I})}^{2} \leq \mathcal{C} \sum_{i=0}^{N-1} (h^{2}||v^{(1)}||_{L^{2}(\mathbb{I}_{i})}^{2} + ||v||_{L^{2}(\mathbb{I}_{i})}^{2}) \leq \mathcal{C}(h^{2}||v^{(1)}||_{L^{2}(\mathbb{I})}^{2} + ||v||_{L^{2}(\mathbb{I})}^{2}).$$

Using the definition of \mathcal{P}^2 and following the similar process above, we can prove the estimate for $||e^{(1)}||_{L^2(\mathbb{I})}$. The proof is completed.

Remark 2. Theorems 2.1-2.3 are also valid for the one dimensional problem (d = 1 in equations (4)-(6)). Compared to the assumption that $kh \to 0$ when proving the convergence order in [50], the condition here is improved (see (8)) Furthermore, the higher order convergence as reported in [50] can be achieved for the 1*D* problem.

Remark 3. By using (34), the interpolation operator $\mathcal{P}^{\tilde{i}}$ ($\tilde{i} = 1, 2$) defined above can also be extended to other cases with higher order with respect to h under the assumption of (8).

4. Numerical experiments

We verify the convergence order in this section. Set the exact solution of (4) to be $\tilde{u} = e^{jkx_1}$ and $\tilde{u} = \tilde{u}_0 e^{jkr\cos\theta}$ with \tilde{u}_0 being incident in the x_3 -direction on a sphere (see Example 2.2 in [31]) when d = 2 and 3, respectively. By the coordinate transformation, we have

$$\tilde{u} = e^{jkx_1} = J_0(kr) + 2\sum_{m=1}^{\infty} j^m J_m(kr) \cos(m\phi),$$

with $J_m(\cdot)$ being the *m*-th degree Bessel function of the first kind, and

$$\tilde{u} = \tilde{u}_0 e^{jkr\cos\theta} = u_0 \sum_{m=0}^{\infty} (2m+1)j^m P_m(\cos\theta)\tilde{J}_m(kr),$$

with $P_m(\cdot)$ being the Lengendre polynomials and $\tilde{J}_m(\cdot)$ being the spherical Bessel functions of the first kind in 2D and 3D, respectively. The corresponding approximation solutions are got according to (52) and (53). Let kh = 0.6, we collect the numerical solution in Table 1, which is good agreement with the theoretical prediction in Section 2. For more numerical results, the reader is referred to [52].

	2D		3D	
1/h	Error	Order	Error	Order
1/100	6.55e-005	1.15	7.65e-004	1.10
1/120	5.31e-005	1.17	6.26e-004	1.29
1/140	4.44e-005	1.17	5.21e-004	1.15
1/160	3.79e-005	1.18	4.46e-004	1.23
1/180	3.30e-005	1.20	3.86e-004	1.22
1/200	2.91e-005	1.19	3.40e-004	1.24

TABLE 1. Convergence order.

5. Conclusions

By using the weighted-test-function method in the finite difference scheme and the spherical harmonics results in 2D and 3D, we established an error estimate for the first-order pollution-free scheme given by [52], which is proposed to solve the Helmholtz equation with high wave numbers in the annulus and hollow sphere domains. The error estimate result reveals that the famous pollution effect can be avoided in these cases. In the present approach, the numerical solutions of the multi-dimensional Helmholtz equation are computed by solving a sequence of one-dimensional problems. Although the number of linear solver is of the order of the wave number, it is important to note that the linear system is a tri-diagonal matrix. Hence, the system of linear equations can be solved effectively by a direct method. Recall that the resulting linear system for a multi-dimensional Helmholtz equation is large and indefinite. Not only it can not be solved efficiently by a direct method, and most iterative methods also have difficulty in computing the resulting indefinite system. It is important to point out that the success of the proposed methodology is due to the problem can be computed by the separation of variables using spherical harmonics. Depending upon the type of boundary conditions, the approach can also be extended to certain multi-dimensional Helmholtz equations in cartesian coordinates. Based on the limitations, we conclude that pollutionfree difference schemes can be applied only to certain multi-dimensional Helmholtz equations.

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