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A new family of fourth-order locally one-dimensional schemes for the three-dimensional wave equation☆

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ABSTRACT

In this paper, we present a new family of locally one-dimensional (LOD) schemes with fourth-order accuracy in both space and time for the three-dimensional (3D) acoustic wave equation. It is well-known that high order explicit schemes offer efficient time steppings but with restrictive CFL conditions; implicit discretization gives unconditional stable schemes but with inefficient time steppings. Our LOD schemes can be seen as a compromise between explicit and implicit schemes, in the way that our schemes have more relax CFL conditions compared with traditional explicit schemes and only require solutions of tridiagonal systems of linear algebraic equations, which is more efficient than implicit schemes. Moreover, the new scheme is four-layer in time and three-layer in space, so that boundary conditions can be imposed in the classical way. The computations of the initial conditions for the three intermediate time layers are explicitly constructed. Furthermore, the stability condition is derived and the restriction for the time step is given explicitly. Finally, numerical examples are completed to show the performance of our new method.

1. Introduction

Wave simulation based on the acoustic wave equation has important applications. For example, wave propagation is usually applied to detect the structures of oil and gas reservoir in geophysics [1]. Thus a fast and accurate simulation technique for the acoustic wave equation is important. There are in literature many numerical methods for wave equations. These include the finite difference method (see, e.g., [2–5]), the finite volume method (see, e.g., [6,7]), the finite element method (see, e.g., [8–11]) and the discontinuous Galerkin method (see, e.g., [12–14]). Each numerical method has its own advantages and disadvantages. For example, the FDM is efficient and is relatively easy to implement code but it is not suitable for irregular domain. And the finite element method can adapt complex topography but has large computational cost. In this paper we focus on the difference method for the three-dimensional acoustic wave equation.

Among the various finite difference (FD) methods, the splitting method is an important technique and in fact it has been a research topic for decades (see, e.g., [5,15–23]). The splitting method decouples a multidimensional differential equation into more basic equations, in which each equation contains a one-dimensional problem. The splitting schemes have been proven to be very efficient in the numerical solution of time-dependent differential equations. There are two splitting ways, i.e., the alternating direction implicit (ADI) method and the locally one-dimensional (LOD) method. Both ADI and LOD methods reduce the multidimensional problem to a sequence of locally one-dimensional problems with tridiagonal

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systems which can be solved easily. The ADI method was first introduced by [15,16] for the heat equation in two space variables and then was applied in three space variables [18,24]. Improved ADI schemes were proposed later [25,26]. A high order version of ADI schemes for the wave equation is also developed [20,27,28]. In [23], the high-order ADI algorithms for time-dependent equations based on Richardson extrapolation are investigated. Currently the ADI schemes have been applied to many problems successfully.

The LOD method was proposed about ten years later than the ADI method. In [29], a LOD method for solving hyperbolic equations in two space dimensions was introduced. The LOD method provides a more competitive option as it has good computational efficiency and can be applied to arbitrary regions [29]. Each decomposed one-dimensional problem in the LOD method has clear physical characteristics. We remark that the aforementioned ADI methods such as the method of Lees [17,18], the high accuracy methods of [27] cannot be written in LOD form. The main difference between ADI and LOD methods is that each one-dimensional problem in LOD only has one spatial variable while it contains several spatial variables in ADI. The high accuracy ADI methods are investigated extensively for wave equations. Nevertheless, the high-order LOD schemes for the 3D acoustic wave equation have not been fully developed. In [5], a new LOD scheme with fourth-order accuracy both in space and time for the 2D acoustic wave equation is developed. We remark that the derivation in our previous 2D work [5] cannot be generalized to three space dimensions obviously, and it is therefore the purpose of this paper to develop a LOD scheme for three space dimensions.

Besides efficiency enhancement using splitting ideas, the construction of higher order schemes is equally important. To construct a FD scheme with high accuracy, two general approaches are typically used. One way is to simply increase the grid stencil of the scheme, and the other way uses compact or Padé approximation (see, e.g., [30–34]). Compared to non-compact FD schemes of the same order of accuracy, compact schemes have a shorter stencil, which provides many desirable properties, such as ease of implementation and ease of imposing boundary conditions. Compact schemes have been widely used with great success (see, e.g., [21,35,36]). In this paper, we present and analyze a new family of LOD schemes with fourth-order accuracy both in space and time for the 3D acoustic wave equation. It is an extension of our previous work on two-dimensional LOD schemes [5]. Our method only uses a three-points stencil in each spatial direction and has the compact advantages. We remark that our approach produces a family of new schemes and only requires a smaller number of tridiagonal systems.

The organization of the paper is as follows. In Section 2, we prescribe detailedly the derivation of the new LOD scheme, including the two groups of parameters choices used in the schemes. In Section 3, we discuss how the intermediate initial conditions are computed. In Section 4, the stability conditions are investigated in detail. In Section 5, numerical results are illustrated to confirm our theoretical findings. Finally, a conclusion is given in Section 6.

2. Theory

2.1. The derivation of new fourth-order LOD scheme

In this section, we will derive our new LOD scheme to solve the acoustic wave equation in three space dimensions. The 3D acoustic wave equation in a homogeneous media can be written as [1]

$$\frac{\partial^2 u}{\partial t^2} = v^2\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right), \tag{2.1}$$

with $(x, y, z, t) \in \overline{\Omega} = \Omega \times [0, T]$, subject to the initial conditions

$$u(x, y, z, 0) = f_1(x, y, z), \qquad \frac{\partial u(x, y, z, 0)}{\partial t} = f_2(x, y, z), \quad (x, y, z) \in \Omega, \tag{2.2}$$

and the boundary conditions

$$u(x, y, z, t) = 0, \quad (x, y, z, t) \in \partial\Omega \times [0, T], \tag{2.3}$$

where $\partial\Omega$ is the boundary of $\Omega \subset \mathbb{R}^3$, v is the wave velocity, and f_1 and f_2 are given functions. We assume that the given initial conditions are sufficiently smooth to achieve high order accuracy of the difference scheme under consideration. In this paper, we consider the Dirichlet boundary conditions. For absorbing boundary conditions in wave simulation, readers can refer to the references (see, e.g., [37–39]). We remark that this is another important research topic and we will not discuss here as it is not the main concern in this paper.

In order to obtain our higher order scheme, we use the following approximation

$$\left.\frac{\partial^2 u}{\partial t^2}\right|_{t=t_n} \approx \frac{au^{n+s_1} - (a+b)u^n + bu^{n+s_2}}{\Delta t^2}, \tag{2.4}$$

where Δt is the time step. Using the Taylor expansion, we find that the coefficients s_1, s_2, a, b must satisfy

$$a = \frac{2}{-s_1(s_2 - s_1)}, \qquad b = \frac{2}{s_2(s_2 - s_1)} \tag{2.5}$$

so that the approximation (2.4) has at least first order accuracy. Using (2.4), we approximate (2.1) by the following four LOD equations:

$$\frac{a_1u^{n-1+s_3}-(a_1+b_1)u^n+b_1u^{n+s_1}}{\Delta t^2}=v^2\frac{c_1\delta_x^2u^n-c_2\delta_x^2u^{n+s_1}-c_3\delta_x^2u^{n-1+s_3}}{h_x^2}, \tag{2.6}$$

$$\frac{a_2u^n-(a_2+b_2)u^{n+s_1}+b_2u^{n+s_2}}{\Delta t^2}=v^2\frac{d_1\delta_y^2u^{n+s_1}-d_2\delta_y^2u^{n+s_2}-d_3\delta_y^2u^n}{h_y^2}, \tag{2.7}$$

$$\frac{a_3u^{n+s_1}-(a_3+b_3)u^{n+s_2}+b_3u^{n+s_3}}{\Delta t^2}=v^2\frac{\tilde{d}_1\delta_y^2u^{n+s_2}-d_2'\delta_y^2u^{n+s_3}-\tilde{d}_3\delta_y^2u^{n+s_1}}{h_y^2}, \tag{2.8}$$

$$\frac{a_4u^{n+s_2}-(a_4+b_4)u^{n+s_3}+b_4u^{n+1}}{\Delta t^2}=v^2\frac{e_1\delta_z^2u^{n+s_3}-e_2\delta_z^2u^{n+1}-e_3\delta_z^2u^{n+s_2}}{h_z^2}, \tag{2.9}$$

where $s_1, s_2, s_3 \in (0, 1)$ and $s_1 < s_2 < s_3$; a_i, b_i $(i = 1, 2, 3, 4)$, and $c_i, d_i, \tilde{d}_i, e_i, s_i$ $(i = 1, 2, 3)$ are coefficients, which will be determined what follows in this subsection and are summarized in Appendix A. In addition, h_x, h_y and h_z are the mesh sizes in x, y and z directions respectively. We rewrite (2.6)–(2.9) as follows:

$$(a_1+c_3\tau_x\delta_x^2)u^{n-1+s_3}+(b_1+c_2\tau_x\delta_x^2)u^{n+s_1}=(a_1+b_1+c_1\tau_x\delta_x^2)u^n, \tag{2.10}$$

$$(a_2+d_3\tau_y\delta_y^2)u^n+(b_2+d_2\tau_y\delta_y^2)u^{n+s_2}=(a_2+b_2+d_1\tau_y\delta_y^2)u^{n+s_1}, \tag{2.11}$$

$$(a_3+\tilde{d}_3\tau_y\delta_y^2)u^{n+s_1}+(b_3+\tilde{d}_2\tau_y\delta_y^2)u^{n+s_3}=(a_3+b_3+\tilde{d}_1\tau_y\delta_y^2)u^{n+s_2}, \tag{2.12}$$

$$(a_4+e_3\tau_z\delta_z^2)u^{n+s_2}+(b_4+e_2\tau_z\delta_z^2)u^{n+1}=(a_4+b_4+e_1\tau_z\delta_z^2)u^{n+s_3}, \tag{2.13}$$

where

$$\tau_x=\frac{v^2\Delta t^2}{h_x^2},\qquad \tau_y=\frac{v^2\Delta t^2}{h_y^2},\qquad \tau_z=\frac{v^2\Delta t^2}{h_z^2}, \tag{2.14}$$

and δ_x^2, δ_y^2 and δ_z^2 are the second-order central difference operators in the x, y and z directions respectively, e.g.,

$$\delta_x^2u_{i,j,k}^n=u_{i+1,j,k}^n-2u_{i,j,k}^n+u_{i-1,j,k}^n. \tag{2.15}$$

Using (2.5) for the LHS of (2.6)–(2.9), we obtain

$$a_1=\frac{2}{(1-s_3)(s_1+1-s_3)},\qquad b_1=\frac{2}{s_1(s_1+1-s_3)}, \tag{2.16}$$

$$a_2=\frac{2}{s_1s_2},\qquad b_2=\frac{2}{(s_2-s_1)s_2}, \tag{2.17}$$

$$a_3=\frac{2}{(s_2-s_1)(s_3-s_1)},\qquad b_3=\frac{2}{(s_3-s_2)(s_3-s_1)}, \tag{2.18}$$

$$a_4=\frac{2}{(s_3-s_2)(1-s_2)},\qquad b_4=\frac{2}{(1-s_3)(1-s_2)}. \tag{2.19}$$

To simplify the notions, we let

$$A=a_1+c_3\tau_x\delta_x^2,\qquad B=b_1+c_2\tau_x\delta_x^2,\qquad C=a_1+b_1+c_1\tau_x\delta_x^2, \tag{2.20}$$

$$D=a_2+d_3\tau_y\delta_y^2,\qquad E=b_2+d_2\tau_y\delta_y^2,\qquad F=a_2+b_2+d_1\tau_y\delta_y^2, \tag{2.21}$$

$$\tilde{D}=a_3+\tilde{d}_3\tau_y\delta_y^2,\qquad \tilde{E}=b_3+\tilde{d}_2\tau_y\delta_y^2,\qquad \tilde{F}=a_3+b_3+\tilde{d}_1\tau_y\delta_y^2, \tag{2.22}$$

$$G=a_4+e_3\tau_z\delta_z^2,\qquad H=b_4+e_2\tau_z\delta_z^2,\qquad I=a_4+b_4+e_1\tau_z\delta_z^2. \tag{2.23}$$

Then from (2.10)–(2.13) we have

$$Du^{n-1} + Eu^{n-1+s_2} = Fu^{n-1+s_1}, \tag{2.24}$$

$$\tilde{D}u^{n-1+s_1} + \tilde{E}u^{n-1+s_3} = \tilde{F}u^{n-1+s_2}, \tag{2.25}$$

$$Gu^{n-1+s_2} + Hu^{n} = Iu^{n-1+s_3}, \tag{2.26}$$

$$Au^{n-1+s_3} + Bu^{n+s_1} = Cu^{n}, \tag{2.27}$$

$$Du^{n} + Eu^{n+s_2} = Fu^{n+s_1}, \tag{2.28}$$

$$\tilde{D}u^{n+s_1} + \tilde{E}u^{n+s_3} = \tilde{F}u^{n+s_2}, \tag{2.29}$$

$$Gu^{n+s_2} + Hu^{n+1} = Iu^{n+s_3}, \tag{2.30}$$

where we remark that (2.24)–(2.26) are obtained from (2.28)–(2.30) with n replaced by $n-1$. Thus from (2.24)–(2.26), we have

$$(F\tilde{F}I - E\tilde{D}I - F\tilde{E}G)u^{n-1+s_3} = D\tilde{D}Gu^{n-1} + (F\tilde{F}H - E\tilde{D}H)u^{n}, \tag{2.31}$$

and from (2.28)–(2.30), we have

$$(F\tilde{F}I - E\tilde{D}I - F\tilde{E}G)u^{n+s_1} = E\tilde{E}Hu^{n+1} + (D\tilde{F}I - D\tilde{E}G)u^{n}. \tag{2.32}$$

Using (2.27), (2.31) and (2.32), we get

$$AD\tilde{D}Gu^{n-1} + BE\tilde{E}Hu^{n+1} = (CF\tilde{F}I - CE\tilde{D}I - CF\tilde{E}G + AE\tilde{D}H + BD\tilde{E}G - AF\tilde{F}H - BD\tilde{F}I)u^{n}. \tag{2.33}$$

On the RHS of (2.33), there are linear combinations of difference operators δ_x^2, δ_y^2 and δ_z^2 acting on u^n. By a direct calculation, it is easy to see that there are no terms corresponding to the discretizations of $\frac{\partial u}{\partial t}\Delta t$ and $\frac{\partial^3 u}{\partial t^3}\Delta t^3$. In order to get a high order scheme, we should let the coefficients of the discrete forms of the following derivatives,

$$\frac{\partial u}{\partial t}\Delta t, \qquad \frac{\partial^3 u}{\partial x^2 \partial t}h_x^2\Delta t, \qquad \frac{\partial^3 u}{\partial y^2 \partial t}h_y^2\Delta t, \qquad \frac{\partial^3 u}{\partial z^2 \partial t}h_z^2\Delta t, \qquad \frac{\partial^5 u}{\partial^4 y \partial t}h_y^4\Delta t \tag{2.34}$$

which are appeared on the LHS of (2.33), be zero. This requirement is equivalent to the following conditions

$$a_1a_2a_3a_4 = b_1b_2b_3b_4, \qquad a_2a_3a_4c_3 = b_2b_3b_4c_2, \tag{2.35}$$

$$a_1a_3a_4d_3 + a_1a_2a_4\tilde{d}_3 = b_1b_3b_4d_2 + b_1b_2b_4\tilde{d}_2, \tag{2.36}$$

$$a_1a_2a_3e_3 = b_1b_2b_3e_2, \qquad a_1a_4d_3\tilde{d}_3 = b_1b_4d_2\tilde{d}_2. \tag{2.37}$$

In order to satisfy (2.35)–(2.37), it is sufficient to satisfy the following five conditions

$$a_1a_2a_3a_4 = b_1b_2b_3b_4, \tag{2.38}$$

$$a_1c_2 = b_1c_3, \tag{2.39}$$

$$a_2d_2 = b_2d_3, \tag{2.40}$$

$$a_3\tilde{d}_2 = b_3\tilde{d}_3, \tag{2.41}$$

$$a_4e_2 = b_4e_3. \tag{2.42}$$

From (2.16)–(2.19), we know (2.38) is always true and so we have

$$AD\tilde{D}G = BE\tilde{E}H. \tag{2.43}$$

Using (2.43) in (2.33), we have

$$\begin{aligned} AD\tilde{D}G(u^{n-1} - 2u^n + u^{n+1}) = {} & (CF\tilde{F}I - CE\tilde{D}I - CF\tilde{E}G + AE\tilde{D}H \\ & + BD\tilde{E}G - AF\tilde{F}H - BD\tilde{F}I - AD\tilde{D}G - BE\tilde{E}H)u^n. \end{aligned} \tag{2.44}$$

Then we obtain

$$\begin{aligned} AD\tilde{D}G(u^{n-1} - 2u^n + u^{n+1}) = {} & (c_x\tau_x\delta_x^2 + c_y\tau_y\delta_y^2 + c_z\tau_z\delta_z^2 + c_{xy}\tau_x\tau_y\delta_x^2\delta_y^2 \\ & + c_{xz}\tau_x\tau_z\delta_x^2\delta_z^2 + c_{yz}\tau_y\tau_z\delta_y^2\delta_z^2 + c_{yy}\tau_y^2\delta_y^2\delta_y^2)u^n + O(h^6), \end{aligned} \tag{2.45}$$

where $c_x, c_y, c_z, c_{xy}, c_{xz}, c_{yz}, c_{yy}$ are the coefficients which can be computed with the help of Matlab. Their detailed expressions are not the key point here. For simplicity and saving space we omit their expressions. Obviously, c_x involves only a_i, b_i $(i = 1, 2, 3, 4)$ and c_1, c_2, c_3. Similarly, c_{xy} involves only a_i, b_i $(i = 1, 2, 3, 4)$, $c_i d_j$ and $c_i\tilde{d}_j$ $(i, j = 1, 2, 3)$. In addition, c_{yy} involves only a_i, b_i $(i = 1, 2, 3, 4)$ and $d_i\tilde{d}_j$ $(i, j = 1, 2, 3)$.

Let

$$L = u^{n+1} - 2u^n + u^{n-1} = \Delta t^2 \frac{\partial^2 u}{\partial t^2} + \frac{\Delta t^4}{12}\frac{\partial^4 u}{\partial t^4} + O(\Delta t^6). \tag{2.46}$$

Then we have

$$\delta_p^2 L = \Delta t^2 h_p^2 \frac{\partial^4 u}{\partial t^2 \partial p^2} + O(\Delta t^2 h^4 + \Delta t^4 h^2), \quad p = x, y, z, \tag{2.47}$$

and

$$\delta_p^2 u^n = h_p^2 \frac{\partial^2 u}{\partial p^2} + \frac{h_p^4}{12}\frac{\partial^4 u}{\partial p^4} + O(h^6), \quad p = x, y, z, \tag{2.48}$$

$$\delta_p^2 \delta_q^2 u^n = h_p^2 h_q^2 \frac{\partial^4 u}{\partial p^2 \partial q^2} + O(h^6), \quad p, q = x, y, z;\ p \neq q, \tag{2.49}$$

$$\delta_y^2 \delta_y^2 u^n = h_y^4 \frac{\partial^4 u}{\partial y^4} + O(h^6). \tag{2.50}$$

where δ_x^2, δ_y^2, and δ_z^2 are the second-order central difference operators defined in (2.15), and h is the maximum spatial step. Using (2.1), we have

$$\frac{\partial^4 u}{\partial t^2 \partial x^2} = v^2\left(\frac{\partial^4 u}{\partial x^4} + \frac{\partial^4 u}{\partial x^2 \partial y^2} + \frac{\partial^4 u}{\partial x^2 \partial z^2}\right), \tag{2.51}$$

$$\frac{\partial^4 u}{\partial t^2 \partial y^2} = v^2\left(\frac{\partial^4 u}{\partial y^4} + \frac{\partial^4 u}{\partial x^2 \partial y^2} + \frac{\partial^4 u}{\partial y^2 \partial z^2}\right), \tag{2.52}$$

$$\frac{\partial^4 u}{\partial t^2 \partial z^2} = v^2\left(\frac{\partial^4 u}{\partial z^4} + \frac{\partial^4 u}{\partial x^2 \partial z^2} + \frac{\partial^4 u}{\partial y^2 \partial z^2}\right), \tag{2.53}$$

$$\frac{\partial^4 u}{\partial t^4} = v^4\left(\frac{\partial^4 u}{\partial x^4} + \frac{\partial^4 u}{\partial y^4} + \frac{\partial^4 u}{\partial z^4} + 2\frac{\partial^4 u}{\partial x^2 \partial y^2} + 2\frac{\partial^4 u}{\partial x^2 \partial z^2} + 2\frac{\partial^4 u}{\partial y^2 \partial z^2}\right). \tag{2.54}$$

Now we use (2.47), (2.48)–(2.50), and (2.51)–(2.54) to simplify (2.45). In order to achieve high order schemes, we obtain the following nine equations by comparing the coefficients of corresponding terms in (2.45):

$$b_1 b_2 b_3 b_4 \Delta t^2 v^2 = c_x \tau_x h_x^2, \tag{2.55}$$

$$b_1 b_2 b_3 b_4 \Delta t^2 v^2 = c_y \tau_y h_y^2, \tag{2.56}$$

$$b_1 b_2 b_3 b_4 \Delta t^2 v^2 = c_z \tau_z h_z^2, \tag{2.57}$$

$$\frac{b_1 b_2 b_3 b_4 \Delta t^4 v^4}{12} + b_2 b_3 b_4 c_2 \tau_x h_x^2 \Delta t^2 v^2 = \frac{c_x \tau_x h_x^4}{12}, \tag{2.58}$$

$$\frac{b_1 b_2 b_3 b_4 \Delta t^4 v^4}{12} + (b_1 b_3 b_4 d_2 + b_1 b_2 b_4 \tilde{d}_2)\tau_y h_y^2 \Delta t^2 v^2 = \frac{c_y \tau_y h_y^4}{12} + c_{yy}\tau_y^2 h_y^4, \tag{2.59}$$

$$\frac{b_1 b_2 b_3 b_4 \Delta t^4 v^4}{12} + b_1 b_2 b_3 e_2 \tau_z h_z^2 \Delta t^2 v^2 = \frac{c_z \tau_z h_z^4}{12}, \tag{2.60}$$

$$\frac{b_1 b_2 b_3 b_4 \Delta t^4 v^4}{6} + \tau_x \Delta t^2 h_x^2 v^2 b_2 b_3 b_4 c_2 + \tau_y \Delta t^2 h_y^2 v^2 (b_1 b_3 b_4 d_2 + b_1 b_2 b_4 \tilde{d}_2) = c_{xy}\tau_x \tau_y h_x^2 h_y^2, \tag{2.61}$$

$$\frac{b_1 b_2 b_3 b_4 \Delta t^4 v^4}{6} + \tau_z \Delta t^2 h_z^2 v^2 b_1 b_2 b_3 e_2 + \tau_y \Delta t^2 h_y^2 v^2 (b_1 b_3 b_4 d_2 + b_1 b_2 b_4 \tilde{d}_2) = c_{yz}\tau_y \tau_z h_y^2 h_z^2, \tag{2.62}$$

$$\frac{b_1 b_2 b_3 b_4 \Delta t^4 v^4}{6} + \tau_x \Delta t^2 h_x^2 v^2 b_2 b_3 b_4 c_2 + \tau_z \Delta t^2 h_z^2 v^2 b_1 b_2 b_3 e_2 = c_{xz}\tau_x \tau_z h_x^2 h_z^2. \tag{2.63}$$

From (2.39), (2.55) and (2.58), we get

$$c_2 = \frac{b_1(1-\tau_x)}{12\tau_x}, \qquad c_3 = \frac{a_1(1-\tau_x)}{12\tau_x}, \qquad c_1 = \frac{2}{s_1 - s_3 + 1} + c_2 + c_3, \tag{2.64}$$

and from (2.42), (2.57) and (2.60), we get

$$e_2 = \frac{b_4(1-\tau_z)}{12\tau_z}, \qquad e_3 = \frac{a_4(1-\tau_z)}{12\tau_z}, \qquad e_1 = \frac{2}{1-s_2} + e_2 + e_3. \tag{2.65}$$

Thus (2.63) can be reduced to

$$s_3^2 - s_3 + \frac{1}{6} = 0, \tag{2.66}$$

and we have

$$s_3 = \frac{1}{2} \pm \frac{\sqrt{3}}{6}. \tag{2.67}$$

Then c_i, e_i $(i = 1, 2, 3)$ are known, so (2.61) and (2.62) are reduced to linear functions of $d_i, \tilde{d}_i$ $(i = 1, 2, 3)$. Eq. (2.56) is also linear and (2.59) is quadratic. Now we have five equations (2.56), (2.59), (2.61), (2.62), (2.63), and seven undetermined coefficients $s_1, s_2, s_3, d_1, d_2, \tilde{d}_1, \tilde{d}_2$, which satisfy

$$d_3 = \frac{a_2}{b_2} d_2, \qquad \tilde{d}_3 = \frac{a_3}{b_3} \tilde{d}_2 \tag{2.68}$$

from (2.38)–(2.42). Thus, there are two degrees of freedom for the choices of the above parameters.

For ease of notion, (2.56), (2.61), (2.62) can be rewritten as:

$$q_{11}d_1 + q_{12}d_2 + p_{11}\tilde{d}_1 + p_{12}\tilde{d}_2 + r_1 = 0, \tag{2.69}$$

$$q_{21}d_1 + q_{22}d_2 + p_{21}\tilde{d}_1 + p_{22}\tilde{d}_2 + r_2 = 0, \tag{2.70}$$

$$q_{31}d_1 + q_{32}d_2 + p_{31}\tilde{d}_1 + p_{32}\tilde{d}_2 + r_3 = 0, \tag{2.71}$$

with

$$\frac{q_{11}}{q_{21}} = \frac{q_{12}}{q_{22}}, \qquad \frac{p_{11}}{p_{21}} = \frac{p_{12}}{p_{22}}, \qquad \frac{q_{11}}{q_{21}} \neq \frac{p_{11}}{p_{21}}, \tag{2.72}$$

$$\frac{q_{11}}{q_{31}} = \frac{q_{12}}{q_{32}}, \qquad \frac{p_{11}}{p_{31}} = \frac{p_{12}}{p_{32}}, \qquad \frac{q_{11}}{q_{31}} \neq \frac{p_{11}}{p_{31}}. \tag{2.73}$$

The fifteen coefficients above, i.e., $p_{11}, p_{12}, p_{21}, p_{22}, p_{31}, p_{32}, q_{11}, q_{12}, q_{21}, q_{22}, q_{31}, q_{32}, r_1, r_2, r_3$, which can be found with the help of Matlab. Their detailed expressions are not important to our derivation here. For simplicity and saving space we omit them.

The combinations $p_{21} \cdot$ (2.69) $- p_{11} \cdot$ (2.70) and $p_{31} \cdot$ (2.69) $- p_{11} \cdot$ (2.71) lead to

$$d_1 - \frac{s_2 d_2}{s_1} + \frac{6s_2^2 - 6s_2 + 1}{3s_2(s_1 - s_2)(s_1 + s_2 - 1)} = 0, \tag{2.74}$$

$$d_1 - \frac{s_2 d_2}{s_1} + \frac{6(s_2 - s_3) + 6(s_2^2 + s_3^2) - 12s_2s_3 + 1}{3s_2(s_1 - s_2)(s_1 + s_2 - 2s_3 + 1)} = 0, \tag{2.75}$$

respectively, which are the relationship between d_1 and d_2. As (2.74) and (2.75) should have identical coefficients, we have

$$s_2(s_3 - 1)(s_1 - s_3)^2(s_2 - s_1)(6s_1s_2 - 3s_2s_3 - 3s_1s_3 + 3s_3 - 1) = 0. \tag{2.76}$$

Since $s_2 \neq 0$, $s_3 \neq 1$ and $s_1 \neq s_2$, we have

$$6s_1s_2 - 3s_2s_3 - 3s_1s_3 + 3s_3 - 1 = 0. \tag{2.77}$$

The combinations $q_{21} \cdot$ (2.69) $- q_{11} \cdot$ (2.70) and $q_{31} \cdot$ (2.69) $- q_{11} \cdot$ (2.71) lead to

$$\tilde{d}_1 + \frac{(s_1 - s_3)\tilde{d}_2}{s_2 - s_1} - \frac{1}{3}\,\frac{1 + 6s_1^2 - 6s_1}{s_2^2 s_1 - s_2^2 s_3 + s_2 s_3 - s_2 s_1 - s_1 s_3 + s_1^2 - s_1^3 + s_1^2 s_3} = 0, \tag{2.78}$$

$$-\frac{1}{3}\,\frac{6s_3^2 + 6s_1^2 + 1 - 12s_1s_3 + 6s_1 - 6s_3}{s_2(s_1 - s_3)(s_2 + 1) + 2s_3^2(s_2 - s_1) - s_1^3 + 3s_1^2 s_3 - 2s_2s_1s_3 + s_1s_3 - s_1^2} + \tilde{d}_1 + \frac{(s_1 - s_3)\tilde{d}_2}{s_2 - s_1} = 0. \tag{2.79}$$

For the same reason, we get

$$6s_1s_2 - 3s_2s_3 - 3s_1s_3 + 3s_3 - 1 = 0. \tag{2.80}$$

Now we only have two equations, i.e., (2.59) and (2.77) or (2.80) and four undetermined coefficients $s_1, s_2, d_2, \tilde{d}_2$. Thus we can obtain a family of LOD schemes. If we choose $d_2 = \tilde{d}_2$ for simplicity, the schemes depend on the choices of the three parameters. In the following, we present two ways to choose the parameters as examples.

2.2. The first group of parameters

Since the summation of four equations (2.6)–(2.9) should be equivalent to wave equation (2.1), we get the condition

$$\frac{1}{c_1-c_2-c_3}+\left(\frac{\lambda}{d_1-d_2-d_3}+\frac{1-\lambda}{\tilde{d}_1-\tilde{d}_2-\tilde{d}_3}\right)+\frac{1}{e_1-e_2-e_3}=1, \tag{2.81}$$

where $\lambda\in(0,1)$ is a parameter. For simplicity we choose $\lambda=1/2$. Noting that

$$d_1-\frac{s_2}{s_1}d_2=d_1-d_2-d_3,\qquad \tilde{d}_1+\frac{(s_1-s_3)\tilde{d}_2}{s_2-s_1}d_2=\tilde{d}_1-\tilde{d}_2-\tilde{d}_3, \tag{2.82}$$

and using (2.74)–(2.75) and (2.78)–(2.79), the condition (2.81) can be reduced to

$$3s_1^2-3s_1+3s_2^2-3s_2+1=0. \tag{2.83}$$

With the assumption of $s_1<s_2<s_3$ and from (2.67) we select

$$s_3=\frac{1}{2}+\frac{\sqrt{3}}{6}. \tag{2.84}$$

Then combining (2.83) and (2.80) we obtain

$$s_1=\frac{1}{4}+\frac{\sqrt{3}}{12}-\frac{\sqrt{2}\sqrt[4]{27}}{12},\qquad s_2=\frac{1}{4}+\frac{\sqrt{3}}{12}+\frac{\sqrt{2}\sqrt[4]{27}}{12}. \tag{2.85}$$

For simplicity, we let $d_2=\tilde{d}_2$. Then we get the approximate solutions of d_2 and $\tilde{d}_2$ from (2.59):

$$d_2=\tilde{d}_2\approx\frac{0.758364}{\tau_y}-0.192754, \tag{2.86}$$

and from (2.40) and (2.41) we have

$$d_3=\frac{a_2}{b_2}d_2,\qquad d_1=\frac{6s_2^2-6s_2+1}{3s_2(s_2-s_1)(s_1+s_2-1)}+d_2+d_3, \tag{2.87}$$

and

$$\tilde{d}_3=\frac{a_3}{b_3}\tilde{d}_2,\qquad \tilde{d}_1=-\frac{6s_1^2-6s_1+1}{3(s_1-s_2)(s_1-s_3)(s_1+s_2-1)}+\tilde{d}_2+\tilde{d}_3, \tag{2.88}$$

respectively. Thus from the discussion in this subsection, we have the following theorem:

Theorem 2.1. *If s_i $(i=1,2,3)$ are given by (2.84) and (2.85), the coefficients a_i and b_i $(i=1,2,3,4)$ are determined by (2.16)–(2.19), c_i $(i=1,2,3)$ by (2.64), e_i $(i=1,2,3)$ by (2.65), d_i and $\tilde{d}_i$ $(i=1,2,3)$ by (2.86)–(2.88), then the new LOD scheme (2.6)–(2.9) has the accuracy of $O(\Delta t^4+h^4)$, where $h=\max\{h_x,h_y,h_z\}$.*

2.3. The second group of parameters

We recall that $0<s_1<s_2<s_3<1$. One notes that $s_3\approx 0.7887$. With the facts we can know s_2 ranges from 0.5774 to 0.7886 approximately. The figure of s_2 will be shown in Section 4. Now we choose $s_2=2/3$ and solve s_1 from (2.77), thus we have the second group of parameters,

$$s_3=\frac{1}{2}+\frac{\sqrt{3}}{6},\qquad s_2=\frac{2}{3},\qquad s_1=\frac{-3+\sqrt{3}}{3(-5+\sqrt{3})}, \tag{2.89}$$

and we have

$$d_2=\tilde{d}_2=\frac{0.7533731}{\tau_y}-0.1915980,\qquad d_3=\frac{a_2}{b_2}d_2, \tag{2.90}$$

$$d_1=\frac{6s_2^2-6s_2+1}{3s_2(s_2-s_1)(s_1+s_2-1)}+d_2+d_3, \tag{2.91}$$

$$\tilde{d}_3=\frac{a_3}{b_3}\tilde{d}_2,\qquad \tilde{d}_1=-\frac{6s_1^2-6s_1+1}{3(s_1-s_2)(s_1-s_3)(s_1+s_2-1)}+\tilde{d}_2+\tilde{d}_3. \tag{2.92}$$

Thus from the discussion above, we have the following theorem:

Theorem 2.2. *If s_i $(i=1,2,3)$ are given by (2.89), the coefficients a_i and b_i $(i=1,2,3,4)$ are determined by (2.16)–(2.19), c_i $(i=1,2,3)$ by (2.64), e_i $(i=1,2,3)$ by (2.65), d_i and $\tilde{d}_i$ $(i=1,2,3)$ by (2.90)–(2.92), then the new LOD scheme (2.6)–(2.9) has the accuracy of $O(\Delta t^4+h^4)$, where $h=\max\{h_x,h_y,h_z\}$.*

3. Initial conditions

In this section, we present how the initial conditions are computed for our new scheme. The initial condition $u(x, y, z, 0)$ or u^0 is given by the first equation in (2.2). We consider how to obtain the initial condition u^{-1} first. Suppose f_1 and f_2 in (2.2) are smooth enough. From

$$\begin{aligned}\frac{u^1 - u^{-1}}{\Delta t} &= 2\left[\left(\frac{\partial u}{\partial t}\right)^0 + \frac{\Delta t^2}{6}\left(\frac{\partial^3 u}{\partial t^3}\right)^0\right] + O(\Delta t^4)\\ &= 2\left[f_2 + \frac{v^2\Delta t^2}{6}\left(\frac{\partial^2 f_2}{\partial x^2} + \frac{\partial^2 f_2}{\partial y^2} + \frac{\partial^2 f_2}{\partial z^2}\right)\right] + O(\Delta t^4),\end{aligned} \tag{3.1}$$

we have the following approximation of u^{-1} with fourth-order accuracy in time

$$u^{-1} = u^1 - 2\Delta t\left[f_2 + \frac{v^2\Delta^2 t}{6}\left(\frac{\partial^2 f_2}{\partial x^2} + \frac{\partial^2 f_2}{\partial y^2} + \frac{\partial^2 f_2}{\partial z^2}\right)\right]. \tag{3.2}$$

Noting that

$$\begin{aligned}\frac{u^1 - 2u^0 + u^{-1}}{\Delta t^2} &= \left(\frac{\partial^2 u}{\partial t^2}\right)^0 + \frac{\Delta t^2}{12}\left(\frac{\partial^4 u}{\partial t^4}\right)^0 + O(\Delta t^4) = v^2\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right)^0\\ &\quad + \frac{v^2\Delta t^2}{12}\left[\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right)^2\right]^0 + O(\Delta t^4)\\ &= v^2\triangle f_1 + \frac{v^2\Delta t^2}{12}\triangle^2 f_1 + O(\Delta t^4),\end{aligned} \tag{3.3}$$

where $\triangle$ is the Laplacian operator and $\triangle^2$ is the biharmonic operator. Using (3.2) and (3.3) to cancel u^{-1}, we then obtain

$$u^1 = u^0 + \Delta t\Big(f_2 + \frac{v^2\Delta t^2}{6}\triangle f_2\Big) + \frac{v^2\Delta t^2}{2}\Big(\triangle f_1 + \frac{v^2\Delta t^2}{12}\triangle^2 f_1\Big). \tag{3.4}$$

The approximation of u^1 with (3.4) reaches fourth-order accuracy in space and time.

Next we will use (2.32) to obtain approximate values of u^{s_1} with error of $O(h^6)$. From (2.32) we have

$$(F\tilde{F}I - E\tilde{D}I - F\tilde{E}G)u^{s_1} = E\tilde{E}Hu^1 + (D\tilde{F}I - D\tilde{E}G)u^0. \tag{3.5}$$

Remove the high order terms of u^{s_1}, u^1, u^0, and notice that there are no terms involving δ_x^2, so (3.5) can be rewritten as:

$$(p + p_y\tau_y\delta_y^2 + p_z\tau_z\delta_z^2 + p_{yz}\tau_y\tau_z\delta_y^2\delta_z^2 + p_{yy}\tau_y\tau_y\delta_y^2\delta_y^2)u^{s_1} = E\tilde{E}Hu^1 + (D\tilde{F}I - D\tilde{E}G)u^0 + O(h^6), \tag{3.6}$$

where $p, p_y, p_z, p_{yz}, p_{yy}$ are the coefficients given by

$$p = (a_2 + b_2)(a_3 + b_3)(a_4 + b_4) - a_3b_2(a_4 + b_4) - a_4b_3(a_2 + b_2), \tag{3.7}$$

$$\begin{aligned}p_y \;=\; & d_1(a_3 + b_3)(a_4 + b_4) + \tilde{d}_1(a_2 + b_2)(a_4 + b_4)\\ & - a_3d_2(a_4 + b_4) - a_4\tilde{d}_2(a_2 + b_2) - b_2\tilde{d}_3(a_4 + b_4) - a_4b_3d_1,\end{aligned} \tag{3.8}$$

$$p_z = e_1(a_2 + b_2)(a_3 + b_3) - b_3e_3(a_2 + b_2) - a_3b_2e_1, \tag{3.9}$$

$$p_{yz} = d_1e_1(a_3 + b_3) + \tilde{d}_1e_1(a_2 + b_2) - \tilde{d}_2e_3(a_2 + b_2) - a_3d_2e_1 - b_3d_1e_3 - b_2\tilde{d}_3e_1, \tag{3.10}$$

$$p_{yy} = d_1\tilde{d}_1(a_4 + b_4) - d_2\tilde{d}_3(a_4 + b_4) - a_4d_1\tilde{d}_2. \tag{3.11}$$

Using $\delta_z^2\delta_z^2$ multiply (3.6), we have

$$\tau_z^2\delta_z^2\delta_z^2u^{s_1} = \frac{1}{p}\delta_z^2\delta_z^2\big[E\tilde{E}Hu^1 + (D\tilde{F}I - D\tilde{E}G)u^0\big] + O(h^6). \tag{3.12}$$

Similarly, we can get $\delta_y^2\delta_y^2u^{s_1}$, $\delta_y^2\delta_z^2u^{s_1}$, $\delta_y^2u^{s_1}$, $\delta_z^2u^{s_1}$ with error $O(h^6)$ in the same procedure. So we have

$$u^{s_1} = \frac{1}{p}\big[E\tilde{E}Hu^1 + (D\tilde{F}I - D\tilde{E}G)u^0 - (p_y\tau_y\delta_y^2 + p_z\tau_z\delta_z^2 + p_{yz}\tau_y\tau_z\delta_y^2\delta_z^2 + p_{yy}\tau_y\tau_y\delta_y^2\delta_y^2)u^{s_1}\big]. \tag{3.13}$$

Solving u^{s_1} we obtain

$$u^{s_1} = \frac{1}{p}\Big[1 - p_y\tau_y\delta_y^2 - p_z\tau_z\delta_z^2 + \frac{\tau_y\tau_y}{p}(p_yp_y + p_{yy})\delta_y^2\delta_y^2 + \frac{\tau_y\tau_z}{p}(p_yp_z + p_{yz})\delta_y^2\delta_z^2 + \frac{p_z^2\tau_z^2}{p}\delta^2\delta^2 z\Big]R, \tag{3.14}$$

where

$$R = E\tilde{E}Hu^1 + (D\tilde{F}I - D\tilde{E}G)u^0. \tag{3.15}$$

4. Stability analysis

In this section, we analyze the stability of our new LOD scheme for the first group of parameters. For the second group of parameters, the analysis is similar. Let

$$u_{i,j,k}^{n} = \mathcal{Z}^{n} e^{\mathrm{i}k_x i h_x} e^{\mathrm{i}k_y j h_y} e^{\mathrm{i}k_z k h_z},$$

then from (2.44) we have

$$\hat{B}\hat{E}\hat{\hat{E}}\hat{H}\mathcal{Z}^{n+1} - \hat{\varphi}\mathcal{Z}^{n} + \hat{A}\hat{D}\hat{\hat{D}}\hat{G}\mathcal{Z}^{n-1} = 0, \tag{4.1}$$

where

$$\hat{\varphi} = \hat{C}\hat{F}\hat{\hat{F}}\hat{I} - \hat{C}\hat{E}\hat{\hat{D}}\hat{I} - \hat{C}\hat{F}\hat{\hat{E}}\hat{G} + \hat{A}\hat{E}\hat{\hat{D}}\hat{H} + \hat{B}\hat{D}\hat{\hat{E}}\hat{G} - \hat{A}\hat{F}\hat{\hat{F}}\hat{H} - \hat{B}\hat{D}\hat{\hat{F}}\hat{I}, \tag{4.2}$$

and

$$\hat{A} = a_1 - 4c_3\tau_x\sigma_x, \qquad \hat{B} = b_1 - 4c_2\tau_x\sigma_x, \qquad \hat{C} = a_1 + b_1 - 4c_1\tau_x\sigma_x, \tag{4.3}$$

$$\hat{D} = a_2 - 4d_3\tau_y\sigma_y, \qquad \hat{E} = b_2 - 4d_2\tau_y\sigma_y, \qquad \hat{F} = a_2 + b_2 - 4d_1\tau_y\sigma_y, \tag{4.4}$$

$$\hat{\hat{D}} = a_3 - 4\tilde{d}_3\tau_y\sigma_y, \qquad \hat{\hat{E}} = b_3 - 4\tilde{d}_2\tau_y\sigma_y, \qquad \hat{\hat{F}} = a_3 + b_3 - 4\tilde{d}_1\tau_y\sigma_y, \tag{4.5}$$

$$\hat{G} = a_4 - 4e_3\tau_z\sigma_z, \qquad \hat{H} = b_4 - 4e_2\tau_z\sigma_z, \qquad \hat{I} = a_4 + b_4 - 4e_1\tau_z\sigma_z, \tag{4.6}$$

with

$$\sigma_x = \sin^2\left(\frac{k_x}{2}\right), \qquad \sigma_y = \sin^2\left(\frac{k_y}{2}\right), \qquad \sigma_z = \sin^2\left(\frac{k_z}{2}\right), \qquad k_x, k_y, k_z \in [-\pi, \pi]. \tag{4.7}$$

Eq. (4.1) can be rewritten as

$$\begin{pmatrix} \hat{B}\hat{E}\hat{\hat{E}}\hat{H} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \mathcal{Z}^{n+1} \\ \mathcal{Z}^{n} \end{pmatrix} = \begin{pmatrix} \hat{\varphi} & -\hat{A}\hat{D}\hat{\hat{D}}\hat{G} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \mathcal{Z}^{n} \\ \mathcal{Z}^{n-1} \end{pmatrix}. \tag{4.8}$$

Since $\hat{A}\hat{D}\hat{\hat{D}}\hat{G} = \hat{B}\hat{E}\hat{\hat{E}}\hat{H}$, we get the amplification matrix

$$\begin{pmatrix} \dfrac{\hat{\varphi}}{\hat{A}\hat{D}\hat{\hat{D}}\hat{G}} & -1 \\ 1 & 0 \end{pmatrix}. \tag{4.9}$$

The eigenvalues of the amplification matrix above should be no more than 1 for stability. Therefore we get the following stability condition:

Theorem 4.1. *The necessary and sufficient stability condition is*

$$\left| \frac{\hat{\varphi}}{\hat{A}\hat{D}\hat{\hat{D}}\hat{G}} \right| \le 2. \tag{4.10}$$

Next, we will derive an explicit restriction of Δt from Theorem 4.1.

To solve inequality (4.10), we need to solve the following two inequalities

$$\hat{\varphi} + 2\hat{A}\hat{D}\hat{\hat{D}}\hat{G} \ge 0, \quad \forall \sigma_x, \sigma_y, \sigma_z \in [0, 1], \tag{4.11}$$

$$\hat{\varphi} - 2\hat{A}\hat{D}\hat{\hat{D}}\hat{G} \le 0, \quad \forall \sigma_x, \sigma_y, \sigma_z \in [0, 1]. \tag{4.12}$$

Both inequalities above are polynomials in the parameters $\tau_x, \tau_y, \tau_z, \sigma_x, \sigma_y, \sigma_z$. To simplify derivation, we assume

$$\tau_x = \tau_y = \tau_z := \tau. \tag{4.13}$$

We remark that this assumption is needed to simplify notations and is not essential for the proof. Let F_1 be the function defined by

$$F_1(\sigma_x, \sigma_y, \sigma_z) := \hat{\varphi} + 2\hat{A}\hat{D}\hat{\hat{D}}\hat{G}. \tag{4.14}$$

If the inequality (4.11) holds, then by taking $\sigma_x = \sigma_y = \sigma_z = 1$, we obtain the following inequality

$$F_1(1, 1, 1) := 350.29\tau^4 + 51586.13\tau^3 + 211496.80\tau^2 - 424063.90\tau + 127558.49 \ge 0. \tag{4.15}$$

Thus, using the CFL condition $\tau \le 1$ and solving the above inequality (4.15), we obtain the following necessary stability condition for the new LOD scheme

$$\tau \le 0.379139. \tag{4.16}$$

To show that the condition (4.16) is also sufficient, we will prove in Theorem 4.4 that the minimum of the function F_1 is attained at

$$\sigma_x = \sigma_y = \sigma_z = 1. \tag{4.17}$$

Since condition (4.16) holds, the inequality (4.15) also holds. Therefore,

$$\hat{\varphi} + 2\hat{A}\hat{D}\hat{\hat{D}}\hat{G} = F_1(\sigma_x, \sigma_y, \sigma_z) \ge F_1(1, 1, 1) \ge 0$$

for all $\sigma_x, \sigma_y, \sigma_z \in [0, 1]$. Hence (4.11) holds.

Next, we will prove Theorem 4.4 and we first need the following lemma.

Lemma 4.2. *Consider the extremum problem*

$$\min_{x,y,z} f(\boldsymbol{x}), \quad \text{s.t. } c_i(\boldsymbol{x}) \ge 0, \tag{4.18}$$

where $f(\boldsymbol{x})$ is a given function, $\boldsymbol{x} = (x, y, z)$, and $c_i(\boldsymbol{x})$ $(i = 1, \dots, 6)$ satisfy the following constraint conditions

$$c_1(x) = x \ge 0, \qquad c_2(x) = 1 - x \ge 0, \qquad c_3(y) = y \ge 0, \tag{4.19}$$

$$c_4(y) = 1 - y \ge 0, \qquad c_5(z) = z \ge 0, \qquad c_6(z) = 1 - z \ge 0. \tag{4.20}$$

If $\nabla f(\boldsymbol{x}) < 0$ for all $\boldsymbol{x}$ and $\boldsymbol{x}^*$ is a minimum point, then $\boldsymbol{x}^* = (1, 1, 1)$.

Proof. As $\boldsymbol{x}^*$ is the minimum point of problem (4.18), there exist λ_i $(i = 1, 2, \dots, 6)$ such that

$$\begin{aligned} &\nabla f(\boldsymbol{x}^*) = \sum_{i=1}^{6} \lambda_i \nabla c_i(\boldsymbol{x}^*), \\ &\lambda_i c_i(\boldsymbol{x}^*) = 0, \qquad \lambda_i \ge 0, \quad i = 1, 2, \dots, 6. \end{aligned} \tag{4.21}$$

Then we have

$$\sum_{i=1}^{6} \lambda_i \nabla c_i(\boldsymbol{x}^*) = \begin{pmatrix} \lambda_1 - \lambda_2 \\ \lambda_3 - \lambda_4 \\ \lambda_5 - \lambda_6 \end{pmatrix} < 0. \tag{4.22}$$

If $c_2(x) \ne 0$, we have $\lambda_2 = 0$, then $\lambda_1 - \lambda_2 = \lambda_1 \ge 0$, which contradicts (4.22). Thus $c_2(x) = 0 \Leftrightarrow x = 1$. Similarly, we have $y = 1$ and $z = 1$. This completes the proof.

Remark 4.3. The conclusion in Lemma 4.2 is independent of the dimension of $\boldsymbol{x}$, i.e., the result holds when $\boldsymbol{x} = (x_1, x_2, \dots, x_n)$ and the constraints are defined by

$$c_1(x_1) = x_1 \ge 0,\ c_2(x_1) = 1 - x_1 \ge 0, \dots,\ c_{2n-1}(x_n) = x_n \ge 0,\ c_{2n}(x_n) = 1 - x_n \ge 0.$$

Theorem 4.4. *Assume (4.16). The minimum of the following problem*

$$\min_{\sigma_x,\sigma_y,\sigma_z} F_1 := \min_{\sigma_x,\sigma_y,\sigma_z} \{\hat{\varphi} + 2\hat{A}\hat{D}\hat{\hat{D}}\hat{G}\}, \quad \forall \sigma_x, \sigma_y, \sigma_z \in [0, 1] \tag{4.23}$$

is attained at $\sigma_x = \sigma_y = \sigma_z = 1$.

Proof. The proof is based on Lemma 4.2. Since F_1 is a polynomial defined on a finite interval, it has a minimum. To show that the minimum of F_1 is achieved at $\sigma_x = \sigma_y = \sigma_z = 1$, we only need to show

$$\frac{\partial F_1}{\partial \sigma_x} < 0, \qquad \frac{\partial F_1}{\partial \sigma_y} < 0, \qquad \frac{\partial F_1}{\partial \sigma_z} < 0 \tag{4.24}$$

according to Lemma 4.2. We will only prove $\frac{\partial F_1}{\partial \sigma_y} < 0$ in the following paragraphs. The proof for $\frac{\partial F_1}{\partial \sigma_x} < 0$ and $\frac{\partial F_1}{\partial \sigma_z} < 0$ follows a similar procedure.

Notice that the highest order term of F_1 is $\sigma_x \sigma_y^2 \sigma_z$. Thus the highest order term of $\frac{\partial F_1}{\partial \sigma_y}$ is $\sigma_x \sigma_y \sigma_z$. Let

$$g(\sigma_x, \sigma_y, \sigma_z) = -\frac{\partial F_1}{\partial \sigma_y}. \tag{4.25}$$

The expressions of F_1 and g can be computed with the help of Matlab and given in Appendix B. By a direct calculation, we have $g(1, 1, 1) > 0$ using the condition (4.16). Using Lemma 4.2, it suffices to show that the function $g(\sigma_x, \sigma_y, \sigma_z)$ reaches its minimum at the point $\sigma_x = \sigma_y = \sigma_z = 1$.

To prove the function $g(\sigma_x, \sigma_y, \sigma_z)$ attains minimum at $\sigma_x = \sigma_y = \sigma_z = 1$, we only need to show

$$\frac{\partial g}{\partial \sigma_x} < 0, \qquad \frac{\partial g}{\partial \sigma_y} < 0, \qquad \frac{\partial g}{\partial \sigma_z} < 0 \tag{4.26}$$

by using Lemma 4.2. We only prove $\frac{\partial g}{\partial \sigma_x} < 0$ in the following. The proofs for $\frac{\partial g}{\partial \sigma_y} < 0$ and $\frac{\partial g}{\partial \sigma_z} < 0$ are similar. We omit them for saving space. Let

$$\tilde{g}_x(\sigma_y, \sigma_z) = -\frac{\partial g}{\partial \sigma_x}, \tag{4.27}$$

where

$$\begin{aligned}
&\tilde{g}_x(\sigma_y, \sigma_z) = P + P_1\sigma_y + P_2\sigma_z + P_3\sigma_y\sigma_z,\\
&P = 157480.14\tau^2 + 515453.1\tau_x + 158804.73,\\
&P_1 = 41552.17\tau^3 - 273072.14\tau^2 - 207332.89\tau - 32533.01,\\
&P_2 = 50305.26\tau^3 - 157921.67\tau^2 - 277687.52\tau - 52934.91,\\
&P_3 = 700.6\tau^4 - 46400.57\tau^3 + 121390.17\tau^2 + 90799.64.
\end{aligned} \tag{4.28}$$

Notice that

$$\tilde{g}_x(1, 1) = P_1 + P_2 + P_3 > 0 \tag{4.29}$$

by the condition (4.16). So $\frac{\partial g}{\partial \sigma_x} < 0$ holds if the minimum of $\tilde{g}_x(\sigma_y, \sigma_z)$ is attained at $\sigma_y = \sigma_z = 1$. Thus, it suffices to prove $\nabla\tilde{g}_x < 0$ by Lemma 4.2. Notice that

$$\frac{\partial \tilde{g}_x}{\partial \sigma_y} = P_1 + P_3\sigma_z \le P_1 + P_3 < 0, \qquad \frac{\partial \tilde{g}_x}{\partial \sigma_z} = P_2 + P_3\sigma_y \le P_2 + P_3 < 0, \tag{4.30}$$

by the condition (4.16). Hence the proof is complete.

We now consider the second inequality (4.12). We have the following theorem.

Theorem 4.5. *The inequality (4.12), i.e.,*

$$F_2 := \hat{\varphi} - 2\hat{A}\hat{D}\hat{\hat{D}}\hat{G} \le 0, \quad \forall \sigma_x, \sigma_y, \sigma_z \in [0, 1] \tag{4.31}$$

is always true under the condition of (4.16), i.e. $\tau \in (0, 0.379139]$.

Proof. First, we recall that $\sigma_x, \sigma_y, \sigma_z$ in $[0, 1]$. Expanding the polynomial F_2 we get

$$\begin{aligned}
F_2(\sigma_x, \sigma_y, \sigma_z) = {} & r_x\sigma_x + r_y\sigma_y + r_z\sigma_z + r_{xy}\sigma_x\sigma_y + r_{yz}\sigma_y\sigma_z + r_{yy}\sigma_y\sigma_y + r_{xz}\sigma_x\sigma_z\\
& + r_{xyz}\sigma_x\sigma_y\sigma_z + r_{yyx}\sigma_y\sigma_y\sigma_x + r_{yyz}\sigma_y\sigma_y\sigma_z + r_{xyyz}\sigma_x\sigma_y\sigma_y\sigma_z \le 0,
\end{aligned} \tag{4.32}$$

where $r_x, r_y, r_z, r_{xy}, r_{xz}, r_{yy}, r_{xyz}, r_{yyx}, r_{yyz}, r_{xyyz}$ are the coefficients given by

$$\begin{aligned}
&r_x = r_y = r_z = -714621.30\tau,\\
&r_{xy} = r_{yz} = 714621.30\tau + 117116.66\tau^2,\\
&r_{xz} = 476414.20\tau, \quad r_{yy} = 238207.10\tau + 117116.66\tau,\\
&r_{xyz} = -397011.83\tau - 78077.78\tau^2 + 36850.77\tau^3,\\
&r_{yyx} = -128201.88\tau - 127216.28\tau^2 + 19725.22\tau^3,\\
&r_{yyz} = -128201.88\tau - 60052.64\tau^2 + 2654.21\tau^3,\\
&r_{xyyz} = 59000.47\tau + 49410.01\tau^2 - 19743.40\tau^3.
\end{aligned} \tag{4.33}$$

Noticing that $\tau \in (0, 0.379139]$ and $\sigma_x, \sigma_y, \sigma_z \in [0, 1]$, we have the following inequalities

$$r_x, r_y, r_z, r_{xyz}, r_{yyx}, r_{yyz} \le 0, \qquad r_{xy}, r_{yz}, r_{yy}, r_{xz}, r_{xyyz} \ge 0, \tag{4.34}$$

$$r_x + \frac{r_{xy}}{2} + \frac{r_{xz}}{2} \le 0, \qquad r_y + \frac{r_{yy}}{2} \le 0, \qquad r_z + \frac{r_{xz}}{2} + \frac{r_{yz}}{2} \le 0, \qquad r_{xyz} + r_{xyyz} \le 0, \tag{4.35}$$

$$r_x + r_y + r_z + \left(r_{xy} + \frac{r_{yyx}}{2}\right) + \left(r_{yz} + \frac{r_{yyz}}{2}\right) + r_{yy} + \left(r_{xz} + \frac{r_{xyz}}{2} + r_{xyyz}\right) \le 0, \tag{4.36}$$

$$r_{xy} + \frac{r_{yyx}}{2} + r_x + \frac{1}{2}\left(r_{xz} + \frac{r_{xyz}}{2} + r_{xyyz}\right) \ge 0, \tag{4.37}$$

$$r_{yz} + \frac{r_{yyz}}{2} + r_z + \frac{1}{2}\left(r_{xz} + \frac{r_{xyz}}{2} + r_{xyyz}\right) \ge 0, \tag{4.38}$$

$$r_x + \frac{1}{2}\left(r_{xz} + \frac{r_{xyz}}{2} + r_{xyyz}\right), \qquad r_z + \frac{1}{2}\left(r_{xz} + \frac{r_{xyz}}{2} + r_{xyyz}\right) \le 0. \tag{4.39}$$

If $\sigma_y \le \frac{1}{2}$, using (4.34) and (4.35) we have

$$F_2 \le \left(r_x + \frac{r_{xy}}{2} + \frac{r_{xz}}{2}\right)\sigma_x + \left(r_y + \frac{r_{yy}}{2}\right)\sigma_y + \left(r_z + \frac{r_{xz}}{2} + \frac{r_{yz}}{2}\right)\sigma_z + (r_{xyz} + r_{xyyz})\sigma_x\sigma_y\sigma_z \le 0. \tag{4.40}$$

If $\sigma_y \ge \frac{1}{2}$, using (4.34), the fact $\sigma_i\sigma_j \le \min(\sigma_i, \sigma_j)$, and (4.36)–(4.39), we can conclude

$$F_2 \le \left[r_x + r_y + r_z + \left(r_{xy} + \frac{r_{yyx}}{2}\right) + \left(r_{yz} + \frac{r_{yyz}}{2}\right) + r_{yy} + \left(r_{xz} + \frac{r_{xyz}}{2} + r_{xyyz}\right)\right]\sigma_y \le 0. \tag{4.41}$$

From (4.40) and (4.41), we know (4.31) holds.

Remark 4.6. The inequality (4.36) is also true for $\tau \in (0, 0.5]$. The inequalities (4.34), (4.35) and (4.37)–(4.39) are also true for $\tau \in (0, 1]$.

From the analysis above we get the following stability condition.

Theorem 4.7. *The sufficient and necessary condition for our new LOD scheme is*

$$\tau \le 0.379139, \tag{4.42}$$

where $\tau_x = \tau_y = \tau_z := \tau$ *with* $\tau = \frac{v^2\Delta t^2}{h^2}$.

Remark 4.8. In order to facilitate computations, the condition (4.42) can be written as

$$\Delta t \le 0.6157\frac{h}{v}, \tag{4.43}$$

where $h = h_x = h_y = h_z := h$. For non-uniform meshes, it becomes

$$\Delta t \le 0.6157\frac{\min\{h_x, h_y, h_z\}}{v}. \tag{4.44}$$

For the second group of parameters, we can derive the stability condition in a similar way as above, we omit the details for saving space. The result is

$$\tau \le 0.379420, \quad \text{or} \quad \Delta t \le 0.6160\frac{h}{v} \tag{4.45}$$

for uniform meshes, and

$$\Delta t \le 0.6160\frac{\min\{h_x, h_y, h_z\}}{v} \tag{4.46}$$

for non-uniform meshes. As we can see, the stability result is very close to that of the first group parameters.

If we choose s_2 as the free parameter, s_1 can be obtained from (2.80) or (2.83). Fig. 4.1(a) shows the parameter s_2 as a function of parameter s_1 and ranges from 0.5774 to 0.7886 when parameter s_1 varies from 0 to 0.211. Once s_1, s_2 and s_3 are given, we can obtain the corresponding stability conditions. Fig. 4.1(b) shows the corresponding stability upper bound of $\sqrt{\tau}$ as a function of parameter s_1.

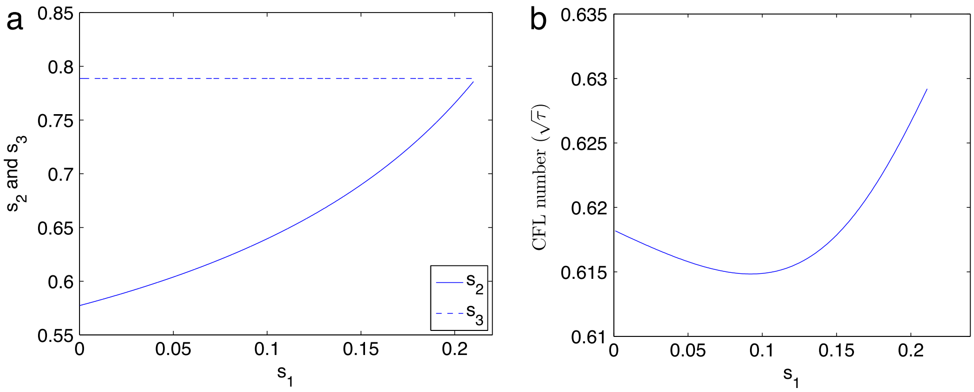

Fig. 4.1. The parameter s_2 (a) and the stability upper bound of $\sqrt{\tau}$ (b) as a function of parameter s_1.

Remark 4.9. From (4.43) and (4.46), we can know the CFL condition $\Delta t v/h$. The CFL number of our method is 0.6157 for the first group parameter or 0.6160 for the second group parameter. Our analysis show that the CFL number of the traditional explicit difference schemes with accuracy $O(\Delta t^2 + h^4)$ and $O(\Delta t^4 + h^4)$ are $\sqrt{\tau} \le 0.5$ and $\sqrt{\tau} \le 0.4640$ respectively. Moreover, the traditional schemes involve at least five nodes in one spatial direction. Hence, we see that our new LOD schemes have narrower stencil and better stability conditions.

We also remark that the dispersion analysis of our new LOD schemes and the corresponding comparisons with classical FD schemes can be carried out very similarly to the 2D case [5]. In [1], the dispersion analysis and comparisons have clearly shown that the new LOD scheme has less errors than the standard FD scheme with accuracy $O(\Delta t^4 + h^4)$. In the 3D case, the theoretical derivation is more complicated and tedious. Moreover, the conclusion is the same. So we do not include them in this paper for saving space.

5. Numerical computations

In this section we will present four numerical examples to illustrate the theoretical results obtained in the previous sections. First we consider a convergence test.

Example 1. For simplicity we set $N_x = N_y = N_z := N$. The exact solution of the wave equation (2.1) is chosen as

$$u(x, y, z, t) = \sin(\pi x)\sin(\pi y)\sin(\pi z)\sin(\sqrt{3}\pi t). \tag{5.1}$$

With this choice, the initial and boundary conditions (2.2) and (2.4) are all zero. Inserting (5.1) into (2.1) yields a source term which excites the wave. To measure the approximation error, we use the L_2 norm

$$\|\cdot\|_2 = \sqrt{\frac{1}{N^3}\left\{\sum_{i=0}^{N_x}\sum_{j=0}^{N_y}\sum_{k=0}^{N_z}\left[u_{i,j,k}^n - u_e(x_i, y_j, z_k, t_n)\right]^2\right\}}, \tag{5.2}$$

and the maximum or L_∞ norm, where $u_e(x_i, y_j, z_k, t^n)$ is the exact solution at time t^n. The convergence order is measured by

$$\mathcal{O}_{L_\nu} = \frac{\log(E^s/E^{s-1})}{\log(h^s/h^{s-1})}, \quad \nu = 2, \infty, \tag{5.3}$$

where $h^s = 1/N$ indicates the mesh spacing h in the sth sequenced meshes and E^s are the corresponding the errors.

In this example, we take the fixed grid ratio $\Delta t/h = 0.2$ and consider the L_2 and L_∞ errors after propagation time 0.2s. In Tables 5.1 and 5.2, we show the errors for the first and second group parameters respectively. The corresponding convergence orders are also given. We can see the convergence order is 4.0. In Fig. 5.1, we show the log–log plots of the L_2 and L_∞ errors for the first group parameters respectively. We found the slopes of the two lines in Fig. 5.1 are both 3.9995. In Fig. 5.2, we show the log–log plots of the L_2 and L_∞ errors for the second group parameters. We found that the slopes of the two lines in Fig. 5.2 are 4.0045 both for L_2 and maximum errors. Thus we see that the rate of convergence of our method is 4.0.

Example 2. The second example is wave simulation in a cubic model ignited by a point source. The computational domain is $\Omega = [0, 5000\text{ m}]^3$. The source is located in the center of the model and its time function is given by

$$S(t) = c(1 - 2000(t - 0.1)^2)e^{-1000(t-0.1)^2}, \tag{5.4}$$

Table 5.1
Numerical L_2 and L_∞ errors of our new LOD scheme with the first group of parameters.

$N_x = N_y = N_z$	L_2 errors	$\mathcal{O}_{L_2}$	L_∞errors	$\mathcal{O}_{L_\infty}$
10	6.764775E−6		1.913367E−5	
20	4.232148E−7	3.998580	1.197032E−6	3.998579
40	2.645645E−8	3.999698	7.483013E−8	3.999698
60	5.226169E−9	3.999903	1.478185E−8	3.999901
80	1.653715E−9	3.999742	4.677424E−9	3.999736
100	6.773635E−10	3.999987	1.915904E−9	3.999927
120	3.267011E−10	3.999320	9.240817E−10	3.999221
140	1.763927E−10	3.998249	4.989516E−10	3.997980

Table 5.2
Numerical L_2 and L_∞ errors of our new LOD scheme with the second group of parameters.

$N_x = N_y = N_z$	L_2 errors	$\mathcal{O}_{L_2}$	L_∞errors	$\mathcal{O}_{L_\infty}$
10	6.723693E−6		1.901728E−5	
20	4.206301E−7	3.998629	1.189722E−6	3.998614
40	2.629440E−8	3.999724	7.437178E−8	3.999725
60	5.193641E−9	4.000149	1.468982E−8	4.000151
80	1.642599E−9	4.001484	4.645982E−9	4.001472
100	6.716766E−10	4.007546	1.899782E−9	4.007570
120	3.224804E−10	4.024398	9.121155E−10	4.024361
140	1.722890E−10	4.066599	4.873121E−10	4.066552

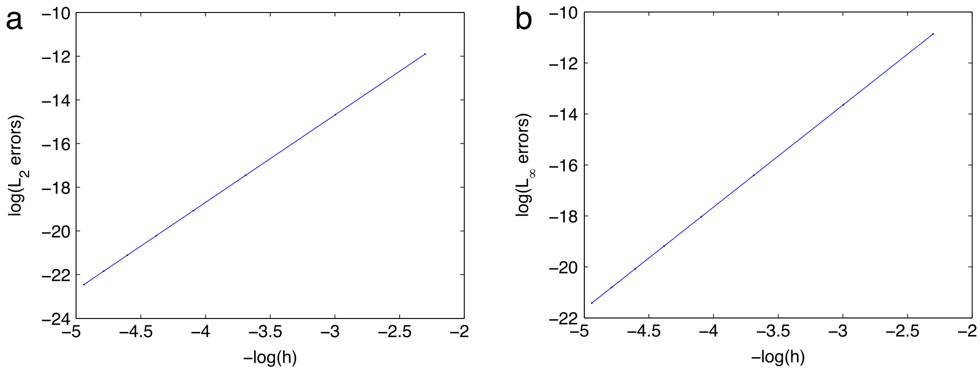

Fig. 5.1. The log–log plots for L_2 errors (left) and L_∞ errors (right) for our new LOD scheme with the first group of parameters. The slopes of the two lines are all 3.9995.

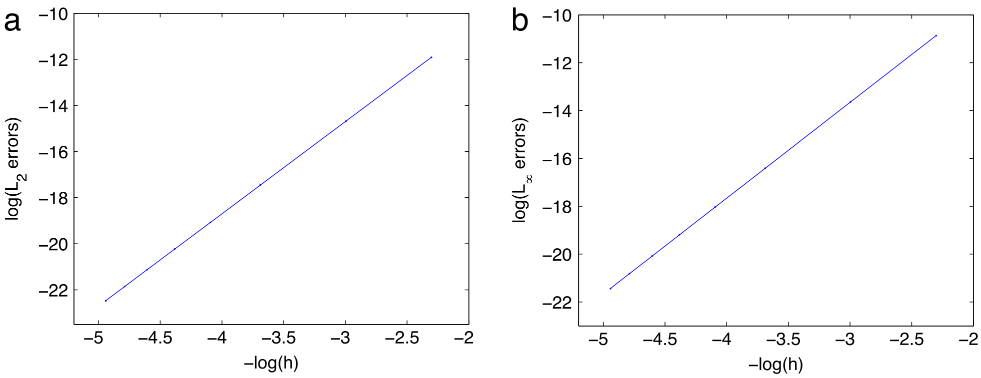

Fig. 5.2. The log–log plots for the L_2 errors (left) and L_∞ errors (right) for our new LOD scheme with the second group of parameters. The slopes of the two lines are all 4.0035.

where $c = 10^6$ is a constant which controls the amplitude. The medium has constant velocity $v = 2500$ m/s. The time step is $\Delta t = 0.002$ s and the space step is $h = 12.5$ m. In this example the first group parameters are used. Fig. 5.3 is the corresponding 3D wavefield snapshot at propagation time 1.26. We find the 2D sections of the 3D snapshot are all circles which is consistent with the physical phenomenon.

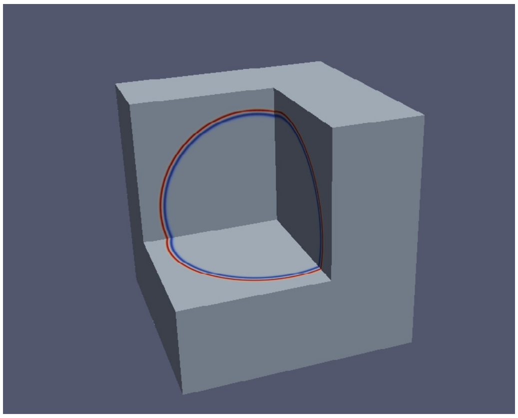

Fig. 5.3. The snapshot of 3D wavefield at 1.26 s.

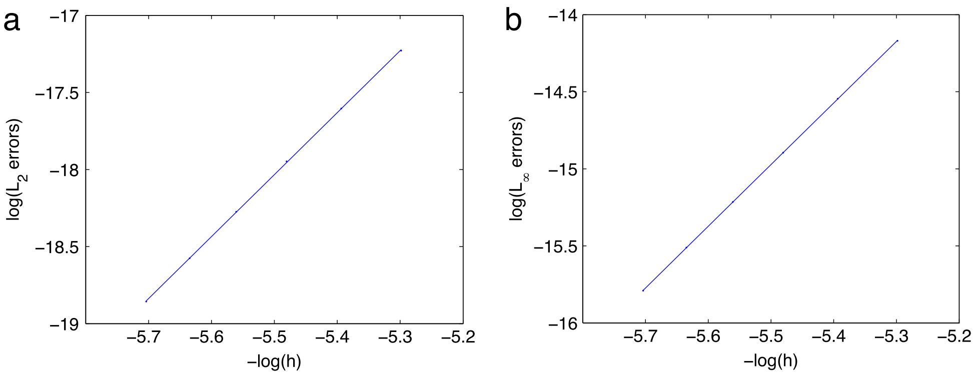

Fig. 5.4. The log–log plots for L_2 errors (left) and L_∞ errors (right). The slopes of the lines are 4.0194 (left) and 3.9993 (right) respectively.

Table 5.3
Numerical L_2 and L_∞ errors of our new LOD scheme with the first group parameter. The time step is fixed $\Delta t = 0.0002$ s.

$N_x = N_y = N_z$	L_2 errors	$\mathcal{O}_{L_2}$	L_∞errors	$\mathcal{O}_{L_\infty}$
200	3.2945E−8	4.0174	7.0218E−7	3.7850
220	2.2629E−8	3.9409	4.8187E−7	3.9504
240	1.6052E−8	3.9467	3.3976E−7	4.0160
260	1.1576E−8	4.0839	2.4677E−7	3.9949
280	8.5614E−9	4.0707	1.8353E−7	3.9956
300	6.4670E−9	4.0633	1.3875E−7	4.0544

Next we investigate the convergence behavior of our method. In Table 5.3 we show the errors measured by the L_2 norm and L_∞ norm for the fixed time step $\Delta t = 0.0002$ s. The corresponding convergence orders are also shown. The analytical or exact solutions are computed by the Cagniard's method [40]. In Fig. 5.4, we show the log–log plots of the errors. We found that the slopes of the lines are 4.0194 and 3.9993 for L_2 and L_∞ errors respectively, which is consistent with our theoretical results. In Table 5.4 we show the L_2 and L_∞ errors for the fixed CFL condition $vh/\Delta t = 0.2$. In Fig. 5.5, we show the log–log plots of the errors. We found that the slopes of the lines are 4.0184 and 3.9993 for L_2 and L_∞ errors respectively. The results show that our method has fourth-order convergence rate. Moreover, the average convergence order for the L_2 errors and L_∞ errors are the same.

6. Conclusions

In this paper, we have presented a new family of locally one-dimensional schemes for solving the three-dimensional acoustic wave equation. Our scheme is fourth-order accurate both in space and time. It is compact and only involves three layer grids in space and only needs to solve tridiagonal system of linear algebraic equation at each time step. Initial conditions are given in detail, which are easy to apply. Moreover, the stability conditions including the explicit restriction for time step are analyzed in detail. The analysis show that the CFL number of our new schemes is more relax compared with explicit schemes. Numerical results are shown to verify the convergence rate which is consistent with our theoretical results.

Table 5.4
Numerical L_2 and L_∞ errors of our new LOD scheme with the first group parameter. The CFL number $vh/\Delta t = 0.2$ is fixed.

$N_x = N_y = N_z$	L_2 errors	$\mathcal{O}_{L_2}$	L_∞ errors	$\mathcal{O}_{L_\infty}$
200	3.2938E−8	4.0168	7.0071E−7	3.7868
220	2.2625E−8	3.9404	4.8082E−7	3.9514
240	1.6049E−8	3.9465	3.3913E−7	4.0123
260	1.1574E−8	4.0839	2.4631E−7	3.9949
280	8.5600E−9	4.0709	1.8311E−7	4.0013
300	6.4692E−9	4.0591	1.3846E−7	4.0510

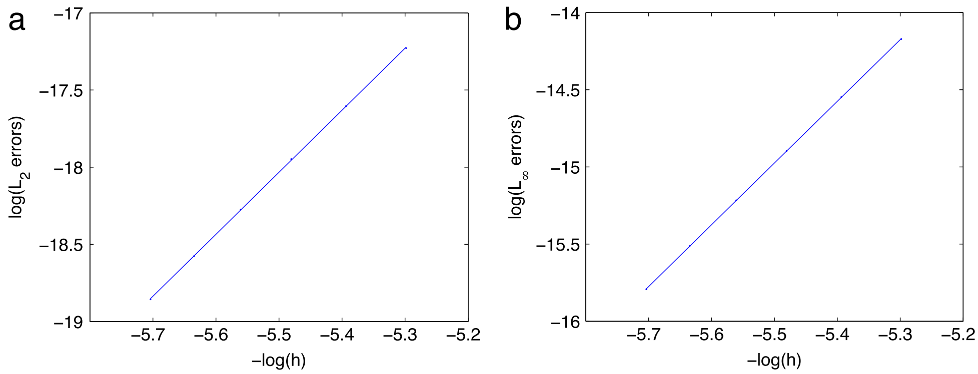

Fig. 5.5. The log–log plots for L_2 errors (left) and L_∞ errors (right) for our new LOD scheme with the first group of parameters. The slopes of the lines are 4.0184 (left) and 3.9993 (right) respectively.

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Appendix A. The coefficients used in (2.6)–(2.9)

The coefficients a_i and b_i $(i = 1, 2, 3, 4)$ are given by

$$a_1 = \frac{2}{(1-s_3)(s_1+1-s_3)}, \qquad a_2 = \frac{2}{s_1 s_2}, \tag{A.1}$$

$$a_3 = \frac{2}{(s_2-s_1)(s_3-s_1)}, \qquad a_4 = \frac{2}{(s_3-s_2)(1-s_2)}, \tag{A.2}$$

$$b_1 = \frac{2}{s_1(s_1+1-s_3)}, \qquad b_2 = \frac{2}{(s_2-s_1)s_2}, \tag{A.3}$$

$$b_3 = \frac{2}{(s_3-s_2)(s_3-s_1)}, \qquad b_4 = \frac{2}{(1-s_3)(1-s_2)}, \tag{A.4}$$

and c_i and e_i $(i = 1, 2, 3)$ are given by

$$c_1 = \frac{2}{s_1-s_3+1} + c_2 + c_3, \qquad c_2 = \frac{b_1(1-\tau_x)}{12\tau_x}, \qquad c_3 = \frac{a_1(1-\tau_x)}{12\tau_x}, \tag{A.5}$$

$$e_1 = \frac{2}{1-s_2} + e_2 + e_3, \qquad e_2 = \frac{b_4(1-\tau_z)}{12\tau_z}, \qquad e_3 = \frac{a_4(1-\tau_z)}{12\tau_z}, \tag{A.6}$$

where $\tau_x = v^2\Delta t^2/h_x^2$, $\tau_y = v^2\Delta t^2/h_y^2$, $\tau_z = v^2\Delta t^2/h_z^2$.

The parameters s_i $(i = 1, 2, 3)$ satisfy the following equation

$$3s_1^2 - 3s_1 + 3s_2^2 - 3s_2 + 1 = 0, \qquad s_3 = \frac{1}{2} + \frac{\sqrt{3}}{6}. \tag{A.7}$$

Thus the solutions of (A.7) form a family of group parameters s_i. Here we present two groups of parameters as examples. The first group is

$$s_1 = \frac{1}{4} + \frac{\sqrt{3}}{12} - \frac{\sqrt{2}\sqrt[4]{27}}{12}, \qquad s_2 = \frac{1}{4} + \frac{\sqrt{3}}{12} + \frac{\sqrt{2}\sqrt[4]{27}}{12}, \qquad s_3 = \frac{1}{2} + \frac{\sqrt{3}}{6}, \tag{A.8}$$

with the corresponding d_i and $\tilde{d}_i$ $(i = 1, 2, 3)$:

$$d_1 = \frac{6s_2^2 - 6s_2 + 1}{3s_2(s_2 - s_1)(s_1 + s_2 - 1)} + d_2 + d_3, \tag{A.9}$$

$$d_2 \approx \frac{0.758364}{\tau_y} - 0.192754, \qquad d_3 = \frac{a_2}{b_2} d_2, \tag{A.10}$$

$$\tilde{d}_1 = -\frac{6s_1^2 - 6s_1 + 1}{3(s_1 - s_2)(s_1 - s_3)(s_1 + s_2 - 1)} + \tilde{d}_2 + \tilde{d}_3, \qquad \tilde{d}_2 \approx d_2, \qquad \tilde{d}_3 = \frac{a_3}{b_3}\tilde{d}_2. \tag{A.11}$$

The second group is

$$s_1 = \frac{-3 + \sqrt{3}}{3(-5 + \sqrt{3})}, \qquad s_2 = \frac{2}{3}, \qquad s_3 = \frac{1}{2} + \frac{\sqrt{3}}{6}, \tag{A.12}$$

with the corresponding d_i and $\tilde{d}_i$ $(i = 1, 2, 3)$:

$$d_1 = \frac{6s_2^2 - 6s_2 + 1}{3s_2(s_2 - s_1)(s_1 + s_2 - 1)} + d_2 + d_3, \tag{A.13}$$

$$d_2 \approx \frac{0.7533731}{\tau_y} - 0.1915980, \qquad d_3 = \frac{a_2}{b_2} d_2, \tag{A.14}$$

$$\tilde{d}_1 = -\frac{6s_1^2 - 6s_1 + 1}{3(s_1 - s_2)(s_1 - s_3)(s_1 + s_2 - 1)} + \tilde{d}_2 + \tilde{d}_3, \qquad \tilde{d}_2 = d_2, \qquad \tilde{d}_3 = \frac{a_3}{b_3}\tilde{d}_2. \tag{A.15}$$

Appendix B. The expressions of F_1 and g in (4.25)

The expression of function $F_1(\sigma_x, \sigma_y, \sigma_z)$ is

$$\begin{aligned} F_1 = {} & 120269.24\sigma_y^2\tau^2 - 476414.2\sigma_y - 238207.1\sigma_z - 238207.1\sigma_x \\ & + 158804.73\sigma_x\sigma_y + 79402.367\sigma_x\sigma_z + 158804.73\sigma_y\sigma_z - 476414.2\sigma_x\tau \\ & - 593530.86\sigma_y\tau - 476414.2\sigma_z\tau - 16266.505\sigma_x\sigma_y^2 - 16266.505\sigma_y^2\sigma_z \\ & + 213400.31\sigma_y^2\tau + 48799.514\sigma_y^2 + 5422.1683\sigma_x\sigma_y^2\sigma_z + 157480.14\sigma_x\sigma_y\tau^2 \\ & - 103666.44\sigma_x\sigma_y^2\tau + 79402.367\sigma_x\sigma_z\tau^2 + 157480.14\sigma_y\sigma_z\tau^2 - 103666.44\sigma_y^2\sigma_z\tau \\ & - 136536.07\sigma_x\sigma_y^2\tau^2 + 20776.084\sigma_x\sigma_y^2\tau^3 - 69372.431\sigma_y^2\sigma_z\tau^2 + 3705.0682\sigma_y^2\sigma_z\tau^3 \\ & - 52934.911\sigma_x\sigma_y\sigma_z + 515453.09\sigma_x\sigma_y\tau + 317609.47\sigma_x\sigma_z\tau + 515453.09\sigma_y\sigma_z\tau \\ & - 277687.52\sigma_x\sigma_y\sigma_z\tau - 157921.67\sigma_x\sigma_y\sigma_z\tau^2 + 45399.818\sigma_x\sigma_y^2\sigma_z\tau \\ & + 50305.26\sigma_x\sigma_y\sigma_z\tau^3 + 60695.086\sigma_x\sigma_y^2\sigma_z\tau^2 - 23200.284\sigma_x\sigma_y^2\sigma_z\tau^3 \\ & + 350.28642\sigma_x\sigma_y^2\sigma_z\tau^4 + 714621.3. \end{aligned} \tag{B.16}$$

The expression of function $g(\sigma_x, \sigma_y, \sigma_z)$ is

$$\begin{aligned} g = {} & 158804.73\sigma_x + 97599.029\sigma_y + 158804.73\sigma_z - 593530.86\tau - 32533.01\sigma_x\sigma_y \\ & - 52934.911\sigma_x\sigma_z - 32533.01\sigma_y\sigma_z + 515453.09\sigma_x\tau + 426800.61\sigma_y\tau \\ & + 515453.09\sigma_z\tau + 157480.14\sigma_x\tau^2 + 240538.48\sigma_y\tau^2 + 157480.14\sigma_z\tau^2 \\ & - 273072.14\sigma_x\sigma_y\tau^2 + 41552.168\sigma_x\sigma_y\tau^3 - 157921.67\sigma_x\sigma_z\tau^2 + 50305.26\sigma_x\sigma_z\tau^3 \\ & - 138744.86\sigma_y\sigma_z\tau^2 + 7410.1364\sigma_y\sigma_z\tau^3 + 10844.337\sigma_x\sigma_y\sigma_z - 207332.89\sigma_x\sigma_y\tau \\ & - 277687.52\sigma_x\sigma_z\tau - 207332.89\sigma_y\sigma_z\tau + 90799.636\sigma_x\sigma_y\sigma_z\tau + 121390.17\sigma_x\sigma_y\sigma_z\tau^2 \\ & - 46400.567\sigma_x\sigma_y\sigma_z\tau^3 + 700.57284\sigma_x\sigma_y\sigma_z\tau^4 - 476414.2. \end{aligned} \tag{B.17}$$

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