A compact high order Alternating Direction Implicit method for three-dimensional acoustic wave equation with variable coefficient

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Abstract
Efficient and accurate numerical simulation of seismic wave propagation is important in various Geophysical applications such as seismic full waveform inversion (FWI) problem. However, due to the large size of the physical domain and requirement on low numerical dispersion, many existing numerical methods are inefficient for numerical modelling of seismic wave propagation in an heterogeneous media. Despite the great efforts that have been devoted during the past decades, it still remains a challenging task in the development of efficient and accurate finite difference method for multi-dimensional acoustic wave equation with variable velocity. In this paper we proposed a Padé approximation based finite difference scheme for solving the acoustic wave equation in three-dimensional heterogeneous media. The new method is obtained by combining the Padé approximation and a novel algebraic manipulation. The efficiency of the new algorithm is further improved through the Alternative Directional Implicit (ADI) method. The stability of the new algorithm has been theoretically proved by energy method. The new method is conditionally stable with a better Courant - Friedrichs - Lewy condition (CFL) condition, which has been verified numerically. Extensive numerical examples have been solved, which demonstrated that the new method is accurate, efficient and stable.

Keywords: Acoustic Wave Equation, Compact Finite Difference Method, Padé Approximation, Alternative Direction Implicit, Heterogenous Media.
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1. Introduction
Finite difference (FD) method has been widely used in various science and engineering applications for several reasons such as easy implementation, high efficiency etc, when the analytical solution is not available. One example is the

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acoustic wave equation when a non-zero point source function is included in the equation. In particular, the high-order FD methods have attracted the interests of many researchers working on seismic modelling (see [3, 6, 23, 29] and references therein) due to the high-order accuracy and effectiveness in suppressing numerical dispersion. Moreover, the number of grid points per wavelength required by higher order FD methods is significantly less than that of the conventional FD methods.

Recently, a great deal of efforts have been devoted to develop high-order FD schemes for the acoustic equations, and many accurate and efficient methods have been developed. Levander [16] addressed the cost-effectiveness of solving real problems using high-order spatial derivatives to allow a more coarse spatial sample rate. In [23], the authors used a plane wave theory and the Taylor series expansion to develop a low dispersion time-space domain FD scheme with error $O(\tau^2 + h^2M)$ for 1-D, 2-D and 3-D acoustic wave equations, where $\tau$ and $h$ represent the time step and spatial grid size, respectively. It was then shown that, along certain fixed directions the error can be improved to $O(\tau^2M + h^2M)$. In [6], Cohen and Poly extended the works of Dablain [7], Shubin and Bell [27] and Bayliss et al. [1] and developed a fourth-order accurate explicit scheme with error of $O(\tau^4 + h^4)$ to solve the heterogeneous acoustic wave equation. Moreover, it has been reported that highly accurate numerical methods are very effective in suppressing the annoying numerical dispersion [11]. High-order FD method is of particular importance for large-scale 3D acoustic wave equation, as it requires less grid points.

These methods are accurate but are non-compact, which give rise to two issues: efficiency and difficulty in boundary condition treatment. For example, the conventional non-compact fourth-order FD scheme requires a five-point stencil in 1D to approximate $u_{xx}$, while in 2D, a 9-point stencil is needed in approximating $\Delta u$. In 3D problem, a 13-point stencil is required to approximate the derivative $u_{xx} + u_{yy} + u_{zz}$ with fourth-order accuracy. To overcome these difficulties, a variety of compact higher-order FD schemes have been developed for hyperbolic, parabolic and elliptical partial differential equations. In [4], the authors developed a family of fourth-order three-point combined difference schemes to approximate the first- and second-order spatial derivatives. In [13], the authors introduced a family of three-level implicit FD schemes which incorporate the locally one-dimensional method. For more recent compact higher-order difference methods, the readers are referred to [28].

For three-dimensional problems, an implicit scheme results in a block tridiagonal system, which is solved at each time step. Direct solution of such large block linear system is very inefficient, therefore, some operator splitting techniques are used to convert the three-dimensional problem into a sequence of one-dimensional problems. One widely used method is the ADI method, which was originally introduced by Peaceman and Rachford [23] to solve parabolic and elliptic equations. Since then a lot of developments have been made over the years for hyperbolic equations [4, 13]. Later, Fairweather and Mitchell [10] developed a fourth-order compact ADI scheme for solving the wave equation. Some other related work can be found in [18, 19]. Combined with Padé approx-
imation of the finite difference operator, some efficient and high-order compact finite difference methods have been developed to solve the acoustic wave equations in 2D and 3D with constant velocity \[8, 20\]. However, when the velocity is a spatially varying function, it is difficult to apply this technique because the algebraic manipulation is not applicable here. Nevertheless, some research work on accurate and low-dispersion numerical simulation of acoustic wave propagation in heterogeneous media have been reported\[33\], in which a layered model consisting of multiple horizontal homogeneous layers was considered, with the method development and stability analysis are based on constant velocity model.

In \[21\] a new fourth-order compact ADI FD scheme was proposed to solve the two-dimensional acoustic wave equation with spatially variable velocity. Here we extended this method and the Padé approximation based high-order compact FD scheme in \[8\] to the 3D acoustic wave equation with non-constant velocity. The new method is compact and efficient, with fourth-order accuracy in both time and space. To our best knowledge, it is the first time that the energy method has been used to conduct theoretical stability analysis of the Padé-approximation based compact scheme. It has been shown that the obtained stability condition (CFL condition) is highly consistent to the CFL condition obtained by other methods.

The rest of the paper is organized as the follows. We first give a brief introduction of the acoustic wave equation and several existing standard second-order central FD schemes, compact high-order FD schemes for spatial derivatives and some other related high-order method in Section 2, then derive the new compact fourth-order ADI FD scheme in Section 3. Stability analysis of the new method is presented in Section 4, which is followed by three numerical examples in Section 5. Finally, the conclusions and some future works are discussed in Section 6.

2. Acoustic wave equation and existing algorithms

Consider the 3D acoustic wave equation

\[
\begin{align*}
\frac{\partial^2 u}{\partial t^2} &= \nabla^2 u + s(x, y, z, t), \\
\frac{\partial u}{\partial t} &= f(x, y, z), \\
\phi &= g(x, y, z, t),
\end{align*}
\]

where \(\nu(x, y, z)\) represents the wave velocity. Here \(\Omega \subset \mathbb{R}^3\) is a finite computational domain and \(s(x, y, z, t)\) is the source function. We denote \(e(x, y, z) = \nu^2(x, y, z)\) for the sake of simple notation.

First assume that \(\Omega\) is a 3D rectangular box : \([x_0, x_1] \times [y_0, y_1] \times [z_0, z_1]\), which is discretized into an \(N_x \times N_y \times N_z\) grid with spatial grid sizes \(h_x, h_y, h_z\). Let \(\tau\) be the time stepsize and \(u^n_{i,j,k}\) denote the numerical solution at the grid point \((x_i, y_j, z_k)\) and time level \(n\tau\). Let’s first define the standard central difference operators

\[
\delta_t^2 u_{i,j,k}^n = u_{i,j,k}^{n-1} - 2u_{i,j,k}^n + u_{i,j,k}^{n+1},
\]
\[ \delta^2_t u_{i,j,k}^n = u_{i-1,j,k}^n - 2u_{i,j,k}^n + u_{i+1,j,k}^n, \]
\[ \delta^2_y u_{i,j,k}^n = u_{i,j-1,k}^n - 2u_{i,j,k}^n + u_{i,j+1,k}^n, \]
\[ \delta^2_z u_{i,j,k}^n = u_{i,j,k-1}^n - 2u_{i,j,k}^n + u_{i,j,k+1}^n. \]

The standard second-order central FD schemes are then given by approximating the second derivatives in Eq. (1). For example,

\[ u_{tt}(x_i, y_j, z_k, t_n) = \frac{1}{\tau^2} \delta^2_t u_{i,j,k}^n + O(\tau^2), \]  
\[ (5) \]
\[ u_{xx}(x_i, y_j, z_k, t_n) = \frac{1}{h^2_x} \delta^2_x u_{i,j,k}^n + O(h^2_x). \]  
\[ (6) \]

The approximations of \( u_{yy} \) and \( u_{zz} \) are similar to Eq. (6).

To improve the method to fourth-order in space, the conventional high-order FD method was derived by approximating the derivatives using more than three points in one direction, which results in larger stencil. For instance, if \( 2M + 1 \) points are used to approximate \( u_{xx} \), one can obtain the following formula

\[ u_{xx}(x_i, y_j, z_k, t_n) \approx \left[a_0 u_{i,j,k}^n + \sum_{m=1}^{M} a_m (u_{i-m,j,k}^n + u_{i+m,j,k}^n)\right]/h^2_x, \]  
\[ (7) \]

which can be as accurate as \((2M)th\) order in \( x \). The conventional high-order FD method is accurate in space but suffers severe numerical dispersion. Another issue is that it requires more computer memory due to the larger stencil for implicit method. Moreover, more points are needed to approximate the boundary condition.

To improve the accuracy in time, a class of time-domain high-order FD methods have been derived by Liu and Sen [23]. The idea of the time-domain high-order FD method is to determine coefficients using time-space domain dispersion. As a result, the coefficient will be a function of \( \frac{\tau}{h} \). It was noted that in 1D case, the time-domain high-order FD method can be as accurate as \((2M)th\) order in both time and space, provided some conditions are satisfied, while for multidimensional case, \((2M)th\) order is also possible along some propagation directions.

To develop a high-order compact ADI FD scheme, we apply the Padé approximation to the second-order central FD operators, so the second derivatives \( u_{tt}, u_{xx}, u_{yy} \) and \( u_{zz} \) can approximated with fourth-order accuracy. For example,

\[ \frac{\delta^2_t}{\tau^2 (1 + \frac{1}{12} \delta^2_t)} u_{i,j,k}^n = u_{tt}(x_i, y_j, z_k, t_n) + O(\tau^4), \]  
\[ (8) \]
\[ \frac{\delta^2_x}{h^2_x (1 + \frac{1}{12} \delta^2_x)} u_{i,j,k}^n = u_{xx}(x_i, y_j, z_k, t_n) + O(h^4_x). \]  
\[ (9) \]

The fourth-order approximations of \( u_{yy} \) and \( u_{zz} \) can be obtained similarly.
Let $\lambda_x = \frac{\delta_t^2}{\delta_x^2}$, $\lambda_y = \frac{\delta_t^2}{\delta_y^2}$, $\lambda_z = \frac{\delta_t^2}{\delta_z^2}$. Substituting the fourth-order Padé approximations into Eq. (1) gives

$$\frac{\delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_x^2} u_{i,j,k}^n = \lambda_x c_{i,j,k} \frac{\delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_x^2} \left[ \frac{\lambda_x c_{i,j,k} \delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_x^2} \right] u_{i,j,k}^n + \lambda_y c_{i,j,k} \frac{\delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_y^2} \left[ \frac{\lambda_y c_{i,j,k} \delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_y^2} \right] u_{i,j,k}^n + \lambda_z c_{i,j,k} \frac{\delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_z^2} \left[ \frac{\lambda_z c_{i,j,k} \delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_z^2} \right] u_{i,j,k}^n + \tau^2 \left[ \frac{\delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_y^2} \right] s_{i,j,k}^n. \quad (10)$$

Truncation error analysis shows that the algorithm is fourth-order accurate in time and space with the truncation error $O(\tau^4 + h_x^4 + h_y^4 + h_z^4)$, provided the solution $u(x, y, z, t)$ and $c(x, y, z)$ satisfy certain smoothness conditions. As shown in [21], the difficulty to develop high-order compact scheme for wave equation with non-constant velocity is that, one can not multiply the operator $(1 + \delta_t^2 \delta_x^2)^{-1}, (1 + \delta_t^2 \delta_y^2)^{-1}, (1 + \delta_t^2 \delta_z^2)^{-1}$ and $(1 + \delta_t^2 \delta_y^2)^{-1}$, which are difficult to implement. To overcome this problem, we develop an algebraic strategy which will be described in the next section.

3. Derivation of the compact high-order ADI method

Now we extend the novel algebraic manipulation introduced in [21] to the three-dimensional acoustic wave equation with variable velocity. We first demonstrate the difficulty in applying the Padé approximation to the finite difference operator for solving the acoustic wave equation with non-constant velocity. Multiplying the operator in Eq. (11) to Eq. (10) yields

$$\left(1 + \frac{\delta_t^2}{12}\right) \left(1 + \frac{\delta_x^2}{12}\right) \left(1 + \frac{\delta_y^2}{12}\right) \left(1 + \frac{\delta_z^2}{12}\right) \delta_t^2 u_{i,j,k}^n c_{i,j,k} \left(1 + \frac{\delta_t^2}{12}\right) \left(1 + \frac{\delta_x^2}{12}\right) \left(1 + \frac{\delta_y^2}{12}\right) \left(1 + \frac{\delta_z^2}{12}\right) \delta_t^2 u_{i,j,k}^n + \lambda_x c_{i,j,k} \frac{\delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_x^2} \left[ \frac{\lambda_x c_{i,j,k} \delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_x^2} \right] u_{i,j,k}^n + \lambda_y c_{i,j,k} \frac{\delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_y^2} \left[ \frac{\lambda_y c_{i,j,k} \delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_y^2} \right] u_{i,j,k}^n + \lambda_z c_{i,j,k} \frac{\delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_z^2} \left[ \frac{\lambda_z c_{i,j,k} \delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_z^2} \right] u_{i,j,k}^n + \tau^2 \left[ \frac{\delta_t^2}{1 + \frac{\delta_t^2}{12} \delta_y^2} \right] s_{i,j,k}^n. \quad (12)$$

We use the first term on the right-hand side to illustrate the issue here. Since $(1 + \frac{\delta_t^2}{12})$, $(1 + \frac{\delta_x^2}{12})$ and $(1 + \frac{\delta_z^2}{12})$ are commutative, we change the order of the
three finite difference operators to obtain

\[
\lambda_x \left( 1 + \frac{1}{12} \delta_x^2 \right) \left( 1 + \frac{1}{12} \delta_y^2 \right) \left( 1 + \frac{1}{12} \delta_z^2 \right) c_{i,j,k} \frac{\delta_x^2}{1 + \frac{1}{12} \delta_x^2} u^n_{i,j,k} = \\
\lambda_x \left( 1 + \frac{1}{12} \delta_x^2 \right) \left( 1 + \frac{1}{12} \delta_y^2 \right) \left( 1 + \frac{1}{12} \delta_z^2 \right) c_{i,j,k} \frac{\delta_x^2}{1 + \frac{1}{12} \delta_x^2} u^n_{i,j,k} = \\
\lambda_x \left( 1 + \frac{1}{12} \delta_x^2 \right) \left( 1 + \frac{1}{12} \delta_y^2 \right) \left( 1 + \frac{1}{12} \delta_z^2 \right) c_{i,j,k} \frac{\delta_x^2}{1 + \frac{1}{12} \delta_x^2} u^n_{i,j,k}.
\]  

As discussed previously, when \( c(x, y, z) \) is non-constant in terms of \( x \), the operator \( (1 + \frac{1}{12} \delta_x^2) \) and \( c_{i,j,k} \) are not commutative. Hence, \( (1 + \frac{1}{12} \delta_x^2) c_{i,j,k} \neq c_{i,j,k} (1 + \frac{1}{12} \delta_x^2) \). Therefore, the operator \( (1 + \frac{1}{12} \delta_x^2) \) does not cancel the operator \( (1 + \frac{1}{12} \delta_x^2)^{-1} \). In other words,

\[
\lambda_x \left( 1 + \frac{1}{12} \delta_x^2 \right) \left( 1 + \frac{1}{12} \delta_y^2 \right) \left( 1 + \frac{1}{12} \delta_z^2 \right) c_{i,j,k} \frac{\delta_x^2}{1 + \frac{1}{12} \delta_x^2} u^n_{i,j,k}
\neq \lambda_x \left( 1 + \frac{1}{12} \delta_x^2 \right) \left( 1 + \frac{1}{12} \delta_y^2 \right) \left( 1 + \frac{1}{12} \delta_z^2 \right) c_{i,j,k} \delta_x^2 u^n_{i,j,k}.
\]  

To solve this problem, a novel factorization technique is used to preserve the compactness and fourth-order convergence of the numerical scheme. Multiplying \( (1 + \frac{1}{12} \delta_x^2) \) to Eq. (10) yields

\[
\delta_x^2 u^n_{i,j,k} = c_{i,j,k} \left[ \lambda_x \left( 1 + \frac{1}{12} \delta_x^2 \right) \frac{\delta_x^2}{1 + \frac{1}{12} \delta_x^2} + \lambda_y \left( 1 + \frac{1}{12} \delta_y^2 \right) \frac{\delta_y^2}{1 + \frac{1}{12} \delta_y^2} + \lambda_z \left( 1 + \frac{1}{12} \delta_z^2 \right) \frac{\delta_z^2}{1 + \frac{1}{12} \delta_z^2} \right] u^n_{i,j,k} + \tau^2 \left( 1 + \frac{1}{12} \delta_x^2 \right) s^n_{i,j,k}.
\]  

Collecting the term \( \delta_x^2 u^n_{i,j,k} \), we have

\[
\left[ 1 - \lambda_x c_{i,j,k} \frac{\delta_x^2}{1 + \frac{1}{12} \delta_x^2} - \lambda_y c_{i,j,k} \frac{\delta_y^2}{1 + \frac{1}{12} \delta_y^2} - \lambda_z c_{i,j,k} \frac{\delta_z^2}{1 + \frac{1}{12} \delta_z^2} \right] \delta_x^2 u^n_{i,j,k} = c_{i,j,k} \left[ \lambda_x \frac{\delta_x^2}{1 + \frac{1}{12} \delta_x^2} + \lambda_y \frac{\delta_y^2}{1 + \frac{1}{12} \delta_y^2} + \lambda_z \frac{\delta_z^2}{1 + \frac{1}{12} \delta_z^2} \right] u^n_{i,j,k} + \tau^2 \left( 1 + \frac{1}{12} \delta_x^2 \right) s^n_{i,j,k}.
\]  

Factoring the left-hand side of Eq. (10) yields

\[
\left[ 1 - c_{i,j,k} \frac{\lambda_x \delta_x^2}{1 + \frac{1}{12} \delta_x^2} \right] \left[ 1 - c_{i,j,k} \frac{\lambda_y \delta_y^2}{1 + \frac{1}{12} \delta_y^2} \right] \left[ 1 - c_{i,j,k} \frac{\lambda_z \delta_z^2}{1 + \frac{1}{12} \delta_z^2} \right] \delta_x^2 u^n_{i,j,k} = \\
\left[ \lambda_x \frac{\delta_x^2}{1 + \frac{1}{12} \delta_x^2} + \lambda_y \frac{\delta_y^2}{1 + \frac{1}{12} \delta_y^2} + \lambda_z \frac{\delta_z^2}{1 + \frac{1}{12} \delta_z^2} \right] u^n_{i,j,k} + \tau^2 \left( 1 + \frac{1}{12} \delta_x^2 \right) s^n_{i,j,k} + ERR.
\]
where the factorization error is given by

\[
ERR = \frac{\lambda_x \lambda_y}{144} \frac{c_{i,j,k} \delta_x^2}{1 + \frac{\delta_x^2}{12}} \frac{c_{i,j,k} \delta_y^2}{1 + \frac{\delta_y^2}{12}} \delta_t^2 u_{i,j,k} + \\
\frac{\lambda_y \lambda_z}{144} \frac{c_{i,j,k} \delta_y^2}{1 + \frac{\delta_y^2}{12}} \frac{c_{i,j,k} \delta_z^2}{1 + \frac{\delta_z^2}{12}} \delta_t^2 u_{i,j,k} + \\
\frac{\lambda_x \lambda_z}{144} \frac{c_{i,j,k} \delta_x^2}{1 + \frac{\delta_x^2}{12}} \frac{c_{i,j,k} \delta_z^2}{1 + \frac{\delta_z^2}{12}} \delta_t^2 u_{i,j,k} - \frac{\lambda_x \lambda_y \lambda_z}{1728} \frac{c_{i,j,k} \delta_x^2}{1 + \frac{\delta_x^2}{12}} \frac{c_{i,j,k} \delta_y^2}{1 + \frac{\delta_y^2}{12}} \frac{c_{i,j,k} \delta_z^2}{1 + \frac{\delta_z^2}{12}} \delta_t^2 u_{i,j,k}.
\] (18)

Using Taylor series, one can verify that \( ERR = O(\tau^6) \), provided that \( c(x, y, z) \) and \( u(x, y, z, t) \) satisfy some conditions on smoothness. The result regarding the order of the truncation error is included in the following theorem.

**Theorem 3.1.** Assume that \( u(x, y, z, t) \in C^{6,6,6,6}_{x,y,z,t}(\Omega \times [0, T]) \) is the solution of the acoustic wave equation defined by Eqs. (17 - 21), and the coefficient satisfies the smoothness condition \( c(x, y, z) \in C^{2,2,2}_{x,y,z}(\Omega) \). Then the truncation error given in Eq. (18) satisfies

\[
ERR = O(\tau^6) + O(h_x^6) + O(h_y^6) + O(h_z^6),
\]

where \( \tau, h_x, h_y \) and \( h_z \) are the step sizes in time, \( x, y \) and \( z \), respectively.

**Proof.** A detailed proof of the theorem is given in Appendix A. \( \square \)

**Remark:** If Eq. (10) is factorized in a different order of \( \delta_x^2 \), \( \delta_y^2 \) and \( \delta_z^2 \), for instance as

\[
\left[ 1 - \frac{c_{i,j,k} \lambda_y \delta_y^2}{12} \frac{\delta_x^2}{1 + \frac{\delta_x^2}{12}} \frac{\delta_y^2}{1 + \frac{\delta_y^2}{12}} \frac{\delta_z^2}{1 + \frac{\delta_z^2}{12}} \right] \left[ 1 - \frac{c_{i,j,k} \lambda_x \delta_x^2}{12} \frac{\delta_x^2}{1 + \frac{\delta_x^2}{12}} \frac{\delta_y^2}{1 + \frac{\delta_y^2}{12}} \right] \left[ 1 - \frac{c_{i,j,k} \lambda_z \delta_z^2}{12} \frac{\delta_x^2}{1 + \frac{\delta_x^2}{12}} \frac{\delta_y^2}{1 + \frac{\delta_y^2}{12}} \right] \delta_t^2 u_{i,j,k} =
\]

\[
c_{i,j,k} \left[ \frac{\lambda_x \delta_x^2}{1 + \frac{\delta_x^2}{12}} \frac{\delta_y^2}{1 + \frac{\delta_y^2}{12}} + \frac{\lambda_y \delta_y^2}{1 + \frac{\delta_y^2}{12}} \frac{\delta_z^2}{1 + \frac{\delta_z^2}{12}} + \frac{\lambda_z \delta_z^2}{1 + \frac{\delta_z^2}{12}} \frac{\delta_x^2}{1 + \frac{\delta_x^2}{12}} \right] u_{i,j,k} + \tau^2 \left( 1 - \frac{\delta_t^2}{12} \right) \delta_t^2 u_{i,j,k} + ERR, (19)
\]

then the factorizing error \( ERR \) is given by

\[
ERR = \frac{\lambda_y}{144} c_{i,j,k} \frac{\delta_y^2}{1 + \frac{\delta_y^2}{12}} \frac{\delta_x^2}{1 + \frac{\delta_x^2}{12}} \delta_t^2 u_{i,j,k} + \frac{\lambda_x}{144} c_{i,j,k} \frac{\delta_x^2}{1 + \frac{\delta_x^2}{12}} \frac{\delta_y^2}{1 + \frac{\delta_y^2}{12}} \delta_t^2 u_{i,j,k} + \frac{\lambda_z}{144} c_{i,j,k} \frac{\delta_z^2}{1 + \frac{\delta_z^2}{12}} \frac{\delta_y^2}{1 + \frac{\delta_y^2}{12}} \delta_t^2 u_{i,j,k} - \frac{1}{1728} \lambda_y c_{i,j,k} \frac{\delta_y^2}{1 + \frac{\delta_y^2}{12}} \frac{\delta_x^2}{1 + \frac{\delta_x^2}{12}} \delta_t^2 u_{i,j,k}, \] (20)

which has the same error estimation as that defined in Eq. (A.10).
Ignoring the factoring error ERR in Eq. (17) leads to the following compact fourth-order FD method

\[
\left[ 1 - \frac{\lambda_x c_{i,j,k}}{12} \frac{\delta_x^2}{1 + \frac{\delta_x^2}{12}} \right] \cdot \left[ 1 - \frac{\lambda_y c_{i,j,k}}{12} \frac{\delta_y^2}{1 + \frac{\delta_y^2}{12}} \right] \cdot \left[ 1 - \frac{\lambda_z c_{i,j,k}}{12} \frac{\delta_z^2}{1 + \frac{\delta_z^2}{12}} \right] \delta_t^n u_{i,j,k}^n
\]

\[
= c_{i,j,k} \left[ \frac{\lambda_x \delta_x^2}{1 + \frac{\delta_x^2}{12}} + \frac{\lambda_y \delta_y^2}{1 + \frac{\delta_y^2}{12}} + \frac{\lambda_z \delta_z^2}{1 + \frac{\delta_z^2}{12}} \right] u_{i,j,k}^n + \tau^2 \left( 1 + \frac{\delta_t^2}{12} \right) s_{i,j,k}^n.
\]

(21)

Using ADI method, Eq. (21) can be efficiently solved in three steps

\[
\left( 1 - \frac{\lambda_x c_{i,j,k}}{12} \frac{\delta_x^2}{1 + \frac{\delta_x^2}{12}} \right) u_{i,j,k}^{**} = \left[ \frac{c_{i,j,k} \lambda_x \delta_x^2}{1 + \frac{\delta_x^2}{12}} + \frac{c_{i,j,k} \lambda_y \delta_y^2}{1 + \frac{\delta_y^2}{12}} + \frac{c_{i,j,k} \lambda_z \delta_z^2}{1 + \frac{\delta_z^2}{12}} \right] u_{i,j,k}^n
\]

\[
+ \tau^2 \left( 1 + \frac{\delta_t^2}{12} \right) s_{i,j,k}^n, \quad 2 \leq j \leq N_y - 1, \quad 2 \leq k \leq N_z - 1,
\]

(22)

\[
\left( 1 - \frac{\lambda_y c_{i,j,k}}{12} \frac{\delta_y^2}{1 + \frac{\delta_y^2}{12}} \right) u_{i,j,k}^{*} = u_{i,j,k}^{**}, \quad 2 \leq i \leq N_x - 1, \quad 2 \leq k \leq N_z - 1,
\]

(23)

\[
\left( 1 - \frac{\lambda_z c_{i,j,k}}{12} \frac{\delta_z^2}{1 + \frac{\delta_z^2}{12}} \right) \delta_t^n u_{i,j,k}^{*} = u_{i,j,k}^*, \quad 2 \leq i \leq N_x - 1, \quad 2 \leq j \leq N_y - 1.
\]

(24)

Apparently the three equations are difficult to implement due to the three operators \( \left( 1 + \frac{\delta_x^2}{12} \right)^{-1} \), \( \left( 1 + \frac{\delta_y^2}{12} \right)^{-1} \), and \( \left( 1 + \frac{\delta_z^2}{12} \right)^{-1} \). To overcome this problem, we apply the following strategy. Firstly, divide both sides of Eq. (22) by \( c_{i,j,k} \), then multiply \( \left( 1 + \frac{\delta_x^2}{12} \right) \), we have

\[
\left[ 1 + \frac{\delta_x^2}{12} \frac{1}{c_{i,j,k}} - \frac{\lambda_x}{12} \frac{\delta_x^2}{c_{i,j,k}} \right] u_{i,j,k}^{**} = \tau^2 \left( 1 + \frac{\delta_t^2}{12} \right) \left( 1 + \frac{\delta_x^2}{c_{i,j,k}} \right) \frac{s_{i,j,k}^n}{c_{i,j,k}}
\]

\[
+ \left[ \lambda_x \delta_x^2 + \lambda_y \left( 1 + \frac{\delta_x^2}{12} \right) \frac{\delta_y^2}{1 + \frac{\delta_y^2}{12}} + \lambda_z \left( 1 + \frac{\delta_x^2}{12} \right) \frac{\delta_z^2}{1 + \frac{\delta_z^2}{12}} \right] u_{i,j,k}^n.
\]

(25)

Eq. (25) is still hard to implement because of the terms \( \frac{\delta_x^2}{1 + \frac{\delta_x^2}{12}} \) and \( \frac{\delta_y^2}{1 + \frac{\delta_y^2}{12}} \). Substituting \( \frac{\delta_y^2}{1 + \frac{\delta_y^2}{12}} u_{i,j,k}^n \) with \( \delta_y \left( 1 - \frac{\delta_y^2}{12} \right) u_{i,j,k}^n \), \( \frac{\delta_x^2}{1 + \frac{\delta_x^2}{12}} u_{i,j,k}^n \) with \( \delta_x \left( 1 - \frac{\delta_x^2}{12} \right) u_{i,j,k}^n \), respectively, we obtain

\[
\left[ 1 + \frac{\delta_x^2}{12} \frac{1}{c_{i,j,k}} - \lambda_x \frac{\delta_x^2}{c_{i,j,k}} \right] u_{i,j,k}^{**} = \tau^2 \left( 1 + \frac{\delta_t^2}{12} \right) \left( 1 + \frac{\delta_x^2}{c_{i,j,k}} \right) \frac{s_{i,j,k}^n}{c_{i,j,k}}
\]

\[
+ \left[ \lambda_x \delta_x^2 + \lambda_y \left( 1 + \frac{\delta_x^2}{12} \right) \delta_y \left( 1 - \frac{\delta_y^2}{12} \right) + \lambda_z \left( 1 + \frac{\delta_x^2}{12} \right) \delta_z \left( 1 - \frac{\delta_z^2}{12} \right) \right] u_{i,j,k}^n.
\]

(26)

for \( 2 \leq j \leq N_y - 1, \quad 2 \leq k \leq N_z - 1 \).
Note the difference between Eq. (25) and Eq. (26) is \( O(h_y^6 + h_z^6) \), therefore, the method is still fourth-order in space. It is worth to mention that the right-hand side of Eq. (26) includes larger stencil in both \( y \) and \( z \) directions. Furthermore, larger stencil needs values of \( u_i^n, j, k \) outside the boundary when \( j = 2, N_y - 1 \) and \( k = 2, N_z - 1 \). To overcome this problem, we use one-sided approximation to approximate the values outside of the boundary. For example, \( u_{i,0,k}^n \) is approximated by a linear combination of \( u_{i,1,k}^n, \cdots, u_{i,4,k}^n \) with fourth-order accuracy. This boundary treatment is not complicated in terms of implementation, since it only involves the values at time level \( n \), which is known. Similarly, dividing \( c_{i,j,k} \) then multiplying \( \left( 1 + \frac{\delta_y^2}{12} \right) \) to both sides of Eq. (28) lead to

\[
\left[ \left( 1 + \frac{\delta_y^2}{12} \right) \frac{1}{c_{i,j,k}} - \lambda_y \frac{\delta_y^2}{12} \right] u_{i,j,k}^n = \left( 1 + \frac{\delta_y^2}{12} \right) \frac{u_{i,j,k}^n}{c_{i,j,k}}
\]

for \( i = 2, 3, \cdots, N_x - 1 \), \( j = 2, 3, \cdots, N_y - 1 \), \( k = 2, 3, \cdots, N_z - 1 \).

Finally, Eq. (24) can be transformed to the equivalent linear system

\[
\left[ \left( 1 + \frac{\delta_z^2}{12} \right) \frac{1}{c_{i,j,k}} - \lambda_z \frac{\delta_z^2}{12} \right] \delta_z^2 u_{i,j,k}^n = \left( 1 + \frac{\delta_z^2}{12} \right) \frac{u_{i,j,k}^n}{c_{i,j,k}}
\]

for \( i = 2, 3, \cdots, N_x - 1 \), \( j = 2, 3, \cdots, N_y - 1 \).

It is noted that Eq. (28) is equivalent to a three-level FD scheme

\[
\left[ \left( 1 + \frac{\delta_y^2}{12} \right) \frac{1}{c_{i,j,k}} - \lambda_y \frac{\delta_y^2}{12} \right] u_{i,j,k}^{n+1} = \left( 1 + \frac{\delta_y^2}{12} \right) \frac{1}{c_{i,j,k}} - \frac{\delta_y^2}{12} \delta_t^2 u_{i,j,k}^n\right] (2u_{i,j,k}^n - u_{i,j,k}^{n-1})
\]

\[
+ \left( 1 + \frac{\delta_z^2}{12} \right) \frac{u_{i,j,k}^n}{c_{i,j,k}} \quad i = 2, 3, \cdots, N_x - 1, \quad j = 2, 3, \cdots, N_y - 1. \quad (29)
\]

By now the three linear systems defined in Eqs. (26, 27, 29) can be efficiently solved using Thomas algorithm. Here some one-sided fourth-order approximations are needed for boundary condition approximations in these equation systems. For example, in Eq. (25), the following fourth-order one-sided approximations are used to approximate \( u_{i,j,1} \) and \( u_{i,j,N_z} \), respectively:

\[
u_{i,j,1} = 4u_{i,j,2} - 6u_{i,j,3} + 4u_{i,j,4} - u_{i,j,5},
\]

\[
u_{i,j,N_z} = 4u_{i,j,N_z-1} - 6u_{i,j,N_z-2} + 4u_{i,j,N_z-3} - u_{i,j,N_z-4},
\]

for \( i = 2, 3, \cdots, N_x - 1, \quad j = 2, 3, \cdots, N_y - 1 \).

The boundary conditions for Eq. (27) can be obtained by setting \( j = 1 \) and \( j = N_y \) in Eq. (28), respectively.

\[
\left( 1 + \frac{\delta_y^2}{12} \right) \frac{u_{i,1,k}^n}{c_{i,1,k}} = \left( 1 + \frac{\delta_z^2}{12} \right) \frac{1}{c_{i,1,k}} - \frac{\delta_z^2}{12} \delta_t^2 u_{i,1,k}^n,
\]

\[
\left( 1 + \frac{\delta_z^2}{12} \right) \frac{u_{i,N_y,k}^n}{c_{i,N_y,k}} = \left( 1 + \frac{\delta_y^2}{12} \right) \frac{1}{c_{i,N_y,k}} - \frac{\delta_y^2}{12} \delta_t^2 u_{i,N_y,k}^n.
\]
Solving the two tridiagonal linear systems we can get the boundary conditions for Eq. (27). Similarly, the boundary conditions needed by Eq. (26) can be obtained by letting \( i = 1 \) and \( i = N_x \), respectively.

The new compact ADI method defined in Eq. (24) is a three-level FD scheme. Therefore, two initial conditions are needed at \( t = 0 \) and \( t = \tau \). To approximate the initial condition at \( t = \tau \) with fourth-order accuracy, we expand \( u(x_i, y_j, z_k, t) \) by the Taylor series at \( t = 0 \) and obtain the following fourth-order approximation

\[
u_{i,j,k}^1 = u_{i,j,k}^0 + \tau \frac{\partial u_{i,j,k}^0}{\partial t} + \frac{\tau^2}{2} \frac{\partial^2 u_{i,j,k}^0}{\partial t^2} + \frac{\tau^3}{6} \frac{\partial^3 u_{i,j,k}^0}{\partial t^3} + \frac{\tau^4}{24} \frac{\partial^4 u_{i,j,k}^0}{\partial t^4} + O(\tau^5), (32)
\]

where the high-order derivatives are derived using the method in [21].

Now we state and prove the main result on the convergence of the compact ADI FD scheme defined in Eq. (21).

**Theorem 3.2.** Assume that \( u(x, y, z, t) \in C^{6,6,6,6}([0, \Omega] \times [0, T]) \) is the solution of the acoustic wave equation defined in Eqs. (17-22), and the coefficient function satisfies the smooth condition \( c(x, y, z) \in C^{2,2,2,2}([\Omega]) \). Then the compact ADI FD scheme defined in Eq. (24) is fourth-order accurate in time and space with the truncation error \( O(\tau^4 + h_x^6 + h_y^6 + h_z^6) \).

**Proof** According to Theorem 3.1, if \( u(x, y, z, t) \) and \( c(x, y, z) \) are sufficiently smooth, the difference between the numerical scheme defined in Eq. (21) and the numerical scheme defined in Eq. (13) is \( O(\tau^4) + O(h_x^6) + O(h_y^6) + O(h_z^6) \).

On the other hand, it is known [21] that the compact Padé approximation FD method defined in Eq. (21) is fourth-order in time and space, with the truncation error \( O(\tau^4) + O(h_x^6) + O(h_y^6) + O(h_z^6) \).

Moreover, one can see that the truncation errors caused by the substitutions

\[
\begin{align*}
\frac{\delta^2_x}{(1 + \frac{\delta^2_x}{12})} & \rightarrow \delta^2_x \left( 1 - \frac{\delta^2_x}{12} \right), \\
\frac{\delta^2_y}{(1 + \frac{\delta^2_y}{12})} & \rightarrow \delta^2_y \left( 1 - \frac{\delta^2_y}{12} \right), \\
\frac{\delta^2_z}{(1 + \frac{\delta^2_z}{12})} & \rightarrow \delta^2_z \left( 1 - \frac{\delta^2_z}{12} \right)
\end{align*}
\]

in Eq. (26) are \( O(h_x^6) \), \( O(h_y^6) \) and \( O(h_z^6) \), respectively. Base on these, the new compact ADI FD scheme is fourth-order in time and space.

**4. Stability Analysis**

It is important that a numerical method is stable when it is applied to solve time-dependent problems. Most of the FD schemes for solving the acoustic wave equation are conditionally stable and subject to constraints on time step. The popular Von Neumann analysis is applicable for constant velocity case only, therefore, in this paper we adopted the energy method in [2] to analyze and prove the stability of the new method.

For the sake of simplicity, assume zero source for the wave equation. Consider the Padé approximation based fourth-order finite difference scheme

\[
\frac{\delta^2_t}{1 + \frac{\delta^2_t}{12}} u_{i,j,k}^{n+1} = c_{i,j,k} \left[ \lambda_x \frac{\delta^2_x}{1 + \frac{\delta^2_x}{12}} + \lambda_y \frac{\delta^2_y}{1 + \frac{\delta^2_y}{12}} + \lambda_z \frac{\delta^2_z}{1 + \frac{\delta^2_z}{12}} \right] u_{i,j,k}^n, (33)
\]
where } \lambda_x = \frac{x^2}{h_x}, \lambda_y = \frac{y^2}{h_y}, \lambda_z = \frac{z^2}{h_z}. \text{ For simplicity we assume } h = h_x = h_y = h_z,
\lambda = \lambda_x = \lambda_y = \lambda_z, \omega = \lambda c_{i,j,k} = \frac{x^2 c_{i,j,k}}{h_x}. \text{ Note that } \omega \text{ is a grid function but independent of time. Then the above scheme becomes}
\begin{equation}
\frac{1}{\omega} \frac{\delta_t^2}{1 + \frac{1}{12} \delta_t^2} u_{i,j,k}^n = \left[ \frac{\delta_x^2}{1 + \frac{1}{12} \delta_x^2} + \frac{\delta_y^2}{1 + \frac{1}{12} \delta_y^2} + \frac{\delta_z^2}{1 + \frac{1}{12} \delta_z^2} \right] u_{i,j,k}^n.
\end{equation}
If we let
\begin{equation}
\mathcal{L} = \frac{\delta_x^2}{1 + \frac{1}{12} \delta_x^2} + \frac{\delta_y^2}{1 + \frac{1}{12} \delta_y^2} + \frac{\delta_z^2}{1 + \frac{1}{12} \delta_z^2}
= T_x + T_y + T_z,
\end{equation}
The scheme can be written as
\begin{equation}
\frac{1}{\omega} \frac{\delta_t^2}{1 + \frac{1}{12} \delta_t^2} u^n = \mathcal{L} u^n,
\end{equation}
where } u^n \text{ is the numerical solution at time level } t_n:
\begin{equation}
u^n = (u_{i,j,k}^n)_{N \times N \times N}.
\end{equation}
Here we assume that } N_x = N_y = N_z = N.
To prove the stability result, we first state the following lemma, which can be found in standard functional analysis textbook such as [30].

\textbf{Lemma 4.1.} Let } f(s) \text{ be a real-valued measurable function, } A \text{ be a self-adjoint operator. Then }
\sigma(f(A)) \subseteq \overline{f(\sigma(A))},
\text{ where } \sigma(A) \text{ is the spectrum of } A, \overline{f(\sigma(A))} \text{ the closure of the set } f(\sigma(A)). \text{ In addition, if } f \text{ is continuous and } \sigma(f(A)) = f(\sigma(A)), \text{ then }
\sigma(f(A)) = f(\sigma(A)).

\textbf{Lemma 4.2.} If } T_x, T_y \text{ and } T_z \text{ are self-adjoint operators in } L^2, \text{ so is the sum }
\mathcal{L} = T_x + T_y + T_z.

\textbf{Proof} \text{ Let }
\begin{equation}
f(s) = \frac{s}{1 + \frac{1}{12} s},
\end{equation}
then } T_x = f(\delta_x^2). \text{ Note that we can write}
\begin{equation}
f(s) = s \cdot \left(1 + \frac{1}{12} s\right)^{-1} = \left(1 + \frac{1}{12} s\right)^{-1} \cdot s,
\end{equation}
which means
\begin{equation}
\delta_x^2 \cdot \left(1 + \frac{1}{12} \delta_x^2\right)^{-1} = f(\delta_x^2) = \left(1 + \frac{1}{12} \delta_x^2\right)^{-1} \cdot \delta_x^2.
\end{equation}
Thus, if we can prove that both $\delta^2_x$ and $(1 + \frac{1}{12} \delta^2_x)^{-1}$ are self-adjoint, then $T_x = f(\delta_x)$, as a product of two commutative self-adjoint operators, is also self-adjoint. It is clear that both $\delta^2_x$ and $1 + \frac{1}{12} \delta^2_x$ are self-adjoint, then $(1 + \frac{1}{12} \delta^2_x)^{-1}$, as an inverse of a self-adjoint operator, is self-adjoint. The proofs for $T_y$ and $T_z$ are similar. Finally $L$ is self-adjoint since it is a sum of three self-adjoint operators. \[\square\]

The spectrum of $\delta^2_x$ with the homogeneous Dirichlet boundary condition is given by

$$\sigma(\delta^2_x) = \left\{ -4 \sin^2 \left( \frac{j \pi}{2(N+1)} \right) \right\} \subset (-4, a(h)],$$

where $N$ is the number of grid points in the $x$-direction, $j = 1, \cdots, N$, $a(h) = -4 \sin^2 \left( \frac{\pi h}{2(N+1)} \right)$. Then lemma 4.1 asserts that the spectrum of $T_x$ is given by

$$\sigma(T_x) = f(\sigma(\delta^2_x)) = \left\{ f \left( -4 \sin^2 \left( \frac{j \pi}{2(N+1)} \right) \right) \right\},$$

where $f(s) = \frac{s}{1 + \frac{s}{12}}$ and $j = 1, \cdots, N$. Since $f(s)$ is increasing when $s > -12$, we have

$$\sigma(T_x) \subset (-6, f(a(h))].$$

We have $f(a(h)) < 0$ since $-12 < a(h) < 0$ when $h$ is small enough. Note that the operators $T_x$, $T_y$, and $T_z$ are actually hermitian matrices, and the fact that the operator $L$ corresponds to a homogeneous Dirichlet problem, then (for instance, see [14])

$$\sigma(L) \subset (-18, 3f(a(h))).$$

Thus, we obtained the coercive condition, which is a direct result of its spectrum estimate,

$$m = -3f(a(h)) \leq -L \leq 18 = M. \quad (38)$$

Remark Note that $h$ is the grid size and should be small enough, then

$$a(h) = -4 \sin^2 \left( \frac{\pi h}{2(N+1)} \right) \approx -\pi^2 h^2$$

Now we state the main result on the stability of the new method in the following theorem.

**Theorem 4.3.** Assume that the solution of the acoustic wave equation Eq. (1) is sufficiently smooth, the new scheme given in Eq. (21) is stable if

$$\max_{1 \leq i,j,k \leq N} \nu_{i,j,k} \frac{\tau}{h} < \frac{1}{\sqrt{3}}.$$ 

**Proof** Here we follow the strategy of [2] to prove the stability. First, let’s denote the $L^2$ norm by $\| \cdot \|$, the inner product on $L^2$ by $\langle \cdot, \cdot \rangle$. 

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From (35), since $\delta_t^2$ commutes with $\mathcal{L}$, we have
\[
\frac{1}{\omega} \delta_t^2 u^n - \frac{1}{12} \mathcal{L} \delta_t^2 u^n = \mathcal{L} u^n.
\] (39)

Define $v^n = u^n - u^{n-1}$, then $\delta_t^2 u^n = v^{n+1} - v^n$, $v^{n+1} + v^n = u^{n+1} - u^{n-1}$. Taking inner product with $v^{n+1} + v^n$ on both sides of Eq. (39), noting that $\mathcal{L}$ is self-adjoint, we have
\[
\langle \frac{1}{\omega} (v^{n+1} - v^n), v^{n+1} + v^n \rangle - \frac{1}{12} \langle \mathcal{L} (v^{n+1} - v^n), v^{n+1} + v^n \rangle = \langle \mathcal{L} u^n, u^{n+1} - u^{n-1} \rangle.
\] (40)

Expanding the right-hand side of Eq. (40) gives
\[
\langle \mathcal{L} u^n, u^{n+1} - u^{n-1} \rangle
= \frac{1}{4} \left[ \langle \mathcal{L} v^n, v^n \rangle - \langle \mathcal{L} v^{n+1}, v^{n+1} \rangle - \langle \mathcal{L} (u^n + u^{n-1}), u^n + u^{n-1} \rangle + \langle \mathcal{L} (u^{n+1} + u^n), u^{n+1} + u^n \rangle \right].
\] (41)

Combining (40) and (41), noting that the cross terms in (40) eliminate since $\mathcal{L}$ is self-adjoint, we have
\[
\frac{1}{\omega} \langle v^n, v^n \rangle + \frac{1}{6} \langle \mathcal{L} v^n, v^n \rangle - \frac{1}{4} \langle \mathcal{L} (u^n + u^{n-1}), u^n + u^{n-1} \rangle
= \frac{1}{\omega} \langle v^{n+1}, v^{n+1} \rangle + \frac{1}{6} \langle \mathcal{L} v^{n+1}, v^{n+1} \rangle - \frac{1}{4} \langle \mathcal{L} (u^{n+1} + u^n), u^{n+1} + u^n \rangle.
\] (42)

If we define
\[
S_n = \frac{1}{\omega} \| v^n \|^2 + \frac{1}{6} \langle \mathcal{L} v^n, v^n \rangle - \frac{1}{4} \langle \mathcal{L} (u^n + u^{n-1}), u^n + u^{n-1} \rangle,
\]
then the above equality is exactly
\[S_n = S_{n+1}.
\]

By the coercivity of $-\mathcal{L}$, $m \leq -\mathcal{L} \leq M$, we have
\[
S_n \geq \frac{1}{\omega} \| v^n \|^2 - \frac{M}{6} \| v^n \|^2 + \frac{m}{4} \| u^n + u^{n-1} \|^2
\] (43)

and
\[
S_n \leq \frac{1}{\omega} \| v^n \|^2 - \frac{m}{6} \| v^n \|^2 + \frac{M}{4} \| u^n + u^{n-1} \|^2.
\] (44)

Thus, $S_n$ is equivalent to the energy given by
\[
\| v^n \|^2 + \| u^n + u^{n-1} \|^2
= \| u^n - u^{n-1} \|^2 + \| u^n + u^{n-1} \|^2
= 2 \| v^n \|^2 + 2 \| u^n \|^2
\]
if and only if
\[ \frac{1}{\omega} > \frac{M}{6}, \]
i.e.
\[ \max_{i,j,k} \nu_{i,j,k}^2 \frac{\tau^2}{h^2} < \frac{6}{M} = \frac{1}{3} \Rightarrow \max_{i,j,k} \nu_{i,j,k} \frac{\tau}{h} < \frac{1}{\sqrt{3}}. \]  
(45)
since \( M = 18 \) by Eq. (38).

Denoted by \( e_n \), the error at time \( t_n \), the above stability analysis shows that the energy of the error \( \|e^n\|^2 + \|e^{n-1}\|^2 \) conserves during the solving process, which means the scheme is conditionally stable, as long as the stability condition in Eq. (45) is satisfied.

For comparison, according to [22], the stability condition for 3-D problem using the standard second-order difference scheme is
\[ \max_{i,j,k} \nu_{i,j,k} \frac{\tau}{h} < \frac{1}{3}. \]
Moreover, the stability condition for the conventional fourth-order FD scheme (it is second-order in time) is
\[ \max_{i,j,k} \nu_{i,j,k} \frac{\tau}{h} < \frac{1}{2}. \]  
(46)

Apparently, the new method has better stability with a larger CFL number. Although in each time step a sequence of tridiagonal linear systems need to be solved to march the numerical solution, the high-order ADI method outperforms other existing methods in terms of the overall efficiency. One can also see that estimated upper bound of \( \frac{\tau}{h} \) is sharp, as demonstrated in the second numerical example.

5. Numerical examples

In this section three numerical examples are solved by the new method to demonstrate the efficiency and accuracy. The exact solutions of the first and second examples are available, so the numerical errors can be calculated to validate the order of convergence and stability condition of the new method. In the third example, the acoustic wave equation with the Ricker’s wavelet source is solved to demonstrate that the new method is effective in suppressing numerical dispersion and efficient and accurate in simulating wave propagation in heterogeneous media. It is worthwhile to mention that in the following numerical examples, all numerical errors are calculated using maximal norm, although the stability and error analysis were conducted in \( L^2 \) norm. Since the maximal and \( L^2 \) norms are equivalent, all conclusions confirmed in maximal norm hold in \( L^2 \) norm.
5.1. Example 1

In this example, the acoustic wave equation is defined on a rectangular domain \( \Omega = [0, \pi] \times [0, \pi] \times [0, \pi] \), and \( t \in [0, T] \),

\[
u_{tt} = \left[ 1 + \left( \frac{x}{\pi} \right)^2 + \left( \frac{y}{\pi} \right)^2 + \left( \frac{z}{\pi} \right)^2 \right] \Delta u + s(x, y, z, t), \quad (x, y, z, t) \in \Omega \times [0, T],
\]

\[
u(x, y, z, 0) = \sin(x) \sin(y) \sin(z), \quad (x, y, z) \in \Omega,
\]

\[
u_t(x, y, z, 0) = 0, \quad (x, y, z) \in \Omega,
\]

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

with the source function given by

\[
s(x, y, z, t) = \left[ 3 + 2 \left( \frac{x}{\pi} \right)^2 + 2 \left( \frac{y}{\pi} \right)^2 + 2 \left( \frac{z}{\pi} \right)^2 \right] \cos(t) \sin(x) \sin(y) \sin(z)
\]

and the analytical solution given by

\[
u(x, y, z, t) = \cos(t) \sin(x) \sin(y) \sin(z).
\]

It is noted that this problem has zero boundary condition, which is chosen to simplify programming. A more general example with non-zero boundary condition will be solved in the next example. In all numerical simulations, the domain \( \Omega \) is divided into an \( N_x \times N_y \times N_z \) grid. The time domain is uniformly divided into \( N_t \) subdomains. To simplify the discussion, uniform grid size \( h \) is used in \( x, y \) and \( z \) directions. To validate the fourth-order convergence in space, we fixed \( \tau = 0.0025 \) so the temporal truncation error is negligible. The errors in maximal norm obtained by using different \( h \) are included in Table 1, which clearly show that the new method is fourth-order accurate in space. Here the numerical order is calculated using the following formula

\[
\text{Conv. Order} = \frac{\log(E(h_1)/E(h_2))}{\log(h_1/h_2)},
\]

where the numerical error \( E(h) \) is defined by

\[
E(h) = \max_{1 \leq i, j, k \leq N_x \times N_y \times N_z} |u(x_i, y_j, z_k, T) - u_{i,j,k}^{N_t}|,
\]

Here \( u(x_i, y_j, z_k, T) \) is the exact solution of \( u \) at the grid point \( (x_i, y_j, z_k) \) and time \( t = T \), and \( u_{i,j,k}^{N_t} \) is the numerical solution at the same grid point and time \( t = T \) that is computed using stepsize \( h \). The numerical error \( E(h, \tau) \) included in Tables 2-5 is defined similarly, with the only difference that the time stepsize \( \tau \) is changed when \( h \) is changed.

It is clear that the errors are reduced roughly by a factor 16 when \( h \) is reduced by a factor 2. We notice that the convergence order is slightly lower than fourth-order, due to the round-off errors. To show that the method is
fourth-order accurate in time, $h$ and $\tau$ are simultaneously reduced by the same factor to ensure that the CFL condition is satisfied, since using very small $h$ to verify the order in time will violate the stability condition. Therefore, we verify the order of convergence in time through the following argument. Suppose the numerical scheme is $p$th-order accurate in time and fourth-order in space, with $p < 4$, halving $h$ and $\tau$ several times, the truncation error in time will become the dominating error, thus the total error will be reduced by a factor of $2^p < 16$ when $h$ and $\tau$ been halved. In the following numerical test cases, we start from $h = \pi/10$, $\tau = 1/16$ (the parameters are chosen to satisfy the stability condition) and each time we halve both $h$ and $\tau$. The result in Table 2 clearly indicates that the total error is reduced by a factor 16 (roughly) when $h$ and $\tau$ are halved, which confirmed that the convergence order in time is fourth-order. Furthermore, it is interesting that the convergence order is slightly higher than

4. One possible explanation is that the truncation errors are canceled during the computation. The new method is an implicit scheme, so the computational cost in each time step is higher than that of the explicit method, however, the overall computational efficiency has been greatly improved due to the high-order convergence and larger time step size $\tau$ being used.

5.2. Example 2

In the second example, we solve a more general acoustic wave equation defined on $[0, \pi] \times [0, \pi] \times [0, \pi] \times [0, T]$ with non-zero boundary conditions. The analytical solution for the following equation

\[ u_{tt} = \left( 1 + \sin^2 x + \sin^2 y + \sin^2 z \right) \left( u_{xx} + u_{yy} + u_{zz} \right) + s(x, y, z, t) \]

is given by

\[ u(x, y, z, t) = e^{-t} \cos(x) \cos(y) \cos(z), \]
where \( s(x, y, z, t) = (4 + 3(\sin^2 x + \sin^2 y + \sin^2 z))e^{-t} \cos(x) \cos(y) \cos(z) \). For this example, the boundary conditions are non-zero. For example, on the plane \( x = 0 \), the boundary condition is given by

\[
u(0, y, z, t) = e^{-t} \cos(y) \cos(z), \quad (y, z) \in [0, \pi] \times [0, \pi], \quad t > 0.
\]

To demonstrate the fourth-order convergence in space and time, we reduce \( \tau \) and \( h \) simultaneously by the same factor and record the numerical error in Table 3.

Table 3: Numerical errors in maximal norm for example 2 with various \( h \) and \( \tau \).

| \((h, \tau)\)     | \((\pi/16, 1/20)\) | \((\pi/32, 1/40)\) | \((\pi/64, 1/80)\) | \((\pi/128, 1/160)\) |
|------------------|---------------------|---------------------|---------------------|---------------------|
| \(E(h, \tau)\)   | 5.1391e-05          | 4.2849e-06          | 3.9569e-07          | 2.9088e-08          |
| \(E(h/2, \tau/2)\) | -11.9935            | 10.8289             | 13.6032             |
| Conv. Order      | -3.5842             | 3.4368              | 3.7659              |
| CPU time(s)      | 6.83                | 22.09               | 128.04              | 806.29              |

We then show that the estimated CFL constraint is sharp. According to the proof, the method is conditionally stable with the CFL condition \( \max_{i,j,k} \nu_{i,j,k} \frac{\tau}{h} < \frac{1}{\sqrt{3}} \). The maximum value of \( \nu \) is given by

\[
u_{\text{max}} = \max_{0 \leq x, y, z \leq \pi} (1 + \sin^2 x + \sin^2 y + \sin^2 z) = 2.
\]

Therefore, the following stability condition

\[
\frac{\tau}{h} < \frac{1}{2\sqrt{3}} \approx 0.288675134594813
\]

is required.

First we choose \( \tau \) and \( h \) such that \( \frac{\tau}{h} \) is slightly less than \( \frac{1}{2\sqrt{3}} \), so the stability condition given by Theorem 4.3 is satisfied. For all test cases in Table 4, we have

\[
\frac{\tau}{h} = \frac{9}{10\pi} \approx 0.286478897565412 < \frac{1}{2\sqrt{3}} \approx 0.288675134594813.
\]

The numerical results in Table 4 confirmed that the numerical method is stable when the stability condition is met. As can be seen, when \( \tau \) and \( h \) are reduced, the numerical error is also reduced, showing a convergence order between 3.25 and 4. The noticeable deviation from a perfect fourth order in convergence is possibly caused by the fact that \( \frac{\tau}{h} \) is very close to the CFL condition. Thus, the CFL condition might be slightly violated due to some random roundoff error, which then deteriorates the convergence order. Nevertheless, the numerical results in Table 4 clearly show that the method is stable when \( \frac{\tau}{h} < \frac{1}{2\sqrt{3}} \).
Table 4: Numerical errors in maximal norm for example 2 with $\frac{\tau}{h} < \frac{1}{2\sqrt{3}}$.

| $(h, \tau)$ | $(\pi/18, 1/20)$ | $(\pi/36, 1/40)$ | $(\pi/54, 1/60)$ | $(\pi/72, 1/80)$ |
|-------------|----------------|----------------|----------------|----------------|
| $E(h, \tau)$| 3.3689e-05     | 2.7867e-06     | 6.9049e-07     | 2.7001e-07     |
| $\frac{E(h_1, \tau_1)}{E(h_2, \tau_2)}$ | -               | 11.9935         | 4.0358         | 2.5573         |
| Conv. Order | -               | 3.5842          | 3.4410         | 3.2638         |

We then numerically validate that the estimated CFL condition is a necessary condition for stability. To this end, we choose $\tau$ and $h$ such that $\frac{\tau}{h}$ is slightly greater than $\frac{1}{2\sqrt{3}}$, thus, the stability condition given by Theorem 4.3 is slightly violated. As shown in Table 4, the ratio $\frac{\tau}{h} = \frac{10}{20\pi} \approx 0.302394 > \frac{1}{2\sqrt{3}}$.

The numerical results clearly show that the method is not stable, as the numerical solution is not convergent, when $\tau$ and $h$ are reduced. Instead, when $\tau$ and $h$ are reduced, the maximal error increases and goes to infinity. Here “×” in the table means that no convergence is obtained.

Table 5: Numerical errors in maximal norm for example 2 with $\frac{\tau}{h} > \frac{1}{2\sqrt{3}}$.

| $(h, \tau)$ | $(\pi/19, 1/20)$ | $(\pi/38, 1/40)$ | $(\pi/57, 1/60)$ | $(\pi/76, 1/80)$ |
|-------------|----------------|----------------|----------------|----------------|
| $E(h, \tau)$| 8.5884e-05     | 1.1864e-05     | 7.2660e-01     | 1.3165e+06     |
| $\frac{E(h_1, \tau_1)}{E(h_2, \tau_2)}$ | -               | 7.2387          | ×              | ×              |
| Conv. Order | -               | 2.8557          | ×              | ×              |

5.3. Example 3

To demonstrate the efficiency of the new method and show the effectiveness in suppressing numerical dispersion, we solve a realistic problem in which the seismic wave is generated by a Ricker wavelet source located at the centre of a three-dimensional domain $[0m, 1280m] \times [0m, 1280m] \times [0m, 800m]$. The velocity model is given by

$$
\nu(x, y, z) = 1200 + 400 \left( \frac{x}{x_{\text{max}}} \right)^2 + 100 \left( \frac{y}{y_{\text{max}}} \right)^2 + 800 \left( \frac{z}{z_{\text{max}}} \right)^2,
$$

where $x_{\text{max}} = 1280m$, $y_{\text{max}} = 1280m$ and $z_{\text{max}} = 800m$, respectively. Therefore, the maximal and minimal wave speeds over the domain are

$$
\nu_{\text{max}} = \max_{x,y,z} \nu(x, y, z) = 2500m/s
$$

and

$$
\nu_{\text{min}} = \min_{x,y,z} \nu(x, y, z) = 1200m/s,
$$
respectively. The Ricker wavelet source function is given by

\[ s(x, y, z, t) = \delta(x - x_0, y - y_0, z - z_0) \left[ 1 - 2\pi^2 f_p^2 (t - d_r)^2 \right] e^{-\pi^2 f_p^2 (t - d_r)^2}, \]

where \( f_p = 10 \text{Hz} \) is the dominant frequency, \( d_r = 0.5/f_p \) is the temporal delay to ensure zero initial conditions. The centre of the domain is located at \((x_0, y_0, z_0) = (640, 640, 400) \text{m} \). The space and time step sizes are chosen to satisfy the CFL condition. Moreover, the Nyquist sampling theorem states that the sampling frequency should be at least twice the highest frequency contained in the signal to avoid aliasing. As a rule of thumb, at least 10 grid points per wavelength are required in finite difference discretization. Simple calculation shows that the minimal wavelength is given by \( \nu_{\text{min}}/f_p = 120 \text{m} \), which sets the upper limit for \( h \) as \( h_{\text{max}} = 12 \text{m} \). On the other hand, the CFL condition indicates that

\[ \nu_{\text{max}} \frac{\tau}{h} < \frac{1}{\sqrt{3}} \Rightarrow \frac{\tau}{h} < \frac{1}{2500 \sqrt{3}} \]

For all numerical simulations of this example, the uniform grid \( h = 10 \text{m} \) and \( \tau = 0.001 \text{s} \) are used to ensure stability and avoid aliasing.

We plot the wavefield snapshots for central slices in \( x-, y- \) and \( z- \) directions at \( t = 0.2 \text{s}, 0.3 \text{s}, 0.4 \text{s} \) and \( t = 0.5 \text{s} \) in Figs. (1-3), respectively. Apparently the computed wave fronts accurately reflect the wave velocity. For example, in Fig. (1) the simulated wavefields accurately describe the wave propagation. The x-sections are the slices of the 3D wavefields at \( x = x_{\text{max}}/2 \). Since the wave velocity increases more rapidly in \( z \) direction than it does in \( y \) direction, we clearly see that the wavefront moves faster in \( z \) direction. Moreover, the wave velocity is a monotone increasing function of \( y \) and \( z \), the wavefronts moves faster at the right side than at the left side, and moves faster in the lower side than in the upper side of the domain.

Fig. (2) shows the snapshots of the wavefields when \( y = y_{\text{max}}/2 \) is fixed. Again, the velocity is a function of two variables \( x \) and \( z \), and the velocity increases faster in \( z \). Clearly the wavefronts moves faster in \( z \) direction. While in the same direction, the wave propagates faster when the variable is at the large side. For example, the wavefront hits the right boundary before it hits the left boundary.

Finally, in Fig. (3) the wavefields slices demonstrate similar wave propagations, which is also expected from theoretical analysis.

In terms of the numerical dispersion, significant improvement can be observed as well. As shown in these figures, there is no visible numerical dispersions, which indicated that the new numerical algorithm is accurate and effective in suppressing numerical dispersion.

6. Conclusion and future work

A compact fourth-order ADI FD scheme has been developed to solve the three-dimensional acoustic wave equation in heterogeneous media. The new
method is efficiently implemented using the ADI technique, which splits the original three-dimensional problem into a series of one-dimensional problems. The fourth-order convergence in time and space has been validated by two numerical examples for which the exact solutions are available. A more realistic problem has been solved to demonstrate that the new method is robust, accurate and efficient in seismic wave propagation simulation. Moreover, the conditional stability of the new method has been rigidly proved for the variable coefficient case. It has been shown that the new method has a larger CFL number than other conventional finite difference methods. Several numerical tests have been performed to verify that the estimated upper bounds of CFL is sharp. It is expected that this new method will find extensive applications in numerical seismic modelling on complex geological models, and seismic inversion problems. In the future we plan to take more realistic boundary conditions for instance the absorbing boundary condition, or the perfectly matched layer boundary condition into consideration.
Figure 2: Snapshots of y-section of wavefields computed by the new fourth-order compact method at (a) t = 0.2 seconds; (b) t = 0.3 seconds; (c) t = 0.4 seconds; (d) t = 0.5 seconds.

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Figure 3: Snapshots of z-section of wavefields computed by the new fourth-order compact method at (a) $t = 0.2$ seconds; (b) $t = 0.3$ seconds; (c) $t = 0.4$ seconds; (d) $t = 0.5$ seconds.

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Appendix A. Proof of Theorem 3.1

Proof:
First, let’s expand $\delta_t^2 u_{i,j,k}^n$ by Taylor series at time $t_n$ and the grid point $(x_i, y_j, z_k)$ as

$$
\delta_t^2 u_{i,j,k}^n \approx u_{i,j,k}^{n+1} - 2 u_{i,j,k}^n + u_{i,j,k}^{n-1}
$$

$$
= \tau^2 \frac{\partial^2 u_{i,j,k}^n}{\partial t^2} + \frac{\tau^4}{12} \frac{\partial^4 u_{i,j,k}^n}{\partial t^4} + \frac{\tau^6}{360} \frac{\partial^6 u_{i,j,k}^n}{\partial t^6} + \tau_n^* \frac{\partial^6 v(x_i, y_j, z_k, t_n)}{\partial y^6},
$$

(A.1)

where $\tau_n^* \in (t_{n-1}, t_{n+1})$.

By Padé approximation, if $v(x, y, z, t)$ is a sufficiently smooth function, we have

$$
\frac{\delta_y^2}{1 + \frac{1}{12} \delta_y^2} \nu_{i,j,k}^n = \delta_y^2 \left( 1 - \frac{\delta_y^2}{12} \right) v_{i,j,k}^n + \frac{h_y^6}{144} \frac{\partial^6 v(x_i, y_j^*, z_k, t_n)}{\partial y^6},
$$

(A.2)

where $y_j^* \in (y_{j-1}, y_{j+1})$.  

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On the other hand,

\[ \delta_y^2 \left( 1 - \frac{1}{12} \delta_y^2 \right) v_{i,j,k}^n = \left( \delta_y^2 - \frac{1}{12} \delta_y^2 \right) v_{i,j,k}^n \]

\[ = -v_{i,j+2,k}^n + 16v_{i,j+1,k}^n - 30v_{i,j,k}^n + 16v_{i,j-1,k}^n - v_{i,j-2,k}^n \]

\[ = h_y^2 \frac{\partial^2 v}{\partial y^2} |_{i,j,k} - \frac{2}{15} h_y^6 \frac{\partial^6 v(x, y_i^*, z_k, t_n)}{\partial y^6}, \quad (A.3) \]

where \( y_i^* \in (y_{j-1}, y_{j+1}) \).

Letting \( v_{i,j,k}^n = \delta^2 u_{i,j,k}^n \) and combining Eq. (A.4) with Eq. (A.3) lead to

\[ \frac{\delta_y^2}{1 + \frac{1}{12} \delta_y^2} \delta^2 u_{i,j,k}^n = h_y^2 \frac{\partial^2 u}{\partial y^2} |_{i,j,k} - \frac{2}{15} h_y^6 \frac{\partial^6 v(x, y_i^*, z_k, t_n)}{\partial y^6} + \frac{h_y^6}{144} \frac{\partial^6 v(x, y_i^*, z_k, t_n)}{\partial y^6}. \quad (A.4) \]

Using Eq. (A.1), it then follows that

\[ \lambda_y c_{i,j,k} \frac{\delta^2}{1 + \frac{1}{12} \delta_y^2} \delta^2 u_{i,j,k}^n \]

\[ = \lambda_y c_{i,j,k} \frac{\delta^2}{1 + \frac{1}{12} \delta_y^2} \left[ \frac{\tau^2}{12} \delta^2 v_{i,j,k}^n + \frac{\tau^4}{12} \delta^4 v_{i,j,k}^n + \frac{\tau^6}{360} \delta^6 v_{i,j,k}^n \right] \]

\[ = \tau^4 \left[ c_{i,j,k} \frac{\partial^4 u}{\partial y^4} |_{i,j,k} \right] + O(h_y^6) + O(\tau^6) + O(\tau^4 h_y^4). \quad (A.5) \]

Further, let \( w(x, y, z, t) = c(x, y, z) \frac{\partial^4 u}{\partial y^4} \), then the first term on the right-hand side of Eq. (18) can be written as

\[ \frac{\lambda_x}{144} c_{i,j,k} \frac{\delta^2}{1 + \frac{1}{12} \delta_x^2} \lambda_y c_{i,j,k} \frac{\delta^2}{1 + \frac{1}{12} \delta_y^2} \delta^2 u_{i,j,k}^n \]

\[ = \tau^4 \frac{c_{i,j,k}}{144} \left[ \frac{\tau^2}{12} \delta^2 v_{i,j,k}^n \right] \frac{w_{i,j,k}^n}{h_x} + O(h_y^6) + O(\tau^6) + O(\tau^4 h_y^4). \quad (A.6) \]

Expanding \( \delta^2 v_{i,j,k}^n \) we obtain

\[ \delta^2 \left( 1 - \frac{1}{12} \delta_y^2 \right) w_{i,j,k}^n \]

\[ = \frac{1}{12} \left[ w_{i-2,j,k}^n + 16w_{i-1,j,k}^n - 30w_{i,j,k}^n + 16w_{i+1,j,k}^n - w_{i+2,j,k}^n \right]. \quad (A.7) \]

Using Taylor series expansion, we can simplify it to

\[ \delta^2 v_{i,j,k}^n = \frac{2h_x^6}{15} \frac{\partial^6 w(x_i^*, y_j^*, z_k, t_n)}{\partial x^6}, \quad (A.8) \]
where \(x_i^* \in (x_{i-1}, x_{i+1})\).

Inserting Eq. (A.8) into Eq. (A.6) leads to

\[
\frac{\lambda_x}{144} c_{i,j,k} \frac{\delta^2 x}{1 + \frac{\delta^2 t}{12}} \frac{\delta^2 y}{\delta z^2} = \tau^4 \frac{c_{i,j,k}}{144} \left[ \tau^4 \left( \frac{\partial^2 w}{\partial x^2} \right)_{i,j,k} \right] + O(\tau^6) + O(h_y^6) + O(\tau^6 h_y^6)
\]

Similarly, we can derive the error estimations of other terms in Eq. (18) as follows:

\[
\frac{\lambda_y}{144} c_{i,j,k} \frac{\delta^2 y}{1 + \frac{\delta^2 t}{12}} \frac{\delta^2 z}{\delta x^2} = \tau^4 \frac{c_{i,j,k}}{144} \left[ \tau^4 \left( \frac{\partial^2 w}{\partial y^2} \right)_{i,j,k} \right] + O(\tau^6) + O(h_z^6)
\]

where

\[
\frac{\partial^2 w}{\partial x^2} = \frac{\partial^2 c}{\partial x^2} \frac{\partial^4 u}{\partial x^2 \partial t^2} + 2 \frac{\partial c}{\partial x} \frac{\partial^5 u}{\partial x \partial y \partial z \partial t^2} + c(x, y, z) \frac{\partial^6 u}{\partial y^2 \partial z^2 \partial t^2},
\]

\[
\frac{\lambda_x}{144} c_{i,j,k} \frac{\delta^2 z}{1 + \frac{\delta^2 t}{12}} \frac{\delta^2 y}{\delta x^2} = \tau^4 \frac{c_{i,j,k}}{144} \left[ \tau^4 \left( \frac{\partial^2 w}{\partial x \partial z} \right)_{i,j,k} \right] + O(\tau^6) + O(h_z^6)
\]

Similarly, we can derive the error estimations of other terms in Eq. (13) as follows:

\[
\frac{\lambda_y}{144} c_{i,j,k} \frac{\delta^2 y}{1 + \frac{\delta^2 t}{12}} \frac{\delta^2 z}{\delta x^2} = \tau^4 \frac{c_{i,j,k}}{144} \left[ \tau^4 \left( \frac{\partial^2 w}{\partial y \partial z} \right)_{i,j,k} \right] + O(\tau^6) + O(h_y^6)
\]

where

\[
\frac{\partial^2 w}{\partial x \partial z} = \frac{\partial^2 c}{\partial x \partial z} \frac{\partial^4 u}{\partial x \partial z \partial t^2} + 2 \frac{\partial c}{\partial x} \frac{\partial^5 u}{\partial x \partial z \partial t^2} + c(x, y, z) \frac{\partial^6 u}{\partial x \partial z \partial t^2},
\]

\[
\frac{\lambda_z}{144} c_{i,j,k} \frac{\delta^2 x}{1 + \frac{\delta^2 t}{12}} \frac{\delta^2 y}{\delta z^2} = \tau^4 \frac{c_{i,j,k}}{144} \left[ \tau^4 \left( \frac{\partial^2 w}{\partial z^2} \right)_{i,j,k} \right] + O(\tau^6) + O(h_y^6)
\]

where

\[
\frac{\lambda_z}{144} c_{i,j,k} \frac{\delta^2 z}{1 + \frac{\delta^2 t}{12}} \frac{\delta^2 y}{\delta x^2} = \tau^4 \frac{c_{i,j,k}}{144} \left[ \tau^4 \left( \frac{\partial^2 w}{\partial z^2 \partial t^2} \right)_{i,j,k} \right] + O(\tau^6) + O(h_y^6)
\]

and

\[
\frac{\lambda_z}{1728} c_{i,j,k} \frac{\delta^2 z}{1 + \frac{\delta^2 t}{12}} \frac{\delta^2 y}{\delta x^2} = \tau^8 \frac{c_{i,j,k}}{1728} \left[ \tau^8 \left( \frac{\partial^2 w}{\partial y^2} \right)_{i,j,k} \right] + O(\tau^6) + O(h_y^6),
\]

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where $\frac{\partial^2 \bar{w}}{\partial y^2}$ is defined in Eq. (A.12). Therefore, the factoring error $ERR$ in Eq. (18) is given by

$$ERR = \bar{M}_t \tau^6 + \bar{M}_x h_x^6 + \bar{M}_y h_y^6 + \bar{M}_z h_z^6,$$

provided that the following functions

$$c(x, y, z), \frac{\partial c(x, y, z)}{\partial x^{m_1} \partial y^{m_2} \partial z^{m_3}}, \frac{\partial^2 c(x, y, z)}{\partial x^{n_1} \partial y^{n_2} \partial z^{n_3}}$$

are bounded in $\Omega$, where the non-negative integers satisfying $m_1 + m_2 + m_3 = 1$ and $n_1 + n_2 + n_3 = 2$. Moreover, the solution $u(x, y, z, t)$ and its derivatives $\frac{\partial^k u(x, y, z, t)}{\partial x^{k_1} \partial y^{k_2} \partial z^{k_3} \partial t^{k_4}}$ are bounded in $\Omega \times [0, T]$, where the non-negative integers satisfy $k_1 + k_2 + k_3 + k_4 = 6$. $\bar{M}_t$, $\bar{M}_x$, $\bar{M}_y$ and $\bar{M}_z$ are positive constants depending on the functions listed above.