



Research article

An efficient GL-ADI general finite difference method for three dimensional nonlocal diffusion equations with anisotropic diffusion coefficients

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Abstract: This paper is concerned with an alternating direction implicit (ADI) general finite difference method (GFDM) for solving three-dimensional nonlocal diffusion equations with anisotropic diffusion coefficients. The Grünwald-Letnikov (GL) approximation is adopted to discretize the Caputo fractional derivatives on uniform grids. This spatial direction is handled by using the general difference method. A fully discrete GL-ADI general difference scheme is strictly constructed. The existence, uniqueness, stability, and convergence of numerical solution are proved. In addition, numerical experiments are carried out to confirm the validity of the theoretical analysis.

Keywords: nonlocal diffusion equation; ADI method; Grünwald-Letnikov scheme; finite difference method; stability and convergence

1. Introduction

As an important subclass of partial differential equations, nonlocal differential equations have significant application in numerous fields such as physics, biology, engineering, environmental science, and finance, see [1–5]. The three-dimensional nonlocal diffusion equations with anisotropic diffusion coefficients studied in this paper are as follows:

$$D_t^\alpha u = \nabla \cdot (\kappa(x, y, z) \nabla u) + \mu u + f(x, y, z, t), \quad (x, y, z) \in \Omega, \quad 0 < t \leq T, \quad (1.1)$$

with boundary and initial conditions

$$u(x, y, z, t) = 0, \quad (x, y, z) \in \partial\Omega, \quad 0 < t \leq T, \quad (1.2)$$

$$u(x, y, z, t) = u_0(x, y, z), \quad (x, y, z) \in \Omega, \quad (1.3)$$

where $\Omega = (0, L_1) \times (0, L_2) \times (0, L_3)$, μ is a positive constant, and

$$\kappa(x, y, z) = \begin{pmatrix} \kappa_1(x) & 0 & 0 \\ 0 & \kappa_2(y) & 0 \\ 0 & 0 & \kappa_3(z) \end{pmatrix}.$$

The coefficient functions satisfy $\kappa_1(x) \in C^2([0, L_1])$, $\kappa_2(y) \in C^2([0, L_2])$, and $\kappa_3(z) \in C^2([0, L_3])$, with $\kappa_1(x) > 0$, $\kappa_2(y) > 0$, and $\kappa_3(z) > 0$ for all x, y, z , and $f \in C([0, T]; L^2(\Omega))$. $D_t^\alpha u$ is defined by

$$D_t^\alpha u(x, y, z, t) = \frac{1}{\Gamma(1-\alpha)} \int_{s=0}^t (t-s)^{-\alpha} \partial_s u(x, y, z, s) ds, \quad 0 < \alpha < 1. \quad (1.4)$$

Equations (1.1)–(1.3) find extensive applications across a broad spectrum of research fields, including heat conduction processes in inhomogeneous media [6, 7]. The governing Eq (1.1) describes a physically rich class of transport phenomena. The fractional derivative $D_t^\alpha u$ models subdiffusion with memory effects, which is commonly observed in porous media, biological tissues, and disordered systems [8]. The reaction term μu with $\mu > 0$ represents linear decay or absorption processes, modeling phenomena such as cell death, drug degradation, or nutrient consumption. The external source f accounts for external inputs such as drug injection or nutrient supply. The anisotropic tensor $\text{diag}(\kappa_1(x), \kappa_2(y), \kappa_3(z))$ characterizes diffusion rates along the x, y , and z directions. This specific functional form arises from an essential feature of layered materials, composites, and crystalline structures [9], where material properties vary directionally with spatial coordinates due to inherent structural layering or aligned microstructures. Specifically, for layered physical media, the diffusion behavior along each coordinate axis only depends on the corresponding spatial coordinate, without coupling effects across different directions. This physical property motivates the choice of the component-separable diffusion tensor in this work, which can accurately characterize the diffusion and transport features inside layered materials [10–12]. Equations (1.1)–(1.3) provide a unified mathematical framework for describing anomalous transport in complex biological and physical systems.

Over the past several decades, researchers have devoted sustained efforts to investigating nonlocal equations, yielding a rich body of theoretical and numerical results [13–15], with the associated regularity theory having achieved considerable maturity [16].

For nonlocal diffusion equations, a broad range of numerical approaches have been established, which include finite difference methods [17–21], finite volume methods [22, 23], collocation methods [24], spectral methods [25], and finite element methods [26]. For multi-dimensional problems, the ADI scheme has emerged as a widely used numerical approach, primarily on account of its ability to mitigate computational complexity and reduce computational cost [27–30].

Although substantial progress has been made in numerical methods for fractional diffusion equations [17–20, 29, 30], existing three-dimensional ADI schemes suffer from several notable limitations. First, the majority of these methods are restricted to constant diffusion coefficients [25, 28], which significantly limits their applicability to real-world problems involving heterogeneous or anisotropic materials. Second, many prior approaches deliver only low temporal convergence orders [31], particularly in the presence of the initial weak singularity that is characteristic of fractional diffusion equations. Third, rigorous theoretical analysis, including stability and convergence proofs, for variable-coefficient three-dimensional problems, is largely absent in [29, 32]. Fourth, the combination of anisotropic diffusion tensors with ADI splitting in the three-dimensional setting has received very

limited attention, with most studies focusing on isotropic or one-dimensional cases [27, 30]. Furthermore, existing GL-ADI schemes in the literature have primarily focused on two-dimensional problems [33, 34]; the extension to three-dimensional problems with spatially varying anisotropic coefficients has not been previously addressed. To the best of our knowledge, this is the first work to develop a fully discrete GL-ADI GFDM for three-dimensional nonlocal diffusion equations with anisotropic coefficients. In contrast, the present work addresses these gaps through the following key improvements. The GL-ADI scheme accommodates spatially varying anisotropic diffusion coefficients $\kappa_1(x)$, $\kappa_2(y)$, and $\kappa_3(z)$, enabling accurate modeling of heterogeneous materials. We provide rigorous proofs of existence, uniqueness, stability, and convergence for the fully discrete scheme, with sharp error estimates demonstrating local convergence order $O(\tau^{\min\{2\alpha, 1\}})$ and global order $O(\tau^\alpha)$. The ADI factorization reduces the three-dimensional problem to a sequence of one-dimensional tridiagonal solves, substantially reducing computational cost while maintaining provable accuracy.

The key contributions of this paper can be summarized as follows.

- We construct a fully discrete GL-ADI GFDM for three-dimensional nonlocal diffusion equations with anisotropic diffusion coefficients, which reduces the problem to a sequence of one-dimensional solves and significantly lowers the computational cost.
- We rigorously prove the existence, uniqueness, stability, and convergence of the proposed scheme, with a sharp error estimate demonstrating a local temporal convergence order of $O(\tau^{\min\{2\alpha, 1\}})$ and a global temporal convergence order of $O(\tau^\alpha)$.

The remainder of this paper is organized as follows. Section 2 details the fundamental definitions, symbols, and lemmas, which serve as the theoretical basis for the subsequent derivation and theoretical analysis of the difference schemes. Section 3 presents the discretization approach and successfully constructs the GL-ADI GFDM. Section 4 performs a rigorous theoretical analysis on the stability and convergence of the proposed scheme. Section 5 verifies the accuracy of the GL-ADI GFDM and the reliability of the theoretical conclusions through numerical experiments. Finally, Section 6 summarizes the key research findings and main contributions of this work.

In this article, the symbol C represents a general constant, which may take different values at different positions, but is always independent of the grid parameters.

2. Preliminary notations and lemmas

This section begins with relevant notations and fundamental lemmas. Let M_1 , M_2 , M_3 , and N denote positive integers. For solving the problem via the GL-ADI GFDM, the solution domain $\Omega \times (0, T]$ is discretized into a grid, where h_1 , h_2 , and h_3 represent the step sizes in the x , y , and z directions, respectively, and τ denotes the time step. The interval $[0, L_1]$ is divided into M_1 equal subintervals, yielding a step size of $h_1 = L_1/M_1$, with node coordinates satisfying $x_j = jh_1$, $j = 0, 1, \dots, M_1$. The interval $[0, L_2]$ is partitioned into M_2 equal subintervals, where the step size is $h_2 = L_2/M_2$ and the node coordinates are given by $y_k = kh_2$, $k = 0, 1, \dots, M_2$. Similarly, the interval $[0, L_3]$ is divided into M_3 equal subintervals with a step size of $h_3 = L_3/M_3$, and the node coordinates satisfy $z_s = sh_3$, $s = 0, 1, \dots, M_3$. The time interval $(0, T]$ is split into N equal subintervals with a time step of $\tau = T/N$, and the time nodes are determined as $t_n = n\tau$, $n = 0, 1, \dots, N$.

Set

$$\bar{\Omega}_h = \{(x_j, y_k, z_s) | 0 \leq j \leq M_1, 0 \leq k \leq M_2, 0 \leq s \leq M_3\}, \quad \Omega_\tau = \{t_n | 0 \leq n \leq N\},$$

and $\Omega_{h\tau} = \Omega_h \times \Omega_\tau$, $\Omega_h = \bar{\Omega}_h \cap \Omega$, and $\partial\Omega_h = \bar{\Omega}_h \cap \partial\Omega$.

Set $x_{j+\frac{1}{2}} = \frac{1}{2}(x_j + x_{j+1})$, $y_{k+\frac{1}{2}} = \frac{1}{2}(y_k + y_{k+1})$, $z_{s+\frac{1}{2}} = \frac{1}{2}(z_s + z_{s+1})$, and $t_{n+\frac{1}{2}} = \frac{1}{2}(t_n + t_{n+1})$. With respect to any grid function $\{\omega_{jks}^n | 0 \leq j \leq M_1, 0 \leq k \leq M_2, 0 \leq s \leq M_3, 0 \leq n \leq N\}$ defined on $\Omega_{h\tau}$, the set of the interior grid indices $\epsilon = \{(j, k, s) | (x_j, y_k, z_s) \in \partial\Omega\}$, we introduce the corresponding formulation

$$\begin{aligned} \delta_x \omega_{j-\frac{1}{2},k,s} &= \frac{1}{h_1} (\omega_{j,k,s} - \omega_{j-1,k,s}), \quad \delta_y \omega_{j,k-\frac{1}{2},s} = \frac{1}{h_2} (\omega_{j,k,s} - \omega_{j,k-1,s}), \quad \delta_z \omega_{j,k,s-\frac{1}{2}} = \frac{1}{h_3} (\omega_{j,k,s} - \omega_{j,k,s-1}), \\ \delta_x^2 \omega_{j-\frac{1}{2},k,s} &= \frac{1}{h_1} (\delta_x \omega_{j+\frac{1}{2},k,s} - \delta_x \omega_{j-\frac{1}{2},k,s}), \quad \delta_y^2 \omega_{j,k-\frac{1}{2},s} = \frac{1}{h_2} (\delta_y \omega_{j,k+\frac{1}{2},s} - \delta_y \omega_{j,k-\frac{1}{2},s}), \\ \delta_z^2 \omega_{j,k,s-\frac{1}{2}} &= \frac{1}{h_3} (\delta_z \omega_{j,k,s+\frac{1}{2}} - \delta_z \omega_{j,k,s-\frac{1}{2}}), \quad \delta_x \delta_y \omega_{j-\frac{1}{2},k-\frac{1}{2},s} = \frac{1}{h_1} (\delta_y \omega_{j,k-\frac{1}{2},s} - \delta_y \omega_{j-1,k-\frac{1}{2},s}), \\ \delta_y \delta_z \omega_{j,k-\frac{1}{2},s-\frac{1}{2}} &= \frac{1}{h_2} (\delta_z \omega_{j,k,s-\frac{1}{2}} - \delta_z \omega_{j,k-1,s-\frac{1}{2}}), \quad \delta_x \delta_z \omega_{j-\frac{1}{2},k,s-\frac{1}{2}} = \frac{1}{h_1} (\delta_z \omega_{j,k,s-\frac{1}{2}} - \delta_z \omega_{j-1,k,s-\frac{1}{2}}), \\ \delta_x \delta_y \delta_z \omega_{j-\frac{1}{2},k-\frac{1}{2},s-\frac{1}{2}} &= \frac{1}{h_1} (\delta_y \delta_z \omega_{j,k-\frac{1}{2},s-\frac{1}{2}} - \delta_y \delta_z \omega_{j-1,k-\frac{1}{2},s-\frac{1}{2}}), \end{aligned}$$

$$\begin{aligned} \mathcal{A}_x \omega_{j,k,s}^n &= \frac{1}{h_1} \left((\kappa_x)_{j+\frac{1}{2}} \frac{\omega_{j+1,k,s}^n - \omega_{j,k,s}^n}{h_1} - (\kappa_x)_{j-\frac{1}{2}} \frac{\omega_{j,k,s}^n - \omega_{j-1,k,s}^n}{h_1} \right), \\ \mathcal{A}_y \omega_{j,k,s}^n &= \frac{1}{h_2} \left((\kappa_y)_{k+\frac{1}{2}} \frac{\omega_{j,k+1,s}^n - \omega_{j,k,s}^n}{h_2} - (\kappa_y)_{k-\frac{1}{2}} \frac{\omega_{j,k,s}^n - \omega_{j,k-1,s}^n}{h_2} \right), \\ \mathcal{A}_z \omega_{j,k,s}^n &= \frac{1}{h_3} \left((\kappa_z)_{s+\frac{1}{2}} \frac{\omega_{j,k,s+1}^n - \omega_{j,k,s}^n}{h_3} - (\kappa_z)_{s-\frac{1}{2}} \frac{\omega_{j,k,s}^n - \omega_{j,k,s-1}^n}{h_3} \right), \end{aligned}$$

where $(\kappa_x)_{j+\frac{1}{2}} = \kappa_1(x_{j+\frac{1}{2}})$, $(\kappa_y)_{k+\frac{1}{2}} = \kappa_2(y_{k+\frac{1}{2}})$, and $(\kappa_z)_{s+\frac{1}{2}} = \kappa_3(z_{s+\frac{1}{2}})$. Define the discrete space as follows:

$$\mathcal{W}_h := \{w | w = w_{j,k,s}, (x_j, y_k, z_s) \in \bar{\Omega}_h\},$$

$$\mathring{\mathcal{W}}_h := \{w \in \mathcal{W}_h \text{ and } w_{j,k,s} = 0 \text{ if } (x_j, y_k, z_s) \in \partial\Omega_h\}.$$

Let $\iota, \eta \in \mathring{\mathcal{W}}_h$. Accordingly, we define the corresponding inner product and norm as follows:

$$\begin{aligned} (\iota, \eta) &= h_1 h_2 h_3 \sum_{j=1}^{M_1-1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3-1} \iota_{jks} \eta_{jks}, \quad \|\iota\| = \sqrt{(\iota, \iota)}, \\ (\delta_x \iota, \delta_x \eta) &= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3-1} (\delta_x \iota_{j-\frac{1}{2},k,s}) (\delta_x \eta_{j-\frac{1}{2},k,s}), \end{aligned}$$

$$\begin{aligned}
(\delta_y \iota, \delta_y \eta) &= h_1 h_2 h_3 \sum_{j=1}^{M_1-1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3-1} (\delta_y \iota_{j,k-\frac{1}{2},s}) (\delta_y \eta_{j,k-\frac{1}{2},s}), \\
(\delta_z \iota, \delta_z \eta) &= h_1 h_2 h_3 \sum_{j=1}^{M_1-1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} (\delta_z \iota_{j,k,s-\frac{1}{2}}) (\delta_z \eta_{j,k,s-\frac{1}{2}}), \\
(\delta_x \delta_y \iota, \delta_x \delta_y \eta) &= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3-1} (\delta_x \delta_y \iota_{j-\frac{1}{2},k-\frac{1}{2},s}) (\delta_x \delta_y \eta_{j-\frac{1}{2},k-\frac{1}{2},s}), \\
(\delta_x \delta_z \iota, \delta_x \delta_z \eta) &= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} (\delta_x \delta_z \iota_{j-\frac{1}{2},k,s-\frac{1}{2}}) (\delta_x \delta_z \eta_{j-\frac{1}{2},k,s-\frac{1}{2}}), \\
(\delta_y \delta_z \iota, \delta_y \delta_z \eta) &= h_1 h_2 h_3 \sum_{j=1}^{M_1-1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\delta_y \delta_z \iota_{j,k-\frac{1}{2},s-\frac{1}{2}}) (\delta_y \delta_z \eta_{j,k-\frac{1}{2},s-\frac{1}{2}}), \\
(\delta_x \delta_y \delta_z \iota, \delta_x \delta_y \delta_z \eta) &= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\delta_x \delta_y \delta_z \iota_{j-\frac{1}{2},k-\frac{1}{2},s-\frac{1}{2}}) (\delta_x \delta_y \delta_z \eta_{j-\frac{1}{2},k-\frac{1}{2},s-\frac{1}{2}}),
\end{aligned}$$

and

$$\begin{aligned}
\|\delta_x \iota\|^2 &= (\delta_x \iota, \delta_x \iota), \quad \|\delta_y \iota\|^2 = (\delta_y \iota, \delta_y \iota), \quad \|\delta_z \iota\|^2 = (\delta_z \iota, \delta_z \iota), \\
\|\delta_x \delta_y \iota\|^2 &= (\delta_x \delta_y \iota, \delta_x \delta_y \iota), \quad \|\delta_y \delta_z \iota\|^2 = (\delta_y \delta_z \iota, \delta_y \delta_z \iota), \quad \|\delta_x \delta_z \iota\|^2 = (\delta_x \delta_z \iota, \delta_x \delta_z \iota), \\
\|\delta_x \delta_y \delta_z \iota\|^2 &= (\delta_x \delta_y \delta_z \iota, \delta_x \delta_y \delta_z \iota).
\end{aligned}$$

The GL approximation of the Caputo fractional derivative is given by [32]

$$\delta_t^\alpha u^n := q_0 u^n - q_{n-1} u^0 - \sum_{l=1}^{n-1} (q_{l-1} - q_l) u^{n-l}, \quad (2.1)$$

where

$$q_l = \frac{\tau^{-\alpha} \Gamma(l+1-\alpha)}{\Gamma(1-\alpha) \Gamma(l+1)}, \quad l = 0, 1, 2, \dots. \quad (2.2)$$

The following positive multipliers Ψ_n are defined herein:

$$\Psi_0 = q_0^{-1}, \quad \Psi_n = q_0^{-1} \sum_{l=1}^n (q_{l-1} - q_l) \Psi_{n-l}, \quad 1 \leq n \leq N. \quad (2.3)$$

Given a mesh function $\{v^i\}_{i=0}^N$, we define the discrete fractional integral operator Υ_t^α :

$$\Upsilon_t^\alpha(v^0) = 0, \quad \Upsilon_t^\alpha(v^n) = \sum_{l=1}^n \Psi_{n-l} v^l \quad \text{for } n = 1, 2, \dots, N. \quad (2.4)$$

Lemma 2.1. [35, Lemma 2.1] Suppose Ψ_n is defined as beforehand in Eq (2.3). It then follows that

$$\Psi_l < C\tau^\alpha(l+1)^{\alpha-1}, \quad l \geq 0, \quad (2.5)$$

$$\sum_{l=1}^n \Psi_{n-l} < Ct_n^\alpha, \quad n = 1, 2, \dots, N. \quad (2.6)$$

Lemma 2.2. [31, Lemma 2] Let $\xi^n \geq 0$ and assume $\lambda > 0$ such that $\tau \leq \frac{1}{2\sqrt[2]{2\Gamma(2-\alpha)\lambda}}$. For the mesh function $\{v^n\}_{n=0}^N$ fulfilling $v_0 \geq 0$, if

$$\delta_t^\alpha v^n \leq \lambda v^n + \xi^n, \quad \text{for } n = 1, \dots, N, \quad (2.7)$$

then one gets

$$v^n \leq 2E_\alpha(2^{\alpha+1}\lambda t_n^\alpha) \left(v^0 + \max_{1 \leq l \leq n} \Psi_{n-l} \xi^l \right), \quad (2.8)$$

where $E_\alpha(t)$ is the Mittag-Leffler function defined by $E_\alpha(t) = \sum_{k=0}^{\infty} \frac{t^k}{\Gamma(1+k\alpha)}$.

Lemma 2.3. [32, Lemma 3] For the mesh functions $\{v^i\}_{i=0}^N$, the following identity holds:

$$\Upsilon_t^\alpha(\delta_t^\alpha v^n) = v^n - v^0 \quad \text{for } n = 1, \dots, N. \quad (2.9)$$

The exact solution u of Eqs (1.1)–(1.3) is assumed to satisfy the following regularity condition [32]:

$$u(x, y, z, t) - u_0(x, y, z) = \sum_{(j,k)_\alpha} \rho_{j,k} t^{j+k\alpha} \phi(x, y, z) + Y(x, y, z, t), \quad (2.10)$$

where $(j, k)_\alpha := \{(j, k) : j, k \in N_0, j + k\alpha < 2\}$, $\rho_{j,k}$ are certain constants with $\rho_{0,0} = 0$, ϕ is a smooth function, and $Y(x, y, z, t) \in C^2[0, T]$ satisfying $Y(x, y, z, 0) = Y_t(x, y, z, 0) = 0$.

Lemma 2.4. [32, Lemma 5] Let $\sigma = \min\{2\alpha, 1\}$. Then, the following result holds:

$$|D_t^\alpha u(t_n) - \delta_t^\alpha u^n| \leq C(n^{-2} + \tau^{\sigma-\alpha} n^{-(1+\alpha-\sigma)} + \tau), \quad 1 \leq n \leq N. \quad (2.11)$$

Lemma 2.5. [36, Lemma 16] For $s = 1, \dots, N$, the sum of the convolution of the approximate error and the product of the positive multiplier $\{\Psi_s\}$ is

$$\sum_{l=1}^s |D_t^\alpha u(t_l) - \delta_t^\alpha u^l| \Psi_{s-l} \leq C\tau t_s^{\alpha-1}. \quad (2.12)$$

Lemma 2.6. [37, Lemma 5.1] For $n = 1, \dots, N$, if

$$v^n \leq v_1 t_n^{-\zeta_1} + v_2 t_n^{-\zeta_2} + \xi \tau \sum_{j=1}^{n-1} t_{n-j}^{\alpha-1} v^j, \quad 1 \leq n \leq N, \quad (2.13)$$

where $\zeta_1, \zeta_2 \in [0, 1)$, $v_1, v_2, \xi \geq 0$, and $\{v^n\}_{n=1}^N$ is a nonnegative sequence, then there exists a constant $C = C(\zeta_1, \zeta_2, \alpha, \xi, t_N)$, and it holds that

$$v^n \leq C(v_1 t_n^{-\zeta_1} + v_2 t_n^{-\zeta_2}), \quad 1 \leq n \leq N. \quad (2.14)$$

3. The formulation of the GL-ADI scheme

Considering the linear problem Eqs (1.1)–(1.3) at points (x_j, y_k, z_s, t_n) , the grid function $f_{j,k,s}^n = f(x_j, y_k, z_s, t_n)$, $U = \{U_{j,k,s}^n | (j, k, s) \in \epsilon, 0 \leq n \leq N\}$ where $U_{j,k,s}^n = u(x_j, y_k, z_s, t_n)$, and $(x_j, y_k, z_s, t_n) \in \Omega_h \times \Omega_\tau$, $0 \leq n \leq N$, one has

$$D_t^\alpha u(x_j, y_k, z_s, t_n) = \nabla \cdot (\kappa(x_j, y_k, z_s) \nabla u(x_j, y_k, z_s, t_n)) + \mu u(x_j, y_k, z_s, t_n) + f(x_j, y_k, z_s, t_n), \quad (3.1)$$

$$(x_j, y_k, z_s) \in \Omega_h, 1 \leq n \leq N,$$

where

$$\begin{aligned} & \nabla \cdot (\kappa(x_j, y_k, z_s) \nabla u(x_j, y_k, z_s, t_n)) \\ &= \nabla \cdot \begin{pmatrix} \kappa_1(x_j) & 0 & 0 \\ 0 & \kappa_2(y_k) & 0 \\ 0 & 0 & \kappa_3(z_s) \end{pmatrix} \begin{pmatrix} \frac{\partial u}{\partial x}(x_j, y_k, z_s, t_n) \\ \frac{\partial u}{\partial y}(x_j, y_k, z_s, t_n) \\ \frac{\partial u}{\partial z}(x_j, y_k, z_s, t_n) \end{pmatrix} \\ &= \nabla \cdot \begin{pmatrix} \kappa_1(x_j) \frac{\partial u}{\partial x}(x_j, y_k, z_s, t_n) \\ \kappa_2(y_k) \frac{\partial u}{\partial y}(x_j, y_k, z_s, t_n) \\ \kappa_3(z_s) \frac{\partial u}{\partial z}(x_j, y_k, z_s, t_n) \end{pmatrix} \\ &= \frac{\partial}{\partial x} \left(\kappa_1(x_j) \frac{\partial u}{\partial x} \right) (x_j, y_k, z_s, t_n) + \frac{\partial}{\partial y} \left(\kappa_2(y_k) \frac{\partial u}{\partial y} \right) (x_j, y_k, z_s, t_n) + \frac{\partial}{\partial z} \left(\kappa_3(z_s) \frac{\partial u}{\partial z} \right) (x_j, y_k, z_s, t_n). \end{aligned} \quad (3.2)$$

Next, we will separate each term in Eq (3.2). First,

$$\begin{aligned} & \frac{\partial}{\partial x} \left(\kappa_1(x_j) \frac{\partial u}{\partial x} \right) (x_j, y_k, z_s, t_n) \\ &= \frac{1}{h_1} \left((\kappa_x)_{j+\frac{1}{2}} \frac{U_{j+1,k,s}^n - U_{j,k,s}^n}{h_1} - (\kappa_x)_{j-\frac{1}{2}} \frac{U_{j,k,s}^n - U_{j-1,k,s}^n}{h_1} \right) + O(h_1^2) \\ &:= \mathcal{A}_x U_{j,k,s}^n + O(h_1^2). \end{aligned} \quad (3.3)$$

Second,

$$\begin{aligned} & \frac{\partial}{\partial y} \left(\kappa_2(y_k) \frac{\partial u}{\partial y} \right) (x_j, y_k, z_s, t_n) \\ &= \frac{1}{h_2} \left((\kappa_y)_{k+\frac{1}{2}} \frac{U_{j,k+1,s}^n - U_{j,k,s}^n}{h_2} - (\kappa_y)_{k-\frac{1}{2}} \frac{U_{j,k,s}^n - U_{j,k-1,s}^n}{h_2} \right) + O(h_2^2), \\ &:= \mathcal{A}_y U_{j,k,s}^n + O(h_2^2). \end{aligned} \quad (3.4)$$

Finally,

$$\begin{aligned} & \frac{\partial}{\partial z} \left(\kappa_3(z_s) \frac{\partial u}{\partial z} \right) (x_j, y_k, z_s, t_n) \\ &= \frac{1}{h_3} \left((\kappa_z)_{s+\frac{1}{2}} \frac{U_{j,k,s+1}^n - U_{j,k,s}^n}{h_3} - (\kappa_z)_{s-\frac{1}{2}} \frac{U_{j,k,s}^n - U_{j,k,s-1}^n}{h_3} \right) + O(h_3^2) \end{aligned} \quad (3.5)$$

$$:= \mathcal{A}_z U_{j,k,s}^n + O(h_3^2).$$

Denote

$$\mathcal{A}_h U_{j,k,s}^n = \mathcal{A}_x U_{j,k,s}^n + \mathcal{A}_y U_{j,k,s}^n + \mathcal{A}_z U_{j,k,s}^n.$$

From Eqs (3.2)–(3.5), we can obtain

$$\nabla \cdot (\kappa(x_j, y_k, z_s) \nabla u(x_j, y_k, z_s, t_n)) = \mathcal{A}_h U_{j,k,s}^n + (R_h)_{j,k,s}^n, \quad (j, k, s) \in \epsilon, 0 \leq n \leq N, \quad (3.6)$$

where

$$|(R_h)_{j,k,s}^n| \leq C(h_1^2 + h_2^2 + h_3^2), \quad (j, k, s) \in \epsilon, 0 \leq n \leq N. \quad (3.7)$$

Substituting Eqs (2.1) and (3.6) into Eq (3.1), we have

$$\delta_t^\alpha U_{j,k,s}^n - \mathcal{A}_h U_{j,k,s}^n - \mu U_{j,k,s}^n = f_{j,k,s}^n + (R_t)_{j,k,s}^n + (R_h)_{j,k,s}^n, \quad (x_j, y_k, z_s) \in \Omega_h, 1 \leq n \leq N, \quad (3.8)$$

$$U_{j,k,s}^0 = u_0(x_j, y_k, z_s), \quad (x_j, y_k, z_s) \in \bar{\Omega}_h, \quad (3.9)$$

$$U_{j,k,s}^n = 0, \quad (x_j, y_k, z_s) \in \partial\Omega_h, \quad 1 \leq n \leq N, \quad (3.10)$$

where $(R_t)_{j,k,s}^n$ is truncation error as follows:

$$(R_t)_{j,k,s}^n := \delta_t^\alpha U_{j,k,s}^n - D_t^\alpha u(x_j, y_k, z_s, t_n), \quad (j, k, s) \in \epsilon, 0 \leq n \leq N. \quad (3.11)$$

To construct the ADI scheme, we add a small term

$$(\theta^2 \mathcal{A}_x \mathcal{A}_y + \theta^2 \mathcal{A}_y \mathcal{A}_z + \theta^2 \mathcal{A}_x \mathcal{A}_z - \theta^3 \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z)(\delta_t^\alpha - \mu) U_{j,k,s}^n$$

on both sides of Eq (3.8), where

$$\theta := (q_0 - \mu)^{-1}. \quad (3.12)$$

We obtain

$$\begin{aligned} & (I + \theta^2 \mathcal{A}_x \mathcal{A}_y + \theta^2 \mathcal{A}_y \mathcal{A}_z + \theta^2 \mathcal{A}_x \mathcal{A}_z - \theta^3 \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z)(\delta_t^\alpha - \mu) U_{j,k,s}^n - \mathcal{A}_h U_{j,k,s}^n \\ & = f_{j,k,s}^n + r_{j,k,s}^n, \quad (x_j, y_k, z_s) \in \Omega_h, 1 \leq n \leq N, \end{aligned} \quad (3.13)$$

where

$$r_{j,k,s}^n = (R_t)_{j,k,s}^n + (R_h)_{j,k,s}^n + (\theta^2 \mathcal{A}_x \mathcal{A}_y + \theta^2 \mathcal{A}_y \mathcal{A}_z + \theta^2 \mathcal{A}_x \mathcal{A}_z - \theta^3 \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z)(\delta_t^\alpha - \mu) U_{j,k,s}^n, \quad (x_j, y_k, z_s) \in \Omega_h, 1 \leq n \leq N. \quad (3.14)$$

The small perturbation terms are chosen precisely so that the operator on the left-hand side of Eq (3.13) admits the factorization

$$I + \theta^2 \mathcal{A}_x \mathcal{A}_y + \theta^2 \mathcal{A}_y \mathcal{A}_z + \theta^2 \mathcal{A}_x \mathcal{A}_z - \theta^3 \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z = (I - \theta \mathcal{A}_x)(I - \theta \mathcal{A}_y)(I - \theta \mathcal{A}_z),$$

which is the key to the ADI splitting.

To ensure $\theta > 0$ in Eq (3.12), we take the time step τ satisfying

$$\tau^\alpha < \frac{1}{\mu}. \quad (3.15)$$

Since $\theta = (q_0 - \mu)^{-1} = O(\tau^\alpha)$, it follows that $\theta^2 = O(\tau^{2\alpha})$ and $\theta^3 = O(\tau^{3\alpha})$. Thus,

$$\left\| \left(\theta^2 \mathcal{A}_x \mathcal{A}_y + \theta^2 \mathcal{A}_y \mathcal{A}_z + \theta^2 \mathcal{A}_x \mathcal{A}_z - \theta^3 \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \right) (\delta_t^\alpha - \mu) U^n \right\| = O(\tau^{2\alpha}). \quad (3.16)$$

Neglecting the small-order terms in Eq (3.13), taking into account Eqs (3.9) and (3.10), and replacing $U_{j,k,s}^n$ with $u_{j,k,s}^n$, we obtain the GL-ADI GFDM

$$\left(I + \theta^2 \mathcal{A}_x \mathcal{A}_y + \theta^2 \mathcal{A}_y \mathcal{A}_z + \theta^2 \mathcal{A}_x \mathcal{A}_z - \theta^3 \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \right) (\delta_t^\alpha - \mu) u_{j,k,s}^n \quad (3.17)$$

$$- \mathcal{A}_h u_{j,k,s}^n = f_{j,k,s}^n, \quad (x_j, y_k, z_s) \in \Omega_h, \quad 1 \leq n \leq N,$$

$$u_{j,k,s}^0 = u_0(x_j, y_k, z_s), \quad (x_j, y_k, z_s) \in \bar{\Omega}_h, \quad (3.18)$$

$$u_{j,k,s}^n = 0, \quad (x_j, y_k, z_s) \in \partial\Omega_h, \quad 1 \leq n \leq N. \quad (3.19)$$

A more conventional ADI representation of Eq (3.17) is presented as follows:

$$(I - \theta \mathcal{A}_x) (I - \theta \mathcal{A}_y) (I - \theta \mathcal{A}_z) u_{j,k,s}^n \quad (3.20)$$

$$= \theta \left(\theta^2 \mathcal{A}_x \mathcal{A}_y + \theta^2 \mathcal{A}_y \mathcal{A}_z + \theta^2 \mathcal{A}_x \mathcal{A}_z - \theta^3 \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \right) \left(\sum_{l=1}^{n-1} (q_{l-1} - q_l) u_{j,k,s}^{n-l} + q_{n-1} u_{j,k,s}^0 \right) + \theta f_{j,k,s}^n.$$

The numerical solution $u_{j,k,s}^n$ of Eq (3.20) can be obtained by solving three decoupled one-dimensional subproblems. For the sake of notational simplicity, we introduce the following definitions:

$$u_{j,k,s}^{**} = (I - \theta \mathcal{A}_z) u_{j,k,s}^n, \quad (j, k, s) \in \epsilon, \quad 0 \leq n \leq N,$$

$$u_{j,k,s}^* = (I - \theta \mathcal{A}_y) u_{j,k,s}^{**}, \quad (j, k, s) \in \epsilon, \quad 0 \leq n \leq N.$$

Given the values $\{u_{j,k,s}^m \mid 0 \leq j \leq M_1, \quad 0 \leq k \leq M_2, \quad 0 \leq s \leq M_3, \quad m = 1, \dots, n-1\}$ at the first $(n-1)$ levels, the intermediate values $\{u_{j,k,s}^* \mid (j, k, s) \in \epsilon\}$ can be computed from Eq (3.21). For any fixed indices k with $1 \leq k \leq M_2 - 1$ and s with $1 \leq s \leq M_3 - 1$, we have

$$\begin{cases} (I - \theta \mathcal{A}_x) u_{j,k,s}^* = \theta \left(\theta^2 \mathcal{A}_x \mathcal{A}_y + \theta^2 \mathcal{A}_y \mathcal{A}_z + \theta^2 \mathcal{A}_x \mathcal{A}_z - \theta^3 \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \right) \\ \quad \left(\sum_{l=1}^{n-1} (q_{l-1} - q_l) u_{j,k,s}^{n-l} + q_{n-1} u_{j,k,s}^0 \right) + \theta f_{j,k,s}^n, \\ u_{0,k,s}^* = (I - \theta \mathcal{A}_y) (I - \theta \mathcal{A}_z) u_{0,k,s}^n, \\ u_{M_1,k,s}^* = (I - \theta \mathcal{A}_y) (I - \theta \mathcal{A}_z) u_{M_1,k,s}^n. \end{cases} \quad (3.21)$$

When $\{u_{j,k,s}^* \mid (j, k, s) \in \epsilon\}$ has been obtained, $\{u_{j,k,s}^{**} \mid (j, k, s) \in \epsilon\}$ is calculated from Eq (3.22). With j ($1 \leq j \leq M_1 - 1$) and s ($1 \leq s \leq M_3 - 1$) being any fixed values, we have

$$\begin{cases} (I - \theta \mathcal{A}_y) u_{j,k,s}^{**} = u_{j,k,s}^* \\ u_{j,0,s}^{**} = (I - \theta \mathcal{A}_z) u_{j,0,s}^n, \\ u_{j,M_2,s}^{**} = (I - \theta \mathcal{A}_z) u_{j,M_2,s}^n. \end{cases} \quad (3.22)$$

When $\{u_{j,k,s}^{**} | (j,k,s) \in \epsilon\}$ has been obtained, $\{u_{j,k,s}^n | (j,k,s) \in \epsilon, 0 \leq n \leq N\}$ on the n th layer is calculated from Eq (3.23). For fixed j ($1 \leq j \leq M_1 - 1$) and k ($1 \leq k \leq M_2 - 1$), with the boundary conditions, we have

$$\begin{cases} (I - \theta \mathcal{A}_z) u_{j,k,s}^n = u_{j,k,s}^{**} \\ u_{j,k,0}^n = 0, u_{j,k,M_3}^n = 0. \end{cases} \quad (3.23)$$

4. Theoretical analysis

4.1. Solution uniqueness

For arbitrary mesh functions $\phi, \varphi \in \mathcal{W}_h$, we define

$$(\phi, \varphi)_\theta = (\phi, \varphi) + \theta^2 (\mathcal{A}_x \mathcal{A}_y \phi, \varphi) + \theta^2 (\mathcal{A}_y \mathcal{A}_z \phi, \varphi) + \theta^2 (\mathcal{A}_x \mathcal{A}_z \phi, \varphi) - \theta^3 (\mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \phi, \varphi), \quad (4.1)$$

and $\|\phi\|_\theta = \sqrt{(\phi, \phi)_\theta}$.

Next, we prove by virtue of the relevant Lemmas 4.1–4.3 that the newly defined binary operation $(\cdot, \cdot)_\theta$ satisfies symmetry, positive definiteness, and linearity. Thus it follows that $(\cdot, \cdot)_\theta$ is a valid inner product on the corresponding space.

Next, we prove that $(\cdot, \cdot)_\theta$ satisfies symmetry.

Lemma 4.1. *For any mesh functions $\phi, \varphi \in \mathcal{W}_h$, one has*

$$\begin{aligned} (\mathcal{A}_x \phi, \varphi) &= (\phi, \mathcal{A}_x \varphi), (\mathcal{A}_y \phi, \varphi) = (\phi, \mathcal{A}_y \varphi), (\mathcal{A}_z \phi, \varphi) = (\phi, \mathcal{A}_z \varphi), \\ (\mathcal{A}_x \mathcal{A}_y \phi, \varphi) &= (\phi, \mathcal{A}_x \mathcal{A}_y \varphi), (\mathcal{A}_y \mathcal{A}_z \phi, \varphi) = (\phi, \mathcal{A}_y \mathcal{A}_z \varphi), (\mathcal{A}_x \mathcal{A}_z \phi, \varphi) = (\phi, \mathcal{A}_x \mathcal{A}_z \varphi) \\ (\mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \phi, \varphi) &= (\phi, \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \varphi). \end{aligned}$$

Proof. The proof is provided in Appendix A.1 for completeness.

Then, we obtain that $(\cdot, \cdot)_\theta$ satisfies positive definiteness.

Lemma 4.2. *For any mesh functions $\phi \in \mathring{\mathcal{W}}_h$,*

$$(\phi, \phi)_\theta \geq 0.$$

Proof. The proof is given in Appendix A.2.

We now prove that $(\cdot, \cdot)_\theta$ satisfies linearity.

Lemma 4.3. *For any mesh functions $\phi_1, \phi_2, \varphi_1, \varphi_2 \in \mathring{\mathcal{W}}_h$, α and $\beta \in (-\infty, +\infty)$, we have*

$$\begin{aligned} (1) \quad & (\alpha \phi_1 + \beta \phi_2, \varphi)_\theta = \alpha (\phi_1, \varphi)_\theta + \beta (\phi_2, \varphi)_\theta, \\ (2) \quad & (\phi, \alpha \varphi_1 + \beta \varphi_2)_\theta = \alpha (\phi, \varphi_1)_\theta + \beta (\phi, \varphi_2)_\theta. \end{aligned}$$

Proof. We prove the first inequality

$$(\alpha \phi_1 + \beta \phi_2, \varphi)_\theta = (\alpha \phi_1 + \beta \phi_2, \varphi) - \theta^2 (\mathcal{A}_x \mathcal{A}_y (\alpha \phi_1 + \beta \phi_2), \varphi) - \theta^2 (\mathcal{A}_y \mathcal{A}_z (\alpha \phi_1 + \beta \phi_2), \varphi)$$

$$\begin{aligned}
& -\theta^2(\mathcal{A}_x\mathcal{A}_z(\alpha\phi_1 + \beta\phi_2), \varphi) - \theta^3(\mathcal{A}_x\mathcal{A}_y\mathcal{A}_z(\alpha\phi_1 + \beta\phi_2), \varphi) \\
& = \alpha(\phi_1, \varphi) + \beta(\phi_2, \varphi) - \theta^2[\alpha(\mathcal{A}_x\mathcal{A}_y\phi_1, \varphi) + \beta(\mathcal{A}_x\mathcal{A}_y\phi_2, \varphi)] - \theta^2[\alpha(\mathcal{A}_y\mathcal{A}_z\phi_1, \varphi) + \beta(\mathcal{A}_y\mathcal{A}_z\phi_2, \varphi)] \\
& \quad - \theta^2[\alpha(\mathcal{A}_x\mathcal{A}_z\phi_1, \varphi) + \beta(\mathcal{A}_x\mathcal{A}_z\phi_2, \varphi)] \\
& \quad - \theta^3[\alpha(\mathcal{A}_x\mathcal{A}_y\mathcal{A}_z\phi_1, \varphi) + \beta(\mathcal{A}_x\mathcal{A}_y\mathcal{A}_z\phi_2, \varphi)] \\
& = \alpha[(\phi_1, \varphi) - \theta^2(\mathcal{A}_x\mathcal{A}_y\phi_1, \varphi) - \theta^2(\mathcal{A}_y\mathcal{A}_z\phi_1, \varphi) - \theta^2(\mathcal{A}_x\mathcal{A}_z\phi_1, \varphi) - \theta^3(\mathcal{A}_x\mathcal{A}_y\mathcal{A}_z\phi_1, \varphi)] \\
& \quad + \beta[(\phi_2, \varphi) - \theta^2(\mathcal{A}_x\mathcal{A}_y\phi_2, \varphi) - \theta^2(\mathcal{A}_y\mathcal{A}_z\phi_2, \varphi) - \theta^2(\mathcal{A}_x\mathcal{A}_z\phi_2, \varphi) - \theta^3(\mathcal{A}_x\mathcal{A}_y\mathcal{A}_z\phi_2, \varphi)] \\
& = \alpha(\phi_1, \varphi)_\theta + \beta(\phi_2, \varphi)_\theta.
\end{aligned}$$

Analogously, the second inequality can be verified by the same line of reasoning, and the proof is thus concluded.

Remark 1. Based on the conclusions of Lemmas 4.1–4.3, we rigorously proved that the newly introduced binary operation $(\cdot, \cdot)_\theta$ possesses the defining characteristics of internal symmetry, positive definiteness, and linearity. Thus, it directly follows that $(\cdot, \cdot)_\theta$ is a valid inner product on the relevant space. Then, the inequalities

$$(\phi, \varphi)_\theta \leq \|\phi\|_\theta \|\varphi\|_\theta \quad (4.2)$$

and

$$\|\phi\| \leq \|\phi\|_\theta \quad (4.3)$$

hold, where $\|\cdot\|_\theta$ represents the norm of the inner product $(\cdot, \cdot)_\theta$.

The newly defined binary operation $(\cdot, \cdot)_\theta$ is a specialized technical tool specifically designed for ADI decomposition. It can integrate the coupling operators in Eq (3.17) into a single norm $\|\cdot\|_\theta$. This avoids the need for separate estimation of cross-terms and simplifies the subsequent analysis process.

Next, we prove the uniqueness of the solutions to Eqs (3.17)–(3.19).

Theorem 4.1. *The difference scheme given by Eqs (3.17)–(3.19) admits a unique solution.*

Proof. The GL-ADI GFDM method divides the 3D problem into three successive one-dimensional subproblems. To prove the uniqueness of the solution for the full system, it is sufficient to verify the invertibility of the coefficient matrices in each of these three substeps. First, we study the elimination steps along the x -direction and find that $\{u_{j,k,s}^* | (j, k, s) \in \epsilon\}$ can be solved from Eq (3.21). For any fixed indices k with $1 \leq k \leq M_2 - 1$ and s with $1 \leq s \leq M_3 - 1$, we have

$$\begin{aligned}
(I - \theta\mathcal{A}_x) u_{j,k,s}^* &= \theta(\theta^2\mathcal{A}_x\mathcal{A}_y + \theta^2\mathcal{A}_y\mathcal{A}_z + \theta^2\mathcal{A}_x\mathcal{A}_z - \theta^3\mathcal{A}_x\mathcal{A}_y\mathcal{A}_z) \\
&\quad \left(\sum_{l=1}^{n-1} (q_{l-1} - q_l) u_{j,k,s}^{n-l} + q_{n-1} u_{j,k,s}^0 \right) + \theta f_{j,k,s}^n, \quad (j, k, s) \in \epsilon, 0 \leq n \leq N.
\end{aligned} \quad (4.4)$$

The expression $\mathcal{A}_x$ is obtained by substituting it in and rearranging it:

$$-\frac{\theta(\kappa_x)_{j-\frac{1}{2}}}{h_1^2} u_{j-1,k,s}^* + \left(1 + \frac{\theta}{h_1^2} ((\kappa_x)_{j-\frac{1}{2}} + (\kappa_x)_{j+\frac{1}{2}}))\right) u_{j,k,s}^* - \frac{\theta(\kappa_x)_{j+\frac{1}{2}}}{h_1^2} u_{j+1,k,s}^* \quad (4.5)$$

$$= \theta \left(\theta^2 \mathcal{A}_x \mathcal{A}_y + \theta^2 \mathcal{A}_y \mathcal{A}_z + \theta^2 \mathcal{A}_x \mathcal{A}_z - \theta^3 \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \right) \left(\sum_{l=1}^{n-1} (q_{l-1} - q_l) u_{j,k,s}^{n-l} + q_{n-1} u_{j,k,s}^0 \right) \\ + \theta f_{j,k,s}^n, \quad (j, k, s) \in \epsilon, 0 \leq n \leq N.$$

Under the conditions $\theta > 0$, $(\kappa_x)_{j+\frac{1}{2}} > 0$, and $(\kappa_x)_{j-\frac{1}{2}} > 0$, it holds that

$$1 + \frac{\theta}{h_1^2} ((\kappa_x)_{j-\frac{1}{2}} + (\kappa_x)_{j+\frac{1}{2}}) > \frac{\theta}{h_1^2} ((\kappa_x)_{j-\frac{1}{2}} + (\kappa_x)_{j+\frac{1}{2}}) \quad (4.6)$$

Therefore, we conclude that the linear Eq (4.5) is strictly diagonally dominant and thus invertible. The $u_{j,k,s}^*$ in Eq (4.4) is the unique solution.

When $\{u_{j,k,s}^* | (j, k, s) \in \epsilon\}$ has been obtained, $\{u_{j,k,s}^{**} | (j, k, s) \in \epsilon\}$ is calculated from Eq (3.22). With j ($1 \leq j \leq M_1 - 1$) and s ($1 \leq s \leq M_3 - 1$) being any fixed values, we have

$$(I - \theta \mathcal{A}_y) u_{j,k,s}^{**} = u_{j,k,s}^*. \quad (4.7)$$

The expression $\mathcal{A}_y$ is obtained by substituting it in and rearranging it:

$$-\frac{\theta(\kappa_y)_{k-\frac{1}{2}}}{h_2^2} u_{j,k-1,s}^{**} + \left(1 + \frac{\theta}{h_2^2} ((\kappa_y)_{k-\frac{1}{2}} + (\kappa_y)_{k+\frac{1}{2}})\right) u_{j,k,s}^{**} - \frac{\theta(\kappa_y)_{k+\frac{1}{2}}}{h_2^2} u_{j,k+1,s}^{**} = u_{j,k,s}^*, \quad (j, k, s) \in \epsilon, 0 \leq n \leq N. \quad (4.8)$$

Under the conditions $\theta > 0$, $(\kappa_y)_{k+\frac{1}{2}} > 0$, and $(\kappa_y)_{k-\frac{1}{2}} > 0$, it holds that

$$1 + \frac{\theta}{h_2^2} ((\kappa_y)_{k-\frac{1}{2}} + (\kappa_y)_{k+\frac{1}{2}}) > \frac{\theta}{h_2^2} ((\kappa_y)_{k-\frac{1}{2}} + (\kappa_y)_{k+\frac{1}{2}}) \quad (4.9)$$

The linear Eq (4.8) is also strictly diagonally dominant and therefore invertible. The $u_{j,k,s}^{**}$ in Eq (4.7) is the unique solution.

When $\{u_{j,k,s}^{**} | (j, k, s) \in \epsilon\}$ has been obtained, $\{u_{j,k,s}^n | (j, k, s) \in \epsilon\}$ on the n th layer is calculated from Eq (3.23). For fixed j ($1 \leq j \leq M_1 - 1$) and k ($1 \leq k \leq M_2 - 1$), we have

$$(I - \theta \mathcal{A}_z) u_{j,k,s}^n = u_{j,k,s}^{**}. \quad (4.10)$$

The expression $\mathcal{A}_z$ is obtained by substituting it in and rearranging it:

$$-\frac{\theta(\kappa_z)_{s-\frac{1}{2}}}{h_3^2} u_{j,k,s-1}^n + \left(1 + \frac{\theta}{h_3^2} ((\kappa_z)_{s-\frac{1}{2}} + (\kappa_z)_{s+\frac{1}{2}})\right) u_{j,k,s}^n - \frac{\theta(\kappa_z)_{s+\frac{1}{2}}}{h_3^2} u_{j,k,s+1}^n = u_{j,k,s}^{**}, \quad (j, k, s) \in \epsilon, 0 \leq n \leq N. \quad (4.11)$$

Under the conditions $\theta > 0$, $(\kappa_z)_{s+\frac{1}{2}} > 0$, and $(\kappa_z)_{s-\frac{1}{2}} > 0$, it holds that

$$1 + \frac{\theta}{h_3^2} ((\kappa_z)_{s-\frac{1}{2}} + (\kappa_z)_{s+\frac{1}{2}}) > \frac{\theta}{h_3^2} ((\kappa_z)_{s-\frac{1}{2}} + (\kappa_z)_{s+\frac{1}{2}}). \quad (4.12)$$

The linear Eq (4.11) is also strictly diagonally dominant and therefore invertible. The $u_{j,k,s}^n$ in Eq (4.10) is the unique solution. The completely discrete GL-ADI GFDM has a unique solution for each step. The strict diagonal dominance established above relies crucially on the homogeneous Dirichlet boundary conditions $u_{0,k,s}^n = u_{M_1,k,s}^n = 0$ (and similarly for y and z), which eliminate boundary terms in the matrices and ensure the tridiagonal structure is strictly diagonally dominant.

4.2. Stability

Theorem 4.2. *The solution corresponding to the GL-ADI scheme governed by Eqs (3.17)–(3.19) fulfills*

$$\|u^n\|_\theta \leq 2E_\alpha \left(2^{\alpha+1} \lambda t_n^\alpha \right) \left(\|u^0\|_\theta + C t_n^\alpha \max_{1 \leq l \leq n} \|f^l\| \right), \quad \text{for } n = 1, 2, \dots, N. \quad (4.13)$$

Proof. By taking the inner product of Eq (3.17) with u^n and substituting Eq (2.1), we derive that

$$\begin{aligned} & \left((I + \theta^2 \mathcal{A}_x \mathcal{A}_y + \theta^2 \mathcal{A}_y \mathcal{A}_z + \theta^2 \mathcal{A}_x \mathcal{A}_z - \theta^3 \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z) \left[(q_0 - \mu)u^n - \sum_{l=1}^{n-1} (q_{l-1} - q_l)u^{n-l} - q_{n-1}u^0 \right], u^n \right) \\ & - (\mathcal{A}_x u^n, u^n) - (\mathcal{A}_y u^n, u^n) - (\mathcal{A}_z u^n, u^n) = (f^n, u^n), \quad n = 1, 2, \dots, N. \end{aligned} \quad (4.14)$$

Leveraging Eq (A.1) from Lemma 4.1, we have

$$\begin{aligned} -(\mathcal{A}_x u^n, u^n) &= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\delta_x u^n_{j-\frac{1}{2},k,s})^2 \geq 0, \\ -(\mathcal{A}_y u^n, u^n) &= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3-1} (\kappa_y)_{k-\frac{1}{2}} (\delta_y u^n_{j,k-\frac{1}{2},s})^2 \geq 0, \\ -(\mathcal{A}_z u^n, u^n) &= h_1 h_2 h_3 \sum_{j=1}^{M_1-1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_z)_{s-\frac{1}{2}} (\delta_z u^n_{j,k,s-\frac{1}{2}})^2 \geq 0, \quad n = 1, 2, \dots, N. \end{aligned}$$

According to the definition of $(\cdot, \cdot)_\theta$ in Eq (4.1), Eq (4.14) can be written as

$$(q_0 - \mu) \|u^n\|_\theta^2 \leq \sum_{l=1}^n (q_{l-1} - q_l) (u^{n-l}, u^n)_\theta + q_{n-1} (u^0, u^n)_\theta + (f^n, u^n), \quad n = 1, 2, \dots, N.$$

Meanwhile, by combining the Cauchy-Schwarz inequality in Eq (4.2) and the condition $\|\cdot\| \leq \|\cdot\|_\theta$ in Eq (4.3), we can arrive at

$$(q_0 - \mu) \|u^n\|_\theta^2 \leq \sum_{l=1}^n (q_{l-1} - q_l) \|u^n\|_\theta \|u^n\|_\theta + q_{n-1} \|u^0\|_\theta \|u^n\|_\theta + \|f^n\| \|u^n\|_\theta, \quad n = 1, 2, \dots, N. \quad (4.15)$$

Upon dividing both sides of Eq (4.15) by the norm $\|u^n\|_\theta$, we obtain

$$(q_0 - \mu) \|u^n\|_\theta \leq \sum_{l=1}^n (q_{l-1} - q_l) \|u^n\|_\theta + q_{n-1} \|u^0\|_\theta + \|f^n\|, \quad n = 1, 2, \dots, N. \quad (4.16)$$

Ultimately, based on the definition of the operator δ_t^α in Eq (2.1), we obtain

$$\delta_t^\alpha \|u^n\|_\theta \leq \|f^n\| + \mu \|u^n\|_\theta, \quad n = 1, 2, \dots, N. \quad (4.17)$$

The above equation satisfies Lemma 2.2, and we obtain

$$\|u^n\|_\theta \leq 2E_\alpha \left(2^{\alpha+1} \lambda t_n^\alpha \right) \left(\|u^0\|_\theta + \max_{1 \leq l \leq n} \|f^l\| \right), \quad \text{for } n = 1, 2, \dots, N. \quad (4.18)$$

Applying Eq (2.5) of Lemma 2.1, we arrive at the desired conclusion

$$\|u^n\|_\theta \leq 2E_\alpha \left(2^{\alpha+1} \lambda t_n^\alpha \right) \left(\|u^0\|_\theta + C t_n^\alpha \max_{1 \leq l \leq n} \|f^l\| \right), \quad \text{for } n = 1, 2, \dots, N. \quad (4.19)$$

4.3. Convergence

We proceed to investigate the error estimate for the numerical scheme given in Eqs (3.17)–(3.19).

Theorem 4.3. Suppose that the linear problem described by Eqs (1.1)–(1.3) admits a solution $u(x, y, z, t)$ that satisfies the regularity condition given in Eq (2.10), and $\{u_{j,k,s}^n | (j, k, s) \in \epsilon, 0 \leq n \leq N\}$ denotes the discrete approximation obtained via the GL-ADI scheme governed by Eqs (3.17)–(3.19). Then, we have

$$\|U_{j,k,s}^n - u_{j,k,s}^n\| \leq C(\tau t_n^{\alpha-1} + \tau^{2\alpha} + h_1^2 + h_2^2 + h_3^2), \quad 1 \leq n \leq N.$$

Proof. Denote $e_{j,k,s}^n = U_{j,k,s}^n - u_{j,k,s}^n$, $(x_j, y_k, z_s) \in \Omega_h$, $n = 1, 2, \dots, N$, and subtracting Eqs (3.17)–(3.19) from Eqs (3.8)–(3.10), one gets the error equations

$$(I + \theta^2 \mathcal{A}_x \mathcal{A}_y + \theta^2 \mathcal{A}_y \mathcal{A}_z + \theta^2 \mathcal{A}_x \mathcal{A}_z - \theta^3 \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z)(\delta_t^\alpha - \mu) e_{j,k,s}^n \quad (4.20)$$

$$- \mathcal{A}_h e_{j,k,s}^n = r_{j,k,s}^n, \quad (x_j, y_k, z_s) \in \Omega_h, \quad 1 \leq n \leq N,$$

$$e_{j,k,s}^0 = 0, \quad (x_j, y_k, z_s) \in \bar{\Omega}_h, \quad (4.21)$$

$$e_{j,k,s}^n = 0, \quad (x_j, y_k, z_s) \in \partial\Omega_h, \quad 1 \leq n \leq N. \quad (4.22)$$

By calculating the inner product between e^n and two sides of Eq (4.20) and using Eq (2.1), we obtain

$$\begin{aligned} & \left((I + \theta^2 \mathcal{A}_x \mathcal{A}_y + \theta^2 \mathcal{A}_y \mathcal{A}_z + \theta^2 \mathcal{A}_x \mathcal{A}_z - \theta^3 \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z) \left[(q_0 - \mu) e^n - \sum_{l=1}^{n-1} (q_{l-1} - q_l) e^{n-l} - q_{n-1} e^0 \right], e^n \right) \\ & - (\mathcal{A}_x e^n, e^n) - (\mathcal{A}_y e^n, e^n) - (\mathcal{A}_z e^n, e^n) = (r^n, e^n), \quad 1 \leq n \leq N. \end{aligned} \quad (4.23)$$

Applying Eq (A.1) from Lemma 4.1, we arrive at

$$\begin{aligned} - (\mathcal{A}_x e^n, e^n) &= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\delta_x e_{j-\frac{1}{2},k,s}^n)^2 \geq 0, \\ - (\mathcal{A}_y e^n, e^n) &= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3-1} (\kappa_y)_{k-\frac{1}{2}} (\delta_y e_{j,k-\frac{1}{2},s}^n)^2 \geq 0, \\ - (\mathcal{A}_z e^n, e^n) &= h_1 h_2 h_3 \sum_{j=1}^{M_1-1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_z)_{s-\frac{1}{2}} (\delta_z e_{j,k,s-\frac{1}{2}}^n)^2 \geq 0, \quad n = 1, 2, \dots, N. \end{aligned}$$

According to the definition of $(\cdot, \cdot)_\theta$ in Eq (4.1), Eq (4.23) can be written as

$$(q_0 - \mu) \|e^n\|_\theta^2 \leq \sum_{l=1}^n (q_{l-1} - q_l) (e^{n-l}, e^n)_\theta + q_{n-1} (e^0, e^n)_\theta + (r^n, e^n), \quad 1 \leq n \leq N.$$

Meanwhile, by applying the Cauchy–Schwarz inequality (4.2) and the condition $\|\cdot\| \leq \|\cdot\|_\theta$ given in Eq (4.3), we can conclude that

$$(q_0 - \mu) \|e^n\|_\theta^2 \leq \sum_{l=1}^n (q_{l-1} - q_l) \|e^n\|_\theta \|e^{n-l}\|_\theta + q_{n-1} \|e^0\|_\theta \|e^n\|_\theta + \|r^n\| \|e^n\|_\theta, \quad 1 \leq n \leq N. \quad (4.24)$$

Dividing both sides of Eq (4.24) by the corresponding norm yields $\|e^n\|_\theta$, we obtain

$$(q_0 - \mu) \|e^n\|_\theta \leq \sum_{l=1}^n (q_{l-1} - q_l) \|e^n\|_\theta + q_{n-1} \|e^0\|_\theta + \|r^n\|, \quad 1 \leq n \leq N. \quad (4.25)$$

Ultimately, based on the definition of the operator δ_t^α in Eq (2.1), Eq (4.25) can be written as

$$\delta_t^\alpha \|e^n\|_\theta \leq \mu \|e^n\|_\theta + \|r^n\|, \quad 1 \leq n \leq N. \quad (4.26)$$

Applying the operator $\mathcal{Y}_t^\alpha$ in Eq (2.4) to both sides of inequality (4.26) yields

$$\mathcal{Y}_t^\alpha (\delta_t^\alpha \|e^n\|_\theta) \leq \mu \sum_{l=1}^n \Psi_{n-l} \|e^l\|_\theta + \sum_{l=1}^n \Psi_{n-l} (\|r^l\|), \quad 1 \leq n \leq N. \quad (4.27)$$

From Lemma 2.3 and noting that $e^0 = 0$, we can conclude

$$\|e^n\|_\theta \leq \mu \sum_{l=1}^n \Psi_{n-l} \|e^l\|_\theta + \sum_{l=1}^n \Psi_{n-l} \|r^l\|, \quad 1 \leq n \leq N. \quad (4.28)$$

where $r_{j,k,s}^n$ in Eq (3.14) satisfies

$$\begin{aligned} \|r^n\| &= \left\| R_t^n + R_h^n + \left(\theta^2 (\mathcal{A}_x \mathcal{A}_y + \mathcal{A}_y \mathcal{A}_z + \mathcal{A}_x \mathcal{A}_z) - \theta^3 \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \right) (\delta_t^\alpha - \mu) U_{jks}^n \right\| \\ &\leq \|R_t^n\| + C(\tau^{2\alpha} + h_1^2 + h_2^2 + h_3^2), \quad 1 \leq n \leq N. \end{aligned} \quad (4.29)$$

Therefore,

$$\|e^n\|_\theta \leq \mu \sum_{l=1}^n \Psi_{n-l} \|e^l\|_\theta + \sum_{l=1}^n \Psi_{n-l} (\|R_t^l\| + C(\tau^{2\alpha} + h_1^2 + h_2^2 + h_3^2)), \quad 1 \leq n \leq N. \quad (4.30)$$

Furthermore, combining Eqs (2.5) and (2.6) and Lemma 2.5, it follows that

$$\begin{aligned} \|e^n\|_\theta &\leq \mu \tau^\alpha \|e^n\|_\theta + \mu \sum_{l=1}^{n-1} \Psi_{n-l} \|e^l\|_\theta + C \tau t_n^{\alpha-1} + C(\tau^{2\alpha} + h_1^2 + h_2^2 + h_3^2) \\ &\leq \mu \tau^\alpha \|e^n\|_\theta + C \mu \tau \sum_{l=1}^{n-1} t_{n-l}^{\alpha-1} \|e^l\|_\theta + C \tau t_n^{\alpha-1} + C(\tau^{2\alpha} + h_1^2 + h_2^2 + h_3^2), \quad 1 \leq n \leq N. \end{aligned} \quad (4.31)$$

Since Eq (3.15) is satisfied, we can further derive from Lemma 2.6 that

$$\|e^n\|_\theta \leq C \tau t_n^{\alpha-1} + C(\tau^{2\alpha} + h_1^2 + h_2^2 + h_3^2), \quad 1 \leq n \leq N.$$

Finally, using Eq (4.3), we are able to derive the desired results:

$$\|e^n\| \leq C \tau t_n^{\alpha-1} + C(\tau^{2\alpha} + h_1^2 + h_2^2 + h_3^2), \quad 1 \leq n \leq N.$$

5. Numerical result

This section presents a numerical experiment to verify the accuracy and computational efficiency of the proposed GL-ADI scheme.

5.1. Example 1

Consider the following linear subdiffusion problem

$$D_t^\alpha u = \nabla \cdot (\kappa(x, y, z) \nabla u) + \mu u + f(x, y, z, t),$$

with the coefficients

$$\kappa(x, y, z) = \begin{pmatrix} 1 + e^{-2x} & 0 & 0 \\ 0 & 1 + e^{-2y} & 0 \\ 0 & 0 & 1 + e^{-2z} \end{pmatrix}, \mu = 0.3,$$

$$\begin{aligned} f(x, y, z, t) = & \Gamma(1 + \alpha) \sin x \sin y \sin z + t^\alpha \sin y \sin z (2e^{-2x} \cos x + (1 + e^{-2x}) \sin x) \\ & + t^\alpha \sin x \sin z (2e^{-2y} \cos y + (1 + e^{-2y}) \sin y) + t^\alpha \sin x \sin y (2e^{-2z} \cos z + (1 + e^{-2z}) \sin z) \\ & - \mu t^\alpha \sin x \sin y \sin z. \end{aligned}$$

An exact solution featuring the inherent typicality of initial weak singularity is given by

$$u(x, y, z, t) = t^\alpha \sin x \sin y \sin z.$$

We specify the computational domain as $\Omega \times (0, T]$, where the spatial domain is $\Omega = (0, \pi) \times (0, \pi) \times (0, \pi)$, and the terminal time is set to $T = 1$. A uniform spatial grid is employed, with the grid spacing satisfying $h = h_1 = h_2 = h_3$. The global temporal error associated with the numerical solution is defined as

$$E_1 = \max_{1 \leq n \leq N} \|u(t_n) - u^n\|,$$

while the local error at the final time $t = T$ is denoted by

$$E_2 = \|u(t_N) - u^N\|.$$

Through numerical experiments, we investigated the errors and the corresponding convergence orders when the parameters $\alpha = 0.4, 0.6, 0.8$. The relevant results are shown in Table 1. This numerical scheme achieves a global temporal convergence order of $O(N^{-\alpha})$. For $\alpha = 0.4, 0.6, 0.8$, the local temporal convergence orders are shown to be $O(N^{-\min\{1, 2\alpha\}})$, which is in good agreement with our theoretical estimates as shown in Table 2. To verify the spatial accuracy, a sufficiently small time step is selected such that the temporal discretization error is negligible compared to the spatial error component. Numerical data in Table 3 verifies second-order spatial convergence of the presented GL-ADI scheme. To further verify the accuracy and efficiency of the method, we compared the GL-ADI method with the L1-ADI method. Tables 1 and 2 present the global error, local error, convergence rate, and CPU time of the GL-ADI method and the L1-ADI method. Figure 1 illustrates the slice contour profiles of numerical solutions at various time levels for Example 5.1 with $\alpha = 0.6$ and $M_1 = M_2 = M_3 = N = 32$. Figure 2 presents the slice contour plots of the errors for Example 5.1 at different time levels, with the parameter $\alpha = 0.8$ and $M_1 = M_2 = M_3 = N = 32$.

Table 1. Comparative study of global L^2 errors and convergence rates for Example 5.1 ($M_1 = M_2 = M_3 = 64$).

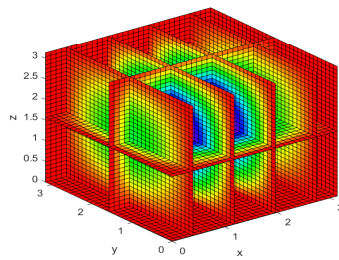
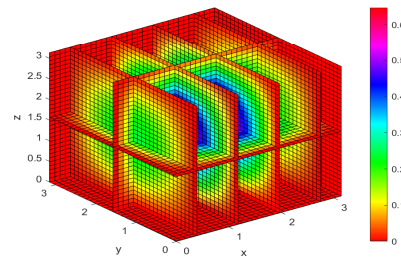
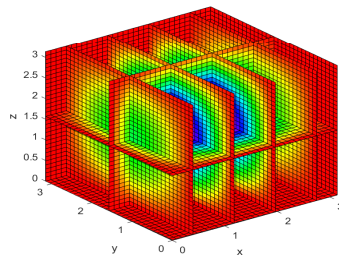
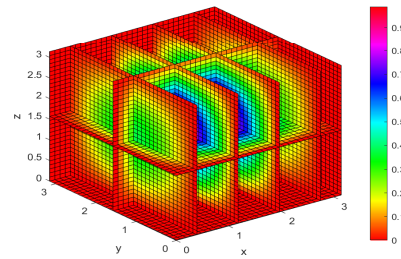
α	N	GL-ADI scheme		L1-ADI scheme	
		E_1	Rate	E_1	Rate
0.4	32	1.058×10^{-1}	–	1.147×10^{-1}	–
	64	6.083×10^{-2}	0.799	7.659×10^{-2}	0.582
	128	3.839×10^{-2}	0.664	5.383×10^{-2}	0.509
	256	2.562×10^{-2}	0.583	3.943×10^{-2}	0.449
0.6	32	3.012×10^{-2}	–	4.584×10^{-2}	–
	64	1.722×10^{-2}	0.807	2.969×10^{-2}	0.627
	128	1.077×10^{-2}	0.677	1.990×10^{-2}	0.577
	256	7.051×10^{-3}	0.611	1.346×10^{-2}	0.564
0.8	32	8.717×10^{-3}	–	1.657×10^{-2}	–
	64	4.677×10^{-3}	0.898	9.746×10^{-3}	0.766
	128	2.673×10^{-3}	0.807	5.839×10^{-3}	0.739
	256	1.551×10^{-3}	0.785	3.471×10^{-3}	0.750

Table 2. Comparative study of local L^2 errors, convergence rates, and CPU times for Example 5.1 ($M_1 = M_2 = M_3 = 64$).

α	N	GL-ADI scheme			L1-ADI scheme		
		E_2	Rate	CPU(s)	E_2	Rate	CPU(s)
0.4	32	1.016×10^{-1}	–	101.419	8.016×10^{-2}	–	153.232
	64	5.569×10^{-2}	0.868	249.558	4.399×10^{-2}	0.866	298.479
	128	3.082×10^{-2}	0.854	706.720	2.441×10^{-2}	0.850	849.709
	256	1.723×10^{-2}	0.839	2253.972	$1.370e \times 10^{-2}$	0.834	2708.792
0.6	32	2.519×10^{-2}	–	95.451	2.047×10^{-2}	–	121.848
	64	$1.066e \times 10^{-2}$	1.241	244.947	8.725×10^{-3}	1.231	300.545
	128	4.637×10^{-3}	1.201	702.317	3.837×10^{-3}	1.185	718.381
	256	2.105×10^{-3}	1.139	2253.270	1.772×10^{-3}	1.115	2239.007
0.8	32	7.068×10^{-3}	–	95.077	7.101×10^{-3}	–	123.255
	64	2.439×10^{-3}	1.535	243.774	2.609×10^{-3}	1.444	304.708
	128	9.527×10^{-4}	1.356	705.730	1.079×10^{-3}	1.274	843.495
	256	4.808×10^{-4}	0.987	2256.413	5.498×10^{-4}	0.973	2259.400

Table 3. Spatial accuracy analysis of Example 5.1 with $\tau = h^2$.

α	$M_1 = M_2 = M_3$	E_1	Rate
0.6	4	1.074×10^{-1}	–
	8	2.551×10^{-2}	2.073
	16	1.591×10^{-2}	2.117
	32	1.082×10^{-2}	2.115
0.8	4	7.369×10^{-2}	–
	8	1.855×10^{-2}	1.990
	16	1.176×10^{-2}	2.041
	32	8.110×10^{-3}	2.039

(a) Numerical solution at $t = 1/4$.(b) Numerical solution at $t = 1/2$.(c) Numerical solution at $t = 3/4$.(d) Numerical solution at $t = 1$.**Figure 1.** Slice contour plots of the numerical approximation at various time points for the Example 5.1 ($\alpha = 0.6, M_1 = M_2 = M_3 = N = 32$).

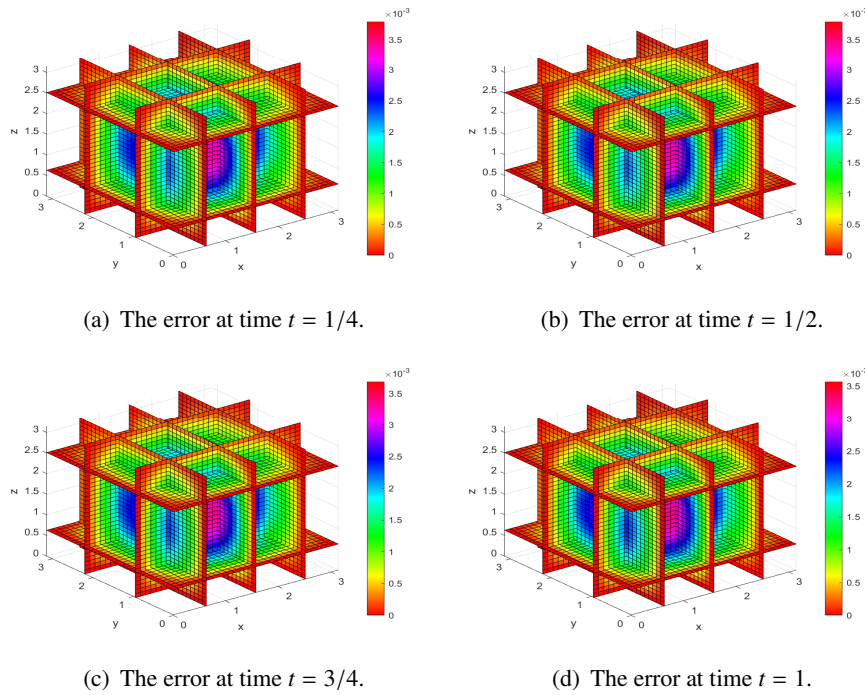


Figure 2. The slice contour plot showing the errors at different time points in the demonstration Example 5.1 ($\alpha = 0.8, M_1 = M_2 = M_3 = N = 32$).

5.2. Example 2

Consider the following linear subdiffusion Eqs (1.1)–(1.3):

$$D_t^\alpha u = \nabla \cdot (\kappa(x, y, z) \nabla u) + \mu u$$

with the coefficients

$$\kappa(x, y, z) = \begin{pmatrix} 1 + \sin^2 x & 0 & 0 \\ 0 & 1 + \sin^2 y & 0 \\ 0 & 0 & 1 + \sin^2 z \end{pmatrix}, \mu = 0.5,$$

and the initial condition

$$u_0(x, y, z) = \frac{1}{2} \sin x \sin y \sin z.$$

The spatial domain is set to $\Omega = (0, \pi)^3$, and the terminal time is chosen as $T = 1$. Since an exact analytical solution to the considered problem is not available, we adopt the two-grid method [38] to evaluate the numerical errors and the associated convergence rates. To this end, we introduce the following definitions:

$$E_3 = \max_{1 \leq n \leq N} \|u^n - q^{2n}\|, \quad E_4 = \|u^N - q^{2N}\|.$$

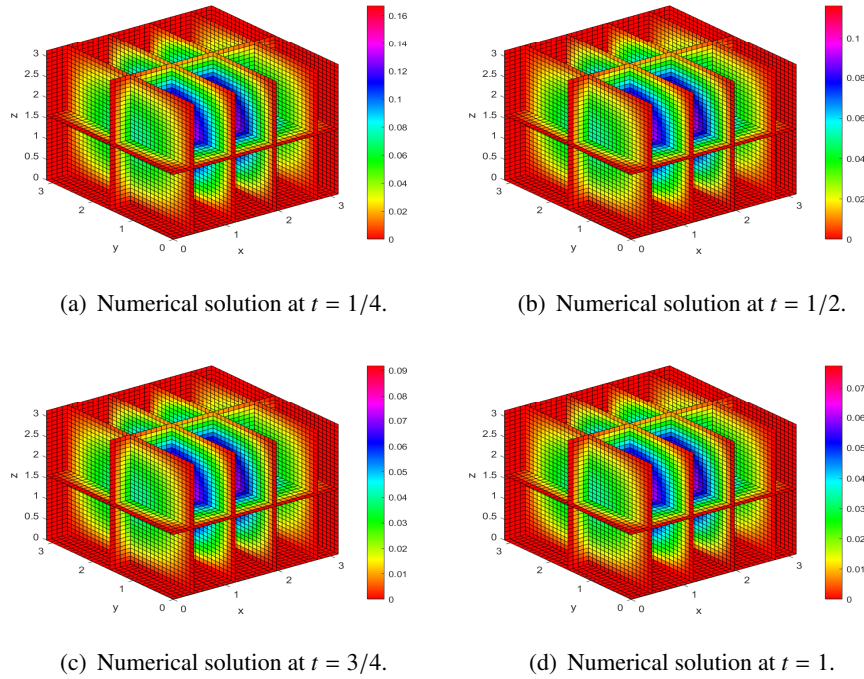


Figure 3. Slice contour plots of the numerical approximation at various time points for the Example 5.2 ($M_1 = M_2 = M_3 = N = 32$).

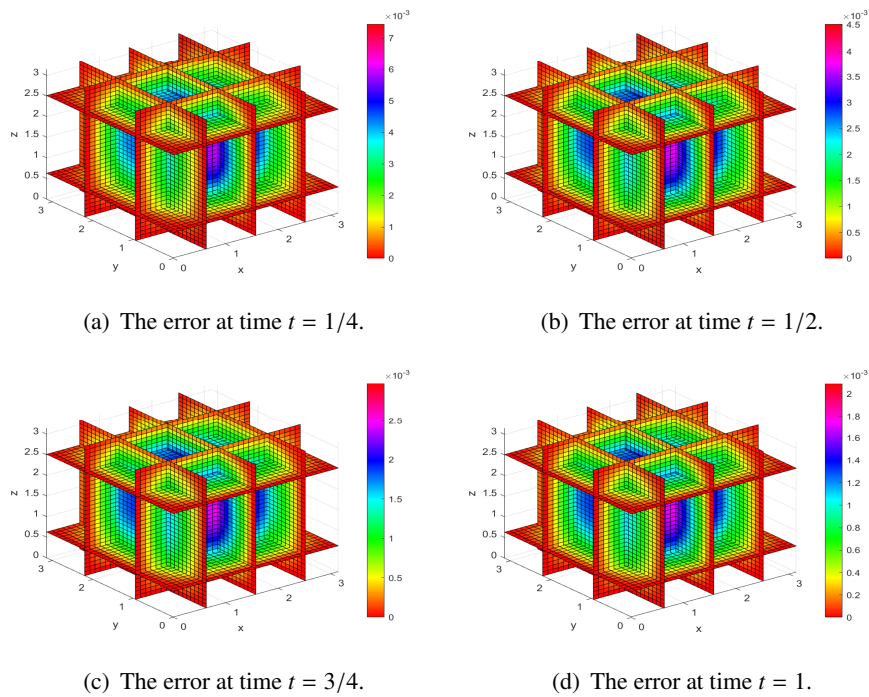


Figure 4. The slice contour plot showing the errors at different time points in the demonstration Example 5.2 ($\alpha = 0.8, M_1 = M_2 = M_3 = N = 32$).

Herein, q^m for $0 \leq m \leq 2N$ represents the numerical solution computed on the refined temporal mesh with grid points $t_m = mT/(2N)$. As shown in Tables 4 and 5, the numerical scheme achieves a global convergence order of $O(N^{-\alpha})$ and a local convergence order of $O(N^{-\min\{2\alpha, 1\}})$, which is in full agreement with the theoretical findings established in Theorem 4.3. Figure 3 presents the slice contour plots of the approximate solutions at different time instants for Example 5.2 with $\alpha = 0.6$ and $M_1 = M_2 = M_3 = N = 32$. Figure 4 presents the slice contour plots of the errors for Example 5.2 at different time levels, with the parameter $\alpha = 0.8$ and $M_1 = M_2 = M_3 = N = 32$.

Table 4. Global L^2 norm error and convergence rate for Example 5.2 ($M_1 = M_2 = M_3 = 32$).

α	N	E_3	Rate
0.4	64	6.336×10^{-2}	–
	128	4.267×10^{-2}	0.571
	256	2.926×10^{-2}	0.544
	512	2.049×10^{-2}	0.514
0.6	64	1.441×10^{-2}	–
	128	9.518×10^{-3}	0.792
	256	6.455×10^{-3}	0.740
	512	4.471×10^{-3}	0.699
0.8	64	8.472×10^{-3}	–
	128	4.091×10^{-3}	1.050
	256	2.030×10^{-3}	1.011
	512	1.021×10^{-3}	0.997

Table 5. Local L^2 norm error and convergence rate for Example 5.2 ($M_1 = M_2 = M_3 = 32$).

α	N	E_4	Rate
0.4	64	2.508×10^{-2}	–
	128	1.325×10^{-2}	0.921
	256	7.140×10^{-2}	0.892
	512	3.909×10^{-2}	0.869
0.6	64	5.181×10^{-3}	–
	128	2.182×10^{-3}	1.1247
	256	9.391×10^{-4}	1.2165
	512	4.098×10^{-4}	1.1962
0.8	64	1.734×10^{-3}	–
	128	7.119×10^{-4}	1.284
	256	3.081×10^{-4}	1.208
	512	1.389×10^{-4}	1.150

6. Conclusions

In this paper, we construct a fully discrete GL-ADI GFDM method for solving three-dimensional non-local diffusion equations with anisotropic diffusion coefficients. The Grünwald-Letnikov formula is adopted to discretize the Caputo time fractional derivative, while a general finite difference scheme is employed for spatial discretization. By virtue of the alternating direction implicit splitting technique, the computational overhead of three-dimensional problems is substantially lowered. Moreover, rigorous theoretical proofs are presented to verify the stability and convergence of the established numerical scheme. Error analysis demonstrates that the scheme achieves a local temporal convergence order of $O(\tau^{\min\{2\alpha, 1\}})$ and a global temporal convergence order of $O(\tau^\alpha)$. Numerical examples are finally carried out to validate the correctness and validity of the theoretical conclusions. Regarding the extension of other boundary conditions and nonlinear problems, this will be left for future research.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare there is no conflict of interest.

Author contributions

The work presented here was performed in collaboration among all authors. Jia Liu: Designed, analyzed, guided the full text, wrote the paper, provided and analyzed the experimental data. Haixiang Zhang: Conceived and designed the research. All authors contributed to and approved the manuscript.

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Appendix A

A. Detailed proofs of Lemmas 4.1 and 4.2

Lemma A.1. For any mesh functions $\phi, \varphi \in \mathcal{W}_h$, one has

$$\begin{aligned}
 (\mathcal{A}_x \phi, \varphi) &= (\phi, \mathcal{A}_x \varphi), (\mathcal{A}_y \phi, \varphi) = (\phi, \mathcal{A}_y \varphi), (\mathcal{A}_z \phi, \varphi) = (\phi, \mathcal{A}_z \varphi), \\
 (\mathcal{A}_x \mathcal{A}_y \phi, \varphi) &= (\phi, \mathcal{A}_x \mathcal{A}_y \varphi), (\mathcal{A}_y \mathcal{A}_z \phi, \varphi) = (\phi, \mathcal{A}_y \mathcal{A}_z \varphi), (\mathcal{A}_x \mathcal{A}_z \phi, \varphi) = (\phi, \mathcal{A}_x \mathcal{A}_z \varphi) \\
 (\mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \phi, \varphi) &= (\phi, \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \varphi).
 \end{aligned}$$

Proof. It follows from the definition of $\mathcal{A}_x$ that

$$\begin{aligned}
 (\mathcal{A}_x \phi, \varphi) &= h_1 h_2 h_3 \sum_{j=1}^{M_1-1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} \frac{1}{h_1} \left((\kappa_x)_{j+\frac{1}{2}} \delta_x \phi_{j+\frac{1}{2},k,s} - (\kappa_x)_{j-\frac{1}{2}} \delta_x \phi_{j-\frac{1}{2},k,s} \right) \cdot \varphi_{j,k,s} \\
 &= h_1 h_2 h_3 \sum_{j=2}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} \frac{1}{h_1} (\kappa_x)_{j-\frac{1}{2}} \delta_x \phi_{j-\frac{1}{2},k,s} \varphi_{j-1,k,s}
 \end{aligned} \tag{A.1}$$

$$\begin{aligned}
& -h_1 h_2 h_3 \sum_{j=1}^{M_1-1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} \frac{1}{h_1} (\kappa_x)_{j-\frac{1}{2}} \delta_x \phi_{j-\frac{1}{2},k,s} \cdot \varphi_{j,k,s} \\
& = -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} \frac{1}{h_1} (\kappa_x)_{j-\frac{1}{2}} \delta_x \phi_{j-\frac{1}{2},k,s} \cdot (\varphi_{j,k,s} - \varphi_{j-1,k,s}) \\
& \quad - h_1 h_2 h_3 \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} \frac{1}{h_1} (\kappa_x)_{j-\frac{1}{2}} \delta_x \phi_{\frac{1}{2},k,s} \cdot \varphi_{0,k,s} \\
& \quad + h_1 h_2 h_3 \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} \frac{1}{h_1} (\kappa_x)_{j-\frac{1}{2}} \delta_x \phi_{M_1-\frac{1}{2},k,s} \cdot \varphi_{M_1,k,s} \\
& = -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} \delta_x \phi_{j-\frac{1}{2},k,s} \cdot \delta_x \varphi_{j-\frac{1}{2},k,s}.
\end{aligned}$$

Further,

$$\begin{aligned}
(\phi, \mathcal{A}_x \varphi) & = h_1 h_2 h_3 \sum_{j=1}^{M_1-1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} \frac{1}{h_1} \left((\kappa_x)_{j+\frac{1}{2}} \delta_x \varphi_{j+\frac{1}{2},k,s} - (\kappa_x)_{j-\frac{1}{2}} \delta_x \varphi_{j-\frac{1}{2},k,s} \right) \cdot \phi_{j,k,s} \quad (\text{A.2}) \\
& = h_1 h_2 h_3 \sum_{j=2}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} \frac{1}{h_1} (\kappa_x)_{j-\frac{1}{2}} \delta_x \varphi_{j-\frac{1}{2},k,s} \phi_{j-1,k,s} \\
& \quad - h_1 h_2 h_3 \sum_{j=1}^{M_1-1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} \frac{1}{h_1} (\kappa_x)_{j-\frac{1}{2}} \delta_x \varphi_{j-\frac{1}{2},k,s} \cdot \phi_{j,k,s}.
\end{aligned}$$

Then,

$$\begin{aligned}
(\phi, \mathcal{A}_x \varphi) & = -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} \frac{1}{h_1} (\kappa_x)_{j-\frac{1}{2}} \delta_x \varphi_{j-\frac{1}{2},k,s} \cdot (\phi_{j,k,s} - \phi_{j-1,k,s}) \quad (\text{A.3}) \\
& \quad - h_1 h_2 h_3 \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} \frac{1}{h_1} (\kappa_x)_{j-\frac{1}{2}} \delta_x \varphi_{\frac{1}{2},k,s} \cdot \phi_{0,k,s} \\
& \quad + h_1 h_2 h_3 \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} \frac{1}{h_1} (\kappa_x)_{j-\frac{1}{2}} \delta_x \varphi_{M_1-\frac{1}{2},k,s} \cdot \phi_{M_1,k,s} \\
& = -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} \delta_x \varphi_{j-\frac{1}{2},k,s} \cdot \delta_x \phi_{j-\frac{1}{2},k,s}.
\end{aligned}$$

Therefore, from Eqs (A.1)–(A.3), we can obtain $(\mathcal{A}_x \phi, \varphi) = (\phi, \mathcal{A}_x \varphi)$.

It follows from the definition of $\mathcal{A}_x, \mathcal{A}_y$ that

$$(\mathcal{A}_x \mathcal{A}_y \phi, \varphi) = -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\delta_x \mathcal{A}_y \phi_{j-\frac{1}{2},k,s}) (\delta_x \varphi_{j-\frac{1}{2},k,s}) \quad (\text{A.4})$$

$$\begin{aligned}
&= -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} \delta_x \frac{1}{h_2} \left((\kappa_y)_{k+\frac{1}{2}} \delta_y \phi_{j-\frac{1}{2}, k+\frac{1}{2}, s} - (\kappa_y)_{k-\frac{1}{2}} \delta_y \phi_{j-\frac{1}{2}, k-\frac{1}{2}, s} \right) (\delta_x \varphi_{j-\frac{1}{2}, k, s}) \\
&= -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=2}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} \frac{1}{h_2} \frac{\delta_y \phi_{j, k-\frac{1}{2}, s} - \delta_y \phi_{j-1, k-\frac{1}{2}, s}}{h_1} (\delta_x \varphi_{j-\frac{1}{2}, k-1, s}) \\
&\quad + h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} \frac{1}{h_2} \frac{\delta_y \phi_{j, k-\frac{1}{2}, s} - \delta_y \phi_{j-1, k-\frac{1}{2}, s}}{h_1} (\delta_x \varphi_{j-\frac{1}{2}, k, s}).
\end{aligned}$$

Then, one has

$$\begin{aligned}
(\mathcal{A}_x \mathcal{A}_y \phi, \varphi) &= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} \frac{\delta_y \phi_{j, k-\frac{1}{2}, s} - \delta_y \phi_{j-1, k-\frac{1}{2}, s}}{h_1} \cdot \frac{\delta_x \varphi_{j-\frac{1}{2}, k, s} - \delta_x \varphi_{j-\frac{1}{2}, k-1, s}}{h_2} \quad (\text{A.5}) \\
&\quad + h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{\frac{1}{2}} \frac{1}{h_2} \frac{\delta_y \phi_{j, \frac{1}{2}, s} - \delta_y \phi_{j-1, \frac{1}{2}, s}}{h_1} (\delta_x \varphi_{j-\frac{1}{2}, 0, s}) \\
&\quad - h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{M_2-\frac{1}{2}} \frac{1}{h_2} \frac{\delta_y \phi_{j, M_2-\frac{1}{2}, s} - \delta_y \phi_{j-1, M_2-\frac{1}{2}, s}}{h_1} (\delta_x \varphi_{j-\frac{1}{2}, M_2, s}) \\
&= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} \delta_x \delta_y \phi_{j-\frac{1}{2}, k-\frac{1}{2}, s} \delta_x \delta_y \varphi_{j-\frac{1}{2}, k-\frac{1}{2}, s}.
\end{aligned}$$

By the same reasoning, we have

$$(\phi, \mathcal{A}_x \mathcal{A}_y \varphi) = h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} \delta_x \delta_y \phi_{j-\frac{1}{2}, k-\frac{1}{2}, s} \delta_x \delta_y \varphi_{j-\frac{1}{2}, k-\frac{1}{2}, s}. \quad (\text{A.6})$$

From Eqs (A.4) to (A.6), we can obtain $(\mathcal{A}_x \mathcal{A}_y \varphi, \phi) = (\varphi, \mathcal{A}_x \mathcal{A}_y \phi)$.

It follows from the definition of $\mathcal{A}_x, \mathcal{A}_y, \mathcal{A}_z$ that

$$\begin{aligned}
(\mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \phi, \varphi) &= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3-1} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\delta_x \delta_y \mathcal{A}_z \phi_{j-\frac{1}{2}, k-\frac{1}{2}, s}) (\delta_x \delta_y \varphi_{j-\frac{1}{2}, k-\frac{1}{2}, s}) \quad (\text{A.7}) \\
&= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3-1} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} \delta_x \delta_y \frac{1}{h_3} \left((\kappa_z)_{s+\frac{1}{2}} \delta_z \phi_{j-\frac{1}{2}, k-\frac{1}{2}, s+\frac{1}{2}} \right. \\
&\quad \left. - (\kappa_z)_{s-\frac{1}{2}} \delta_z \phi_{j-\frac{1}{2}, k-\frac{1}{2}, s-\frac{1}{2}} \right) (\delta_x \delta_y \varphi_{j-\frac{1}{2}, k-\frac{1}{2}, s}) \\
&= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=2}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} \frac{1}{h_3} \frac{\delta_x \delta_z \phi_{j, k, s-\frac{1}{2}} - \delta_x \delta_z \phi_{j-1, k, s-\frac{1}{2}}}{h_1} (\delta_x \delta_y \varphi_{j-\frac{1}{2}, k-\frac{1}{2}, s-1}) \\
&\quad - h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3-1} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} \frac{1}{h_3} \frac{\delta_x \delta_z \phi_{j, k, s-\frac{1}{2}} - \delta_x \delta_z \phi_{j-1, k, s-\frac{1}{2}}}{h_1} (\delta_x \delta_y \varphi_{j-\frac{1}{2}, k-\frac{1}{2}, s})
\end{aligned}$$

$$\begin{aligned}
&= -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} \frac{\delta_x \delta_z \phi_{j,k,s-\frac{1}{2}} - \delta_x \delta_z \phi_{j-1,k,s-\frac{1}{2}}}{h_1} \\
&\quad \cdot \frac{\delta_x \delta_y \varphi_{j-\frac{1}{2},k-\frac{1}{2},s} - \delta_x \delta_y \varphi_{j-\frac{1}{2},k-\frac{1}{2},s-1}}{h_3} \\
&\quad - h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{\frac{1}{2}} \frac{1}{h_3} \frac{\delta_x \delta_z \phi_{j,k,\frac{1}{2}} - \delta_x \delta_z \phi_{j-1,k,\frac{1}{2}}}{h_1} (\delta_x \delta_y \varphi_{j-\frac{1}{2},k,0}) \\
&\quad + h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{M_3-\frac{1}{2}} \frac{1}{h_3} \frac{\delta_x \delta_z \phi_{j,k,M_3-\frac{1}{2}} - \delta_x \delta_z \phi_{j-1,k,M_3-\frac{1}{2}}}{h_1} (\delta_x \delta_y \varphi_{j-\frac{1}{2},k,M_3}) \\
&= -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} \delta_x \delta_y \delta_z \phi_{j-\frac{1}{2},k-\frac{1}{2},s-\frac{1}{2}} \delta_x \delta_y \delta_z \varphi_{j-\frac{1}{2},k-\frac{1}{2},s-\frac{1}{2}}.
\end{aligned}$$

By applying the same method, we can obtain

$$(\phi, \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \varphi) = -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} \delta_x \delta_y \delta_z \phi_{j-\frac{1}{2},k-\frac{1}{2},s-\frac{1}{2}} \delta_x \delta_y \delta_z \varphi_{j-\frac{1}{2},k-\frac{1}{2},s-\frac{1}{2}}. \quad (\text{A.8})$$

Then, from Eqs (A.7) and (A.8), we can obtain $(\mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \phi, \varphi) = (\phi, \mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \varphi)$.

Similarly, it can be proved that

$$(\mathcal{A}_y \phi, \varphi) = (\phi, \mathcal{A}_y \varphi), (\mathcal{A}_z \phi, \varphi) = (\phi, \mathcal{A}_z \varphi), (\mathcal{A}_y \mathcal{A}_z \phi, \varphi) = (\phi, \mathcal{A}_y \mathcal{A}_z \varphi), (\mathcal{A}_x \mathcal{A}_z \phi, \varphi) = (\phi, \mathcal{A}_x \mathcal{A}_z \varphi).$$

Lemma A.2. For any mesh functions $\phi \in \mathring{\mathcal{W}}_h$,

$$(\phi, \phi)_\theta \geq 0.$$

Proof. According to the definition of $(\cdot, \cdot)_\theta$ in Eq (4.1), one gets

$$(\phi, \phi)_\theta = (\phi, \phi) + \theta^2 (\mathcal{A}_x \mathcal{A}_y \phi, \phi) + \theta^2 (\mathcal{A}_y \mathcal{A}_z \phi, \phi) + \theta^2 (\mathcal{A}_x \mathcal{A}_z \phi, \phi) - \theta^3 (\mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \phi, \phi). \quad (\text{A.9})$$

Let us first analyze $(\mathcal{A}_x \mathcal{A}_y \phi, \phi)$ in Eq (A.9):

$$\begin{aligned}
(\mathcal{A}_x \mathcal{A}_y \phi, \phi) &= -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\delta_x \mathcal{A}_y \phi_{j-\frac{1}{2},k,s}) (\delta_x \phi_{j-\frac{1}{2},k,s}) \\
&= -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} \delta_x \frac{1}{h_2} ((\kappa_y)_{k+\frac{1}{2}} \delta_y \phi_{j-\frac{1}{2},k+\frac{1}{2},s} - (\kappa_y)_{k-\frac{1}{2}} \delta_y \phi_{j-\frac{1}{2},k-\frac{1}{2},s}) (\delta_x \phi_{j-\frac{1}{2},k,s}) \\
&= -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=2}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} \frac{1}{h_2} \frac{\delta_y \phi_{j,k-\frac{1}{2},s} - \delta_y \phi_{j-1,k-\frac{1}{2},s}}{h_1} (\delta_x \phi_{j-\frac{1}{2},k-1,s}) \\
&\quad + h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2-1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} \frac{1}{h_2} \frac{\delta_y \phi_{j,k-\frac{1}{2},s} - \delta_y \phi_{j-1,k-\frac{1}{2},s}}{h_1} (\delta_x \phi_{j-\frac{1}{2},k,s})
\end{aligned} \quad (\text{A.10})$$

$$\begin{aligned}
&= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} \frac{\delta_y \phi_{j,k-\frac{1}{2},s} - \delta_y \phi_{j-1,k-\frac{1}{2},s}}{h_1} \cdot \frac{\delta_x \phi_{j-\frac{1}{2},k,s} - \delta_x \phi_{j-\frac{1}{2},k-1,s}}{h_2} \\
&\quad + h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{\frac{1}{2}} \frac{1}{h_2} \frac{\delta_y \phi_{j,\frac{1}{2},s} - \delta_y \phi_{j-1,\frac{1}{2},s}}{h_1} (\delta_x \phi_{j-\frac{1}{2},0,s}) \\
&\quad - h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{M_2-\frac{1}{2}} \frac{1}{h_2} \frac{\delta_y \phi_{j,M_2-\frac{1}{2},s} - \delta_y \phi_{j-1,M_2-\frac{1}{2},s}}{h_1} (\delta_x \phi_{j-\frac{1}{2},M_2,s}) \\
&= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} \delta_x \delta_y \phi_{j-\frac{1}{2},k-\frac{1}{2},s} \delta_x \delta_y \phi_{j-\frac{1}{2},k-\frac{1}{2},s} \\
&= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\delta_x \delta_y \phi_{j-\frac{1}{2},k-\frac{1}{2},s})^2 \geq 0.
\end{aligned}$$

Similarly,

$$\begin{aligned}
(\mathcal{A}_y \mathcal{A}_z \phi, \phi) &= h_2 h_3 h_1 \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} \sum_{j=1}^{M_1} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} \delta_y \delta_z \phi_{j,k-\frac{1}{2},s-\frac{1}{2}} \delta_y \delta_z \phi_{j,k-\frac{1}{2},s-\frac{1}{2}} \\
&= h_2 h_3 h_1 \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} \sum_{j=1}^{M_1} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} (\delta_y \delta_z \phi_{j,k-\frac{1}{2},s-\frac{1}{2}})^2 \geq 0,
\end{aligned} \tag{A.11}$$

and

$$\begin{aligned}
(\mathcal{A}_x \mathcal{A}_z \phi, \phi) &= h_1 h_3 h_2 \sum_{j=1}^{M_1} \sum_{s=1}^{M_3} \sum_{k=1}^{M_2} (\kappa_x)_{j-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} \delta_x \delta_z \phi_{j-\frac{1}{2},k,s-\frac{1}{2}} \delta_x \delta_z \phi_{j-\frac{1}{2},k,s-\frac{1}{2}} \\
&= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} (\delta_x \delta_z \phi_{j-\frac{1}{2},k,s-\frac{1}{2}})^2 \geq 0.
\end{aligned} \tag{A.12}$$

Then, we conduct an analysis $(\mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \phi, \phi)$ in Eq (A.9):

$$\begin{aligned}
(\mathcal{A}_x \mathcal{A}_y \mathcal{A}_z \phi, \phi) &= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3-1} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\delta_x \delta_y \mathcal{A}_z \phi_{j-\frac{1}{2},k-\frac{1}{2},s}) (\delta_x \delta_y \phi_{j-\frac{1}{2},k-\frac{1}{2},s}) \\
&= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3-1} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} \delta_x \delta_y \frac{1}{h_3} \left((\kappa_z)_{s+\frac{1}{2}} \delta_z \phi_{j-\frac{1}{2},k-\frac{1}{2},s+\frac{1}{2}} \right. \\
&\quad \left. - (\kappa_z)_{s-\frac{1}{2}} \delta_z \phi_{j-\frac{1}{2},k-\frac{1}{2},s-\frac{1}{2}} \right) (\delta_x \delta_y \phi_{j-\frac{1}{2},k-\frac{1}{2},s}) \\
&= h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=2}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} \frac{1}{h_3} \frac{\delta_x \delta_z \phi_{j,k,s-\frac{1}{2}} - \delta_x \delta_z \phi_{j-1,k,s-\frac{1}{2}}}{h_1} (\delta_x \delta_y \phi_{j-\frac{1}{2},k-\frac{1}{2},s-1}) \\
&\quad - h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3-1} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} \frac{1}{h_3} \frac{\delta_x \delta_z \phi_{j,k,s-\frac{1}{2}} - \delta_x \delta_z \phi_{j-1,k,s-\frac{1}{2}}}{h_1} (\delta_x \delta_y \phi_{j-\frac{1}{2},k-\frac{1}{2},s})
\end{aligned} \tag{A.13}$$

$$\begin{aligned}
&= -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} \frac{\delta_x \delta_z \phi_{j,k,s-\frac{1}{2}} - \delta_x \delta_z \phi_{j-1,k,s-\frac{1}{2}}}{h_1} \\
&\quad \cdot \frac{\delta_x \delta_y \phi_{j-\frac{1}{2},k-\frac{1}{2},s} - \delta_x \delta_y \phi_{j-\frac{1}{2},k-\frac{1}{2},s-1}}{h_3} \\
&\quad - h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{\frac{1}{2}} \frac{1}{h_3} \frac{\delta_x \delta_z \phi_{j,k,\frac{1}{2}} - \delta_x \delta_z \phi_{j-1,k,\frac{1}{2}}}{h_1} (\delta_x \delta_y \phi_{j-\frac{1}{2},k,0}) \\
&\quad + h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{M_3-\frac{1}{2}} \frac{1}{h_3} \frac{\delta_x \delta_z \phi_{j,k,M_3-\frac{1}{2}} - \delta_x \delta_z \phi_{j-1,k,M_3-\frac{1}{2}}}{h_1} (\delta_x \delta_y \phi_{j-\frac{1}{2},k,M_3}) \\
&= -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} \delta_x \delta_y \delta_z \phi_{j-\frac{1}{2},k-\frac{1}{2},s-\frac{1}{2}} \delta_x \delta_y \delta_z \phi_{j-\frac{1}{2},k-\frac{1}{2},s-\frac{1}{2}} \\
&= -h_1 h_2 h_3 \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \sum_{s=1}^{M_3} (\kappa_x)_{j-\frac{1}{2}} (\kappa_y)_{k-\frac{1}{2}} (\kappa_z)_{s-\frac{1}{2}} (\delta_x \delta_y \delta_z \phi_{j-\frac{1}{2},k-\frac{1}{2},s-\frac{1}{2}})^2 \geq 0.
\end{aligned}$$

From Eqs (A.10)–(A.13), we can obtain

$$(\phi, \phi)_\theta \geq 0.$$



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