

## An Efficient Second-Order Finite Volume ADI Method for Nonlinear Three-Dimensional Space-Fractional Reaction-Diffusion Equations

Bingyin Zhang<sup>1</sup>, Hongfei Fu<sup>2,\*</sup>, Xueting Liang<sup>1</sup>, Jun Liu<sup>1</sup>  
and Jiansong Zhang<sup>1</sup>

<sup>1</sup> College of Science, China University of Petroleum (East China), Qingdao, Shandong 266580, China

<sup>2</sup> School of Mathematical Sciences, Ocean University of China, Qingdao, Shandong 266100, China

Received 5 May 2021; Accepted (in revised version) 2 December 2021

---

**Abstract.** In this paper, a three-dimensional time-dependent nonlinear Riesz space-fractional reaction-diffusion equation is considered. First, a linearized finite volume method, named BDF-FV, is developed and analyzed via the discrete energy method, in which the space-fractional derivative is discretized by the finite volume element method and the time derivative is treated by the backward differentiation formulae (BDF). The method is rigorously proved to be convergent with second-order accuracy both in time and space with respect to the discrete and continuous  $L^2$  norms. Next, by adding high-order perturbation terms in time to the BDF-FV scheme, an alternating direction implicit linear finite volume scheme, denoted as BDF-FV-ADI, is proposed. Convergence with second-order accuracy is also strictly proved under a rough temporal-spatial stepsize constraint. Besides, efficient implementation of the ADI method is briefly discussed, based on a fast conjugate gradient (FCG) solver for the resulting symmetric positive definite linear algebraic systems. Numerical experiments are presented to support the theoretical analysis and demonstrate the effectiveness and efficiency of the method for large-scale modeling and simulations.

**AMS subject classifications:** 65M08, 65M12, 65M15

**Key words:** Nonlinear space-fractional reaction-diffusion equation, finite volume method, ADI, convergence, efficient implementation.

---

\*Corresponding author.

Emails: s19090043@s.upc.edu.cn (B. Zhang), fhf@ouc.edu.cn (H. Fu), s20090006@s.upc.edu.cn (X. Liang), liujun@upc.edu.cn (J. Liu), jszhang@upc.edu.cn (J. Zhang)

## 1 Introduction

In the past decades, nonlinear space-fractional differential equations (s-FDEs) have been shown to provide an adequate and accurate description for challenging phenomena such as long-range interaction and anomalously diffusive transport in various science and engineering fields. For example, the fractional Allen-Cahn equation [2, 12] was applied to describe the mesoscale morphological pattern formation and interface motion; the fractional FitzHugh-Nagumo model [3] was used to represent impulse propagation in nerve membranes; and the fractional Bloch-Torrey equation [21] has been successfully used in magnetic resonance. However, in most case it is not available to obtain the analytical solutions [15,32] for fractional differential equations. Therefore, efficient numerical modeling becomes extremely urgent and important. Up to now, there has been an increasing interest in developing and analyzing efficient numerical methods, see [4, 7, 16, 19, 20, 23, 24, 28, 31, 35, 37, 38] and the references therein.

Due to the local conservation property, the finite volume (FV) method is particularly suitable for modeling and simulation of conservative type s-FDEs. Hejazi and Moroney [10] presented a finite volume approximation to the one-dimensional time-space fractional advection-dispersion equation, and showed that this method performs better than finite difference method for the considered problem with variable coefficient, since it deals with the equation directly in a conservative form. A preconditioned Lanczos method which uses finite volume spatial discretization for space-fractional reaction-diffusion equations was proposed and verified to be suitable for unstructured meshes in [36]. Liu et al. [20] presented a finite volume method for the space-fractional diffusion equation with variable coefficients and nonlinear source term. Simmons and Yang [27] developed a novel finite volume discretization based on non-uniform meshes for two-sided fractional diffusion equations with Riemann-Liouville derivative and proved the stability of the scheme. In order to obtain second-order temporal accuracy, some numerical techniques like Crank-Nicolson method [8, 38] and backward differentiation formulae (BDF) [5, 13] were considered for related fractional models. In particular, Fu et al. presented second-order Crank-Nicolson FV approximations for the two-dimensional s-FDEs [8], and for the three-dimensional nonlinear distributed-order s-FDEs [41]. Corresponding unconditional stability and error estimates in discrete energy norms were rigorously studied. However, the FV scheme coupling with the BDF method for nonlinear space-fractional models has not been studied yet.

In this paper, we are interested in the following three-dimensional nonlinear Riesz space-fractional reaction-diffusion equation (s-FRDEs) with orders  $\alpha$  ( $1 < \alpha < 2$ ) in  $x$ -direction,  $\beta$  ( $1 < \beta < 2$ ) in  $y$ -direction and  $\gamma$  ( $1 < \gamma < 2$ ) in  $z$ -direction [6, 13]:

$$\frac{\partial u}{\partial t} - d_x \frac{\partial^\alpha u(\mathbf{x}, t)}{\partial |x|^\alpha} - d_y \frac{\partial^\beta u(\mathbf{x}, t)}{\partial |y|^\beta} - d_z \frac{\partial^\gamma u(\mathbf{x}, t)}{\partial |z|^\gamma} = f(u) + g(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Omega \times (0, T], \quad (1.1a)$$

$$u(\mathbf{x}, t) = 0, \quad (\mathbf{x}, t) \in \partial\Omega \times [0, T], \quad u(\mathbf{x}, 0) = u^0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \quad (1.1b)$$

where  $T < \infty$  is the final time instant,  $\partial\Omega$  is the boundary of  $\Omega \subset \mathbb{R}^3$  and  $\mathbf{x} = (x, y, z)$ .

Generally speaking, numerical methods based on fully-implicit discretization for the nonlinear model (1.1a)–(1.1b) are usually proved to be *unconditionally* stable and convergent. However, one has to solve a system of nonlinear equations [12, 41], in which an extra iterative process must be imposed at each time level. To reduce the computational costs, many linearized numerical methods are developed. For example, Cheng et al. [6] presented a second-order Newton linearized compact difference scheme for the two-dimensional analogs of (1.1a), under the assumption that  $f(u) \in C^2(\mathbb{R})$ . Hu and Cao [13] utilized the BDF and temporal extrapolation techniques, and proposed a compact ADI scheme for the same model under the global Lipschitz continuous assumption of  $f(u)$ . Combining the fourth-order compact operator in space discretization, a linearized compact difference scheme was proposed in [40] for the two-dimensional nonlinear space-fractional Schrödinger equation, and then a compact ADI scheme was also presented and analyzed. The main purposes of this paper are (i) to develop an efficient linearized second-order accurate finite volume method for the three-dimensional model (1.1a) under assumption  $f(u) \in C^1(\mathbb{R})$ , and (ii) to establish corresponding convergence analysis under a weak temporal-spatial stepsize constraint. For discretization of the time derivative, we shall also use the two-step BDF scheme combined with second-order temporal extrapolation technique; while for the spatial counterpart, the linear finite volume element method is adopted.

From the perspective of computation, there will be huge computational complexity and storage problem when numerically solving multi-dimensional time-dependent models. To overcome these challenges, the alternating direction implicit (ADI) techniques, which reduce the solution of a multi-dimensional large-scale problem to a series of independent one-dimensional small-scale subproblems, have deserved great increasing research interests. For instance, Tadjeran and Meerschaert [29] proposed a second-order ADI difference method for the two-dimensional s-FDEs, and stability was discussed by using a spectral analysis method. Zhao et al. [40] established a fourth-order compact ADI difference scheme for the two-dimensional space-fractional Schrödinger equation. In [38], Zeng et al. developed an ADI Galerkin-Legendre spectral method for the two-dimensional nonlinear s-FRDEs and proved its stability and convergence. After that, Zhang et al. [39] extended this ADI method to the two-dimensional advection-diffusion equation with the Riesz space distributed-order derivative. Recently, Liu et al. [18] constructed and analyzed a second-order ADI finite volume method for the two-dimensional linear s-FDEs. Besides, due to the non-local nature of fractional derivatives, numerical methods for s-FDEs usually yield dense stiffness matrices which require  $\mathcal{O}(N^2)$  memory and  $\mathcal{O}(N^3)$  computational complexity per time step using the direct Gaussian elimination (GE) solver, where  $N$  is the total number of spatial unknowns. Wang et al. [33] then developed a fast ADI difference method, which only requires computational work of  $\mathcal{O}(N \log^2 N)$  per time step and memory of  $\mathcal{O}(N)$  without losing any accuracy. The idea was also adopted in e.g., [14, 18, 34]. These works inspire us to propose an efficient finite volume ADI method, denoted as BDF-FV-ADI, for the three-dimensional nonlinear s-FRDEs. Most importantly, it is well known that the ADI method is well suitable for

large-scale modeling and simulations via parallel computing.

The rest of this paper is organized as follows. In Section 2, some preliminary lemmas are presented. In Section 3, we propose the BDF-FV scheme and analyze the second-order convergence in the discrete and continuous  $L^2$  norms. Then, the BDF-FV-ADI method and corresponding error estimate are carefully discussed in Section 4, and also efficient implementation of the ADI method is briefly analyzed. In Section 5, we carry out several numerical experiments to verify the effectiveness and efficiency of the proposed method. Finally, we draw a brief conclusion. In the following, we use  $C$  to represent a general positive constant, which can be different under different circumstances.

## 2 Preliminaries

Let  $\Omega := (x_L, x_R) \times (y_L, y_R) \times (z_L, z_R)$  be the interested domain. In model (1.1a),  $u(\mathbf{x}, t)$  usually represents concentration, mass, or other physical quantities of interest,  $f(u) \in C^1(\mathbb{R})$  is a nonlinear reaction term and  $g(\mathbf{x}, t)$  is a given source or sink term. Besides,  $d_x, d_y$  and  $d_z$  are three positive constant-diffusivity coefficients. Moreover, the Risez space-fractional derivative  $\frac{\partial^\alpha u(\mathbf{x}, t)}{\partial |x|^\alpha}$  is defined by [25]

$$\frac{\partial^\alpha u(\mathbf{x}, t)}{\partial |x|^\alpha} := -\frac{1}{2\cos(\alpha\pi/2)} \frac{\partial}{\partial x} \left( \frac{\partial^{\alpha-1} u(\mathbf{x}, t)}{\partial_+ x^{\alpha-1}} - \frac{\partial^{\alpha-1} u(\mathbf{x}, t)}{\partial_- x^{\alpha-1}} \right),$$

with

$$\begin{aligned} \frac{\partial^{\alpha-1} u(\mathbf{x}, t)}{\partial_+ x^{\alpha-1}} &:= \frac{1}{\Gamma(2-\alpha)} \frac{\partial}{\partial x} \int_{x_L}^x \frac{u(\mathbf{x}, t)}{(x-s)^{\alpha-1}} ds, \\ \frac{\partial^{\alpha-1} u(\mathbf{x}, t)}{\partial_- x^{\alpha-1}} &:= -\frac{1}{\Gamma(2-\alpha)} \frac{\partial}{\partial x} \int_x^{x_R} \frac{u(\mathbf{x}, t)}{(s-x)^{\alpha-1}} ds. \end{aligned}$$

For simplicity of presentation, we denote

$$\mathcal{D}^{\alpha-1} := \frac{\partial^{\alpha-1}}{\partial_+ x^{\alpha-1}} - \frac{\partial^{\alpha-1}}{\partial_- x^{\alpha-1}}.$$

The Risez derivatives  $\frac{\partial^\beta u(\mathbf{x}, t)}{\partial |y|^\beta}$  and  $\frac{\partial^\gamma u(\mathbf{x}, t)}{\partial |z|^\gamma}$  in other two directions can be defined in a similar way.

Let  $M$  be a positive integer and define a uniform temporal partition of  $[0, T]$  with  $t_m := m\tau$  for  $m = 0, 1, \dots, M$ , such that the temporal stepsize  $\tau := T/M$ . Denote the set of temporal partition  $\mathbb{I}_t := \{1, 2, \dots, M\}$ . For  $m=1$ , we approximate the time derivative by the first-order BDF (Backward Euler) method, i.e.,  $g'(t_1) \approx (g(t_1) - g(t_0))/\tau$ ; while for  $m \geq 2$ , we approximate it by the second-order BDF method, i.e.,

$$g'(t_m) \approx (3g(t_m) - 4g(t_{m-1}) + g(t_{m-2}))/2\tau.$$

Then the following lemma holds.

**Lemma 2.1** ([30]). *Let*

$$D_t u(\mathbf{x}, t_m) := \begin{cases} \frac{u(\mathbf{x}, t_1) - u(\mathbf{x}, t_0)}{\tau}, & m = 1, \\ \frac{3u(\mathbf{x}, t_m) - 4u(\mathbf{x}, t_{m-1}) + u(\mathbf{x}, t_{m-2})}{2\tau}, & m \geq 2. \end{cases} \quad (2.1)$$

Then, for  $u(\mathbf{x}, \cdot) \in C^3([0, T])$ , it holds

$$\frac{\partial u(\mathbf{x}, t_m)}{\partial t} = D_t u(\mathbf{x}, t_m) + r_t^m, \quad m \in \mathbb{I}_t,$$

such that

$$|r_t^m| = \begin{cases} \mathcal{O}(\tau), & m = 1, \\ \mathcal{O}(\tau^2), & m \geq 2. \end{cases}$$

At each time level  $t_m$ , the nonlinear reaction term can be approximated by the linear extrapolation method [13]

$$f(u(\mathbf{x}, t_m)) \approx \hat{f}(u(\mathbf{x}, t_m)) := \begin{cases} f(u(\mathbf{x}, t_0)), & m = 1, \\ f(2u(\mathbf{x}, t_{m-1}) - u(\mathbf{x}, t_{m-2})), & m \geq 2. \end{cases} \quad (2.2)$$

**Lemma 2.2.** *Let  $r_n^m := f(u(\mathbf{x}, t_m)) - \hat{f}(u(\mathbf{x}, t_m))$ . Then, if  $f(u) \in C^1(\mathbb{R})$  and  $u(\mathbf{x}, \cdot) \in C^2[0, T]$ , it holds*

$$|r_n^m| = \begin{cases} \mathcal{O}(\tau), & m = 1, \\ \mathcal{O}(\tau^2), & m \geq 2. \end{cases}$$

Let  $\mathbf{A} \otimes \mathbf{B}$  represents the Kronecker product of two matrices  $\mathbf{A}$  and  $\mathbf{B}$ . We review the following well-known conclusions which are required in the analysis.

**Lemma 2.3** ([17]). *Suppose  $\mathbf{A}$  and  $\mathbf{B}$  are two real symmetric positive definite matrices, then both  $\mathbf{A} \otimes \mathbf{B}$  and  $\mathbf{B} \otimes \mathbf{A}$  are symmetric positive definite.*

**Lemma 2.4** ([11]). *Let  $\mathbf{A} \in \mathbb{R}^{m \times n}$ ,  $\mathbf{B} \in \mathbb{R}^{r \times s}$ ,  $\mathbf{C} \in \mathbb{R}^{n \times p}$  and  $\mathbf{D} \in \mathbb{R}^{s \times t}$ . Then*

$$(\mathbf{A} \otimes \mathbf{B})(\mathbf{C} \otimes \mathbf{D}) = \mathbf{AC} \otimes \mathbf{BD}.$$

The following lemma can be proved directly from Lemma 2.4.

**Lemma 2.5.** *Let  $\{\mathbf{A}_i\}_{i=1}^2 \in \mathbb{R}^{m \times m}$ ,  $\{\mathbf{B}_i\}_{i=1}^2 \in \mathbb{R}^{n \times n}$  and  $\{\mathbf{C}_i\}_{i=1}^2 \in \mathbb{R}^{r \times r}$ . Accordingly, let  $\mathbf{I}_\kappa$  be the identity matrix of order  $\kappa$  for  $\kappa = m, n$  and  $r$ , we have*

$$\begin{aligned} & (\mathbf{A}_1 \pm \mathbf{A}_2) \otimes (\mathbf{B}_1 \pm \mathbf{B}_2) \otimes (\mathbf{C}_1 \pm \mathbf{C}_2) \\ &= \left( (\mathbf{A}_1 \pm \mathbf{A}_2) \otimes \mathbf{I}_n \otimes \mathbf{I}_r \right) \left( \mathbf{I}_m \otimes (\mathbf{B}_1 \pm \mathbf{B}_2) \otimes \mathbf{I}_r \right) \left( \mathbf{I}_m \otimes \mathbf{I}_n \otimes (\mathbf{C}_1 \pm \mathbf{C}_2) \right). \end{aligned} \quad (2.3)$$

### 3 The BDF-FV method and its error estimate

In this section, we are committed to establishing the finite volume space discretization of the three-dimensional nonlinear Riesz s-FRDEs model (1.1a)–(1.1b) combined with the second-order BDF time discretization and the linear extrapolation technique. Meanwhile, we shall prove the corresponding convergence analysis.

#### 3.1 Derivation of the BDF-FV scheme

First, note that at each time level  $t_m$ , model (1.1a) can be rewritten as

$$\begin{aligned}
 D_t u(\mathbf{x}, t_m) - d_x \frac{\partial^\alpha u(\mathbf{x}, t_m)}{\partial |x|^\alpha} - d_y \frac{\partial^\beta u(\mathbf{x}, t_m)}{\partial |y|^\beta} - d_z \frac{\partial^\gamma u(\mathbf{x}, t_m)}{\partial |z|^\gamma} \\
 = \hat{f}(u(\mathbf{x}, t_m)) + g(\mathbf{x}, t_m) + r_n^m + r_t^m,
 \end{aligned}
 \tag{3.1}$$

where the temporal truncation errors  $r_t^m$  and  $r_n^m$  satisfy Lemmas 2.1–2.2.

Let  $N_x, N_y$  and  $N_z$  be three given positive integers. The domain  $\Omega$  is uniformly divided by  $x_i := x_L + ih_x, y_j := y_L + jh_y, z_k := z_L + kh_z$  for  $i = 0, 1, \dots, N_x + 1, j = 0, 1, \dots, N_y + 1$  and  $k = 0, 1, \dots, N_z + 1$ , such that the spatial mesh sizes  $h_x := (x_R - x_L) / (N_x + 1), h_y := (y_R - y_L) / (N_y + 1)$  and  $h_z := (z_R - z_L) / (N_z + 1)$ . Denote the sets of spatial partitions as  $\mathbb{I}_x := \{1, 2, \dots, N_x\}, \mathbb{I}_y := \{1, 2, \dots, N_y\}$  and  $\mathbb{I}_z := \{1, 2, \dots, N_z\}$ . Moreover, let  $x_{i-1/2} := (x_{i-1} + x_i) / 2, y_{j-1/2} := (y_{j-1} + y_j) / 2, z_{k-1/2} := (z_{k-1} + z_k) / 2$  and define the control volume element  $\Omega_{i,j,k} := [x_{i-1/2}, x_{i+1/2}] \times [y_{j-1/2}, y_{j+1/2}] \times [z_{k-1/2}, z_{k+1/2}]$  for each  $i \in \mathbb{I}_x, j \in \mathbb{I}_y$  and  $k \in \mathbb{I}_z$ .

Let  $\mathcal{S}_h(\Omega)$  be the space of continuous and piecewise linear functions with respect to the spatial partition, which vanishes at the boundary  $\partial\Omega$ . Besides, let  $u_{i,j,k}^m$  be the finite volume approximations to the true solution  $u(x_i, y_j, z_k, t_m)$  for  $i \in \mathbb{I}_x, j \in \mathbb{I}_y$  and  $k \in \mathbb{I}_z$  at time  $t_m, m \in \mathbb{I}_t$ . Then the finite volume solution  $u_h(\mathbf{x}, t_m) \in \mathcal{S}_h(\Omega)$  of model (1.1a) can be expressed as

$$u_h(\mathbf{x}, t_m) := \sum_{l \in \mathbb{I}_x} \sum_{r \in \mathbb{I}_y} \sum_{s \in \mathbb{I}_z} u_{l,r,s}^m \phi_l^x(x) \phi_r^y(y) \phi_s^z(z),
 \tag{3.2}$$

where  $\phi_l^x(x), \phi_r^y(y)$  and  $\phi_s^z(z)$  are the standard Lagrange piecewise linear nodal basis functions along the  $x$ -,  $y$ - and  $z$ -directions, respectively. Basically, we have the following conclusions for the basis functions.

**Lemma 3.1** ([7, 41]). *For each piecewise linear nodal basis function  $\phi_l^x(x), l \in \mathbb{I}_x$ , we have*

$$\int_{x_{i-1/2}}^{x_{i+1/2}} \phi_l^x(x) dx = \frac{h_x}{8} \begin{cases} 1, & |l-i|=1, \\ 6, & l=i, \\ 0, & \text{else,} \end{cases}$$

$$\mathcal{D}^{\alpha-1}\phi_l^x(x)\Big|_{x=x_{i-1/2}} = \frac{1}{h_x^{\alpha-1}\Gamma(3-\alpha)} \begin{cases} -s_{l-i+1}^{(\alpha)}, & l > i, \\ s_0^{(\alpha)} - s_1^{(\alpha)}, & l = i, \\ s_1^{(\alpha)} - s_0^{(\alpha)}, & l = i-1, \\ s_{i-l}^{(\alpha)}, & l < i-1, \end{cases}$$

$$\mathcal{D}^{\alpha-1}\phi_l^x(x)\Big|_{x=x_{i+1/2}} = \frac{1}{h_x^{\alpha-1}\Gamma(3-\alpha)} \begin{cases} -s_{l-i}^{(\alpha)}, & l > i+1, \\ s_0^{(\alpha)} - s_1^{(\alpha)}, & l = i+1, \\ s_1^{(\alpha)} - s_0^{(\alpha)}, & l = i, \\ s_{i-l+1}^{(\alpha)}, & l < i, \end{cases}$$

where

$$s_i^{(\alpha)} = \begin{cases} \left(\frac{1}{2}\right)^{2-\alpha}, & i = 0, \\ \left(\frac{3}{2}\right)^{2-\alpha} - 2\left(\frac{1}{2}\right)^{2-\alpha}, & i = 1, \\ \left(i + \frac{1}{2}\right)^{2-\alpha} - 2\left(i - \frac{1}{2}\right)^{2-\alpha} + \left(i - \frac{3}{2}\right)^{2-\alpha}, & 2 \leq i \leq N_x. \end{cases}$$

**Remark 3.1.** Similar conclusions for the basis functions  $\phi_r^y(y), r \in \mathbb{I}_y$  and  $\phi_s^z(z), s \in \mathbb{I}_z$  can be derived by a small modification of Lemma 3.1, in which parameters  $(h_x, N_x, \alpha)$  are replaced by  $(h_y, N_y, \beta)$  and  $(h_z, N_z, \gamma)$ , respectively.

Now we consider the finite volume element approximation of model (1.1a). Integrating both sides of the governing equation (3.1) over each  $\Omega_{i,j,k}$  with  $u(\mathbf{x}, t_m)$  replaced by  $u_h(\mathbf{x}, t_m)$  in (3.2), and then dropping the temporal truncation errors give rise to the linearly implicit BDF-FV scheme:

$$\begin{aligned} & \sum_{l \in \mathbb{I}_x} \sum_{r \in \mathbb{I}_y} \sum_{s \in \mathbb{I}_z} D_t u_{l,r,s}^m \int_{\Omega_{i,j,k}} \phi_l^x(x) \phi_r^y(y) \phi_s^z(z) dx \\ & + \frac{d_x}{2\cos(\alpha\pi/2)} \sum_{l \in \mathbb{I}_x} \sum_{r \in \mathbb{I}_y} \sum_{s \in \mathbb{I}_z} u_{k,r,s}^m \left[ \mathcal{D}^{\alpha-1}\phi_l^x(x)\Big|_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \phi_r^y(y) dy \int_{z_{k-1/2}}^{z_{k+1/2}} \phi_s^z(z) dz \right] \\ & + \frac{d_y}{2\cos(\beta\pi/2)} \sum_{l \in \mathbb{I}_x} \sum_{r \in \mathbb{I}_y} \sum_{s \in \mathbb{I}_z} u_{l,r,s}^m \left[ \mathcal{D}^{\beta-1}\phi_r^y(y)\Big|_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} \phi_l^x(x) dx \int_{z_{k-1/2}}^{z_{k+1/2}} \phi_s^z(z) dz \right] \\ & + \frac{d_z}{2\cos(\gamma\pi/2)} \sum_{l \in \mathbb{I}_x} \sum_{r \in \mathbb{I}_y} \sum_{s \in \mathbb{I}_z} u_{l,r,s}^m \left[ \mathcal{D}^{\gamma-1}\phi_s^z(z)\Big|_{z_{k-1/2}}^{z_{k+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} \phi_l^x(x) dx \int_{y_{j-1/2}}^{y_{j+1/2}} \phi_r^y(y) dy \right] \\ & = h_x h_y h_z \left[ \mathcal{N}_{i,j,k}^m + \mathcal{L}_{i,j,k}^m \right], \end{aligned} \tag{3.3}$$

where

$$\mathcal{N}_{i,j,k}^m := \frac{1}{h_x h_y h_z} \int_{\Omega_{i,j,k}} \hat{f}(u_h(\mathbf{x}, t_m)) d\mathbf{x}, \quad \mathcal{L}_{i,j,k}^m := \frac{1}{h_x h_y h_z} \int_{\Omega_{i,j,k}} g(\mathbf{x}, t_m) d\mathbf{x}. \quad (3.4)$$

Next, we reformulate the finite volume scheme (3.3) into a compact matrix form. Let  $\mathbf{U}^m, \mathcal{N}^m$  and  $\mathcal{L}^m$  be  $N := N_x N_y N_z$ - dimensional vectors defined by

$$\mathbf{U}^m := \left[ u_{1,1,1}^m, \dots, u_{N_x,1,1}^m, \dots, u_{1,N_y,1}^m, \dots, u_{N_x,N_y,1}^m, \dots, u_{1,1,N_z}^m, \dots, u_{N_x,N_y,N_z}^m \right]^\top, \quad (3.5a)$$

$$\mathcal{N}^m := \left[ \mathcal{N}_{1,1,1}^m, \dots, \mathcal{N}_{N_x,1,1}^m, \dots, \mathcal{N}_{1,N_y,1}^m, \dots, \mathcal{N}_{N_x,N_y,1}^m, \dots, \mathcal{N}_{1,1,N_z}^m, \dots, \mathcal{N}_{N_x,N_y,N_z}^m \right]^\top, \quad (3.5b)$$

$$\mathcal{L}^m := \left[ \mathcal{L}_{1,1,1}^m, \dots, \mathcal{L}_{N_x,1,1}^m, \dots, \mathcal{L}_{1,N_y,1}^m, \dots, \mathcal{L}_{N_x,N_y,1}^m, \dots, \mathcal{L}_{1,1,N_z}^m, \dots, \mathcal{L}_{N_x,N_y,N_z}^m \right]^\top. \quad (3.5c)$$

Furthermore, let  $\mathbf{A}_x$  and  $\mathbf{B}_x$  be respectively the mass matrix and stiffness matrix of order  $N_x$  as

$$\mathbf{A}_x := \frac{1}{8} \begin{bmatrix} 6 & 1 & \dots & \dots & 0 \\ 1 & 6 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & 1 & 6 & 1 \\ 0 & \dots & \dots & 1 & 6 \end{bmatrix}, \quad \mathbf{B}_x := \begin{bmatrix} q_1^{(\alpha)} & q_2^{(\alpha)} & \dots & \dots & q_{N_x}^{(\alpha)} \\ q_2^{(\alpha)} & q_1^{(\alpha)} & q_2^{(\alpha)} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & q_2^{(\alpha)} & q_1^{(\alpha)} & q_2^{(\alpha)} \\ q_{N_x}^{(\alpha)} & \dots & \dots & q_2^{(\alpha)} & q_1^{(\alpha)} \end{bmatrix}, \quad (3.6)$$

with

$$q_i^{(\alpha)} = \begin{cases} 2(s_0^{(\alpha)} - s_1^{(\alpha)}), & i=1, \\ s_1^{(\alpha)} - s_0^{(\alpha)} - s_2^{(\alpha)}, & i=2, \\ s_{i-1}^{(\alpha)} - s_i^{(\alpha)}, & 3 \leq i \leq N_x. \end{cases}$$

Similarly, we can define the matrices  $\mathbf{A}_y$  and  $\mathbf{B}_y$  of order  $N_y$ , and  $\mathbf{A}_z$  and  $\mathbf{B}_z$  of order  $N_z$ , just with  $(\alpha, N_x)$  being replaced by  $(\beta, N_y)$  and  $(\gamma, N_z)$ .

Let

$$\eta_\alpha := \frac{d_x}{2\cos(\alpha\pi/2)\Gamma(3-\alpha)} \frac{\tau}{h_x^\alpha},$$

$$\eta_\beta := \frac{d_y}{2\cos(\beta\pi/2)\Gamma(3-\beta)} \frac{\tau}{h_y^\beta},$$

$$\eta_\gamma := \frac{d_z}{2\cos(\gamma\pi/2)\Gamma(3-\gamma)} \frac{\tau}{h_z^\gamma}.$$

Then the matrix form of the BDF-FV scheme (3.3) reads as:

$$\begin{aligned} & (\mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x) \hat{D}_t \mathbf{U}^m + (\eta_\alpha \mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x + \eta_\beta \mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x + \eta_\gamma \mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x) \mathbf{U}^m \\ & = \tau(\mathcal{N}^m + \mathcal{L}^m), \end{aligned} \quad (3.7)$$



for  $m \in \mathbb{I}_t$ , where

$$\hat{D}_t \mathbf{U}^m := \begin{cases} \mathbf{U}^1 - \mathbf{U}^0, & m = 1, \\ \frac{3\mathbf{U}^m - 4\mathbf{U}^{m-1} + \mathbf{U}^{m-2}}{2}, & m \geq 2. \end{cases}$$

The following lemma follows immediately from [8].

**Lemma 3.2.** *The mass matrices  $\mathbf{A}_x$ ,  $\mathbf{A}_y$  and  $\mathbf{A}_z$  and the stiffness matrices  $\mathbf{B}_x$ ,  $\mathbf{B}_y$  and  $\mathbf{B}_z$  are all symmetric positive definite.*

**Remark 3.2.** Lemmas 2.3 and 3.2 further imply that the Kronecker products  $\mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x$ ,  $\mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x$ ,  $\mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x$  and  $\mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x$  in (3.7) are all symmetric positive definite. Besides,  $\mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x$ ,  $\mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x$ ,  $\mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x$  and  $\mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x$  are also symmetric positive definite. These facts play an important role in the following convergence estimates.

**Remark 3.3.** We have proposed a linearized second-order finite volume scheme (3.3), which avoids the solution of a nonlinear algebra system resulting from the fully-implicit finite volume discretization of the nonlinear Riesz s-FRDE model (1.1a). However, at each time level  $t_m$  ( $m \in \mathbb{I}_t$ ), one still has to solve a large-scale and dense  $N$ -by- $N$  linear algebra system (3.7). It is well-known that if the traditional GE solver is adopted for the solution of (3.7), the memory requirement is of order  $\mathcal{O}(N^2)$  and the computational complexity is of order  $\mathcal{O}(N^3)$ . This is deemed computationally challenging for large-scale modeling of multi-dimensional s-FRDEs, compared with the one-dimensional analogs.

However, note that the matrices  $\mathbf{A}_x$ ,  $\mathbf{A}_y$  and  $\mathbf{A}_z$  are all tri-diagonal, and  $\mathbf{B}_x$ ,  $\mathbf{B}_y$  and  $\mathbf{B}_z$  are all symmetric positive definite and Topelitz [9]. Based on these special matrix structures, using the same idea of Zheng et al. [41], we can develop a fast version Krylov subspace iterative method for the BDF-FV scheme (3.7), in which the computational complexity can be reduced to  $\mathcal{O}(N \log N)$  per iteration and meanwhile the total memory requirement is reduced to  $\mathcal{O}(N)$ . As it is not the main concern of this paper, we refer readers to [41] for the details.

### 3.2 Error estimate of the BDF-FV scheme

In this subsection, we prove the convergence of the BDF-FV scheme (3.7) via the discrete energy method. Throughout the paper, just like [6, 40], we assume that there exists a positive constant  $K$  such that

$$\max_{\mathbf{x} \in \Omega} |u(\mathbf{x}, t_m)| \leq K, \quad m \in \mathbb{I}_t. \tag{3.8}$$

Define mesh grid space

$$\mathcal{V}_h = \{ \mathbf{v} \mid \mathbf{v} = \{v_{i,j,k}\}, i \in \mathbb{I}_x, j \in \mathbb{I}_y, k \in \mathbb{I}_z \}.$$

For any  $\mathbf{v}, \mathbf{w} \in \mathcal{V}_h$ , define the discrete  $L^2$  inner product and discrete  $L^2$  and  $L^\infty$  norms as follows:

$$(\mathbf{v}, \mathbf{w}) := h_x h_y h_z \mathbf{w}^\top \mathbf{v} = h_x h_y h_z \sum_{i \in \mathbb{I}_x} \sum_{j \in \mathbb{I}_y} \sum_{k \in \mathbb{I}_z} v_{i,j,k} w_{i,j,k}, \tag{3.9a}$$

$$\|\mathbf{v}\| := \sqrt{(\mathbf{v}, \mathbf{v})}, \quad \|\mathbf{v}\|_\infty := \max_{i \in \mathbb{I}_x, j \in \mathbb{I}_y, k \in \mathbb{I}_z} |v_{i,j,k}|. \tag{3.9b}$$

Moreover, we introduce the following weighted discrete inner product and norm

$$(\mathbf{v}, \mathbf{w})_{\mathcal{K}} := (\mathcal{K}\mathbf{v}, \mathbf{w}) = h_x h_y h_z \mathbf{w}^\top \mathcal{K}\mathbf{v}, \quad \|\mathbf{v}\|_{\mathcal{K}} := \sqrt{(\mathbf{v}, \mathbf{v})_{\mathcal{K}}}, \tag{3.10}$$

for any positive definite matrix  $\mathcal{K}$  of order  $N$ . In particular, by Remark 3.2 we define

$$\|\mathbf{v}\|_A := \|\mathbf{v}\|_{\mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x}, \tag{3.11a}$$

$$\|\mathbf{v}\|_E := \left( \eta_\alpha \|\mathbf{v}\|_{\mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x}^2 + \eta_\beta \|\mathbf{v}\|_{\mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x}^2 + \eta_\gamma \|\mathbf{v}\|_{\mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x}^2 \right)^{1/2}. \tag{3.11b}$$

The following lemma states the equivalence of the norms  $\|\cdot\|_A$  and  $\|\cdot\|$ .

**Lemma 3.3** ([41]). *The  $\|\cdot\|$  and  $\|\cdot\|_A$  norms are equivalent with the following relation holds*

$$\frac{1}{2\sqrt{2}} \|\mathbf{v}\| \leq \|\mathbf{v}\|_A \leq \|\mathbf{v}\|, \quad \mathbf{v} \in \mathcal{V}_h.$$

Let  $\Pi_h$  be the standard Lagrange piecewise linear interpolation operator [26], i.e.,

$$\Pi_h g(\mathbf{x}) := \sum_{l \in \mathbb{I}_x} \sum_{r \in \mathbb{I}_y} \sum_{s \in \mathbb{I}_z} g(x_l, y_r, z_s) \phi_l^x(x) \phi_r^y(y) \phi_s^z(z), \tag{3.12}$$

where  $\phi_l^x(x)$ ,  $\phi_r^y(y)$  and  $\phi_s^z(z)$  are the Lagrange piecewise linear basis functions. Denote

$$r_I^m := u(\mathbf{x}, t_m) - \Pi_h u(\mathbf{x}, t_m), \quad m \in \mathbb{I}_t.$$

Then, for  $u(\cdot, t) \in C^2(\Omega)$  we have

$$|r_I^m| = \mathcal{O}\left(h_x^2 + h_y^2 + h_z^2\right). \tag{3.13}$$

For  $n \in \mathbb{N} \cup \{0\}$  and  $\theta > 0$ , define

$$\mathcal{L}^{n+\theta}(\mathbb{R}) = \left\{ \varphi(z) \in L^1(\mathbb{R}) \mid \int_{-\infty}^{\infty} (1+|\omega|)^{n+\theta} |\mathcal{F}(\omega)| d\omega < \infty \right\},$$

where

$$\mathcal{F}(\omega) = \int_{-\infty}^{\infty} \varphi(z) e^{i\omega z} dz$$

denotes the Fourier transform of  $\varphi(z)$ .

Denote the spatial truncation errors

$$r_x^m := \mathcal{D}^{\alpha-1}r_I^m, \quad r_y^m := \mathcal{D}^{\beta-1}r_I^m, \quad r_z^m := \mathcal{D}^{\gamma-1}r_I^m.$$

Moreover, for fixed  $y \in [y_L, y_R], z \in [z_L, z_R]$  and  $t \in [0, T]$ , define

$$\tilde{u}(\mathbf{x}, t) = \begin{cases} u(\mathbf{x}, t), & x \in [x_L, x_R], \\ 0, & x \notin [x_L, x_R], \end{cases}$$

for fixed  $x \in [x_L, x_R], z \in [z_L, z_R]$  and  $t \in [0, T]$ , define

$$\hat{u}(\mathbf{x}, t) = \begin{cases} u(\mathbf{x}, t), & y \in [y_L, y_R], \\ 0, & y \notin [y_L, y_R], \end{cases}$$

for fixed  $x \in [x_L, x_R], y \in [y_L, y_R]$  and  $t \in [0, T]$ , define

$$\check{u}(\mathbf{x}, t) = \begin{cases} u(\mathbf{x}, t), & z \in [z_L, z_R], \\ 0, & z \notin [z_L, z_R]. \end{cases}$$

Then the following lemma holds.

**Lemma 3.4** ([18]). *Assume that for each fixed  $t \in [0, T]$ , the zero extension functions  $\tilde{u}(\cdot, y, z, t) \in \mathcal{L}^{2+\alpha}(\mathbb{R}), \hat{u}(x, \cdot, z, t) \in \mathcal{L}^{2+\beta}(\mathbb{R})$  and  $\check{u}(x, y, \cdot, t) \in \mathcal{L}^{2+\gamma}(\mathbb{R})$ . Then*

$$\left| r_x^m \Big|_{x=x_{i-\frac{1}{2}}}^{x=x_{i+\frac{1}{2}}} \right| = \mathcal{O}(h_x^3), \quad \left| r_y^m \Big|_{y=y_{j-\frac{1}{2}}}^{y=y_{j+\frac{1}{2}}} \right| = \mathcal{O}(h_y^3), \quad \left| r_z^m \Big|_{z=z_{k-\frac{1}{2}}}^{z=z_{k+\frac{1}{2}}} \right| = \mathcal{O}(h_z^3).$$

Next, we turn to the estimate of the BDF-FV scheme (3.7). We see from the governing equation (3.1) that the exact solution  $u(\mathbf{x}, t_m)$  satisfies the following formula

$$\begin{aligned} & \int_{\Omega_{i,j,k}} D_t u(\mathbf{x}, t_m) d\mathbf{x} + \frac{d_x}{2\cos(\alpha\pi/2)} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{z_{k-1/2}}^{z_{k+1/2}} \left[ \mathcal{D}^{\alpha-1} u(\mathbf{x}, t_m) \Big|_{x_{i-1/2}}^{x_{i+1/2}} \right] dy dz \\ & + \frac{d_y}{2\cos(\beta\pi/2)} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{z_{k-1/2}}^{z_{k+1/2}} \left[ \mathcal{D}^{\beta-1} u(\mathbf{x}, t_m) \Big|_{y_{j-1/2}}^{y_{j+1/2}} \right] dx dz \\ & + \frac{d_z}{2\cos(\gamma\pi/2)} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \left[ \mathcal{D}^{\gamma-1} u(\mathbf{x}, t_m) \Big|_{z_{k-1/2}}^{z_{k+1/2}} \right] dx dy \\ & = h_x h_y h_z \left[ \tilde{\mathcal{N}}_{i,j,l}^m + \mathcal{L}_{i,j,l}^m + r_t^m + r_n^m \right], \end{aligned} \tag{3.14}$$

where

$$\tilde{\mathcal{N}}_{i,j,l}^m := \frac{1}{h_x h_y h_z} \int_{\Omega_{i,j,k}} \hat{f}(u(\mathbf{x}, t_m)) d\mathbf{x}. \tag{3.15}$$

Let  $\mathbf{u}^m := \{u(x_i, y_j, z_k, t_m)\} \in \mathcal{V}_h$  be the exact solution vector of (1.1a) at  $t=t_m$ . Now replacing  $u(\mathbf{x}, t_m)$  on the left-hand side of (3.14) by its Lagrange linear interpolation  $\Pi_h u(\mathbf{x}, t_m)$ , it follows from (3.13) and Lemma 3.4 that the exact solution vector  $\mathbf{u}^m$  also satisfies a similar formula of (3.3) with an extra local spatial truncation error

$$|r_s^m| = \mathcal{O}\left(h_x^2 + h_y^2 + h_z^2\right). \tag{3.16}$$

That means in matrix form the error  $\mathbf{e}^m := \mathbf{u}^m - \mathbf{U}^m$  satisfies

$$\begin{aligned} & (\mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x) \hat{D}_t \mathbf{e}^m \\ & + (\eta_\alpha \mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x + \eta_\beta \mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x + \eta_\gamma \mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x) \mathbf{e}^m \\ & = \tau \left( \tilde{\mathcal{N}}^m - \mathcal{N}^m + \mathbf{R}^m \right), \end{aligned} \tag{3.17}$$

for  $m \in \mathbb{I}_t$ , where  $\mathbf{R}^m = (r_t^m + r_n^m + r_s^m) \mathbf{E}$  and  $\mathbf{E} = [1, 1, \dots, 1]^\top$ .

**Lemma 3.5.** *Let  $\mathcal{N}^m, \tilde{\mathcal{N}}^m \in \mathcal{V}_h$  with elements defined by (3.4) and (3.15), respectively. If  $f(\cdot) \in C^1(\mathbb{R})$ , then we have*

$$\|\tilde{\mathcal{N}}^m - \mathcal{N}^m\|^2 \leq \begin{cases} \mathcal{O}\left(h_x^2 + h_y^2 + h_z^2\right)^2, & m = 1, \\ 128L^2 \|\mathbf{2e}^{m-1} - \mathbf{e}^{m-2}\|_A^2 + \mathcal{O}\left(h_x^2 + h_y^2 + h_z^2\right)^2, & m \geq 2, \end{cases}$$

provided that the the finite volume solutions  $u_h(\mathbf{x}, t_{m-1})$  and  $u_h(\mathbf{x}, t_{m-2})$  are bounded. Here the constant  $L := \max |f'(\cdot)|$  is finite which depends on the solutions  $u_h(\mathbf{x}, t_{m-1})$  and  $u_h(\mathbf{x}, t_{m-2})$ .

*Proof.* First, for the initial time we take  $u_h(\mathbf{x}, t_0) = \Pi_h u^0(\mathbf{x})$  which yields

$$\begin{aligned} \left| \tilde{\mathcal{N}}_{i,j,k}^1 - \mathcal{N}_{i,j,k}^1 \right| &= \left| \frac{1}{h_x h_y h_z} \int_{\Omega_{i,j,k}} [f(u^0(\mathbf{x})) - f(u_h^0(\mathbf{x}))] d\mathbf{x} \right| \\ &\leq \frac{1}{h_x h_y h_z} \int_{\Omega_{i,j,k}} |f(u^0(\mathbf{x})) - f(\Pi_h u^0(\mathbf{x}))| d\mathbf{x} \\ &\leq \frac{1}{h_x h_y h_z} \int_{\Omega_{i,j,k}} L |r_I^0| d\mathbf{x} \leq C \left( h_x^2 + h_y^2 + h_z^2 \right), \end{aligned}$$

where the interpolation estimate (3.13) is utilized in the last step, and  $L$  is finite because the initial value  $u_h(\mathbf{x}, t_0) = \Pi_h u^0(\mathbf{x})$  is bounded. With the help of the above inequality, we then directly have

$$\|\tilde{\mathcal{N}}^1 - \mathcal{N}^1\|^2 = h_x h_y h_z \sum_{i \in \mathbb{I}_x} \sum_{j \in \mathbb{I}_y} \sum_{k \in \mathbb{I}_z} \left| \tilde{\mathcal{N}}_{i,j,k}^1 - \mathcal{N}_{i,j,k}^1 \right|^2 \leq C \left( h_x^2 + h_y^2 + h_z^2 \right), \tag{3.18}$$

which proves the case for  $m = 1$ .

Next, we pay special attention on the estimate of  $\|\widetilde{\mathcal{N}}^m - \mathcal{N}^m\|$  for  $m \geq 2$ . By the mean value theorem

$$\begin{aligned} \|\widetilde{\mathcal{N}}^m - \mathcal{N}^m\|^2 &= h_x h_y h_z \sum_{i \in \mathbb{I}_x} \sum_{j \in \mathbb{I}_y} \sum_{k \in \mathbb{I}_z} \left[ \frac{1}{h_x h_y h_z} \int_{\Omega_{i,j,k}} f\left(2u(\mathbf{x}, t_{m-1}) - u(\mathbf{x}, t_{m-2})\right) \right. \\ &\quad \left. - f\left(2u_h(\mathbf{x}, t_{m-1}) - u_h(\mathbf{x}, t_{m-2})\right) \right]^2 d\mathbf{x} \\ &\leq L^2 \sum_{i \in \mathbb{I}_x} \sum_{j \in \mathbb{I}_y} \sum_{k \in \mathbb{I}_z} \int_{\Omega_{i,j,k}} \left| (2u(\mathbf{x}, t_{m-1}) - u(\mathbf{x}, t_{m-2})) \right. \\ &\quad \left. - (2u_h(\mathbf{x}, t_{m-1}) - u_h(\mathbf{x}, t_{m-2})) \right|^2 d\mathbf{x}, \end{aligned}$$

for  $f(\cdot) \in C^1(\mathbb{R})$ , provided that the numerical solutions  $u_h(\mathbf{x}, t_{m-1})$  and  $u_h(\mathbf{x}, t_{m-2})$  are bounded.

Note that on each control volume element  $\Omega_{i,j,k}$ , by triangle inequality we have

$$\begin{aligned} &\left| (2u(\mathbf{x}, t_{m-1}) - u(\mathbf{x}, t_{m-2})) - (2u_h(\mathbf{x}, t_{m-1}) - u_h(\mathbf{x}, t_{m-2})) \right| \\ &\leq \left| (2u(\mathbf{x}, t_{m-1}) - u(\mathbf{x}, t_{m-2})) - (2\Pi_h u(\mathbf{x}, t_{m-1}) - \Pi_h u(\mathbf{x}, t_{m-2})) \right| \\ &\quad + \left| (2\Pi_h u(\mathbf{x}, t_{m-1}) - \Pi_h u(\mathbf{x}, t_{m-2})) - (2u_h(\mathbf{x}, t_{m-1}) - u_h(\mathbf{x}, t_{m-2})) \right| \\ &= \left| 2r_I^{m-1} - r_I^{m-2} \right| + \left| 2e_h(\mathbf{x}, t_{m-1}) - e_h(\mathbf{x}, t_{m-2}) \right|, \end{aligned}$$

where

$$e_h(\mathbf{x}, t_m) := \Pi_h u(\mathbf{x}, t_m) - u_h(\mathbf{x}, t_m),$$

and thus

$$\begin{aligned} \|\widetilde{\mathcal{N}}^m - \mathcal{N}^m\|^2 &\leq 2L^2 \sum_{i \in \mathbb{I}_x} \sum_{j \in \mathbb{I}_y} \sum_{k \in \mathbb{I}_z} \int_{\Omega_{i,j,k}} \left| 2r_I^{m-1} - r_I^{m-2} \right|^2 d\mathbf{x} \\ &\quad + 2L^2 \sum_{i \in \mathbb{I}_x} \sum_{j \in \mathbb{I}_y} \sum_{k \in \mathbb{I}_z} \int_{\Omega_{i,j,k}} \left| 2e_h(\mathbf{x}, t_{m-1}) - e_h(\mathbf{x}, t_{m-2}) \right|^2 d\mathbf{x} \\ &=: I_1 + I_2. \end{aligned} \tag{3.19}$$

While for the first term of (3.19), by interpolation estimate (3.13), it is bounded by

$$I_1 \leq C \left( h_x^2 + h_y^2 + h_z^2 \right)^2. \tag{3.20}$$

Next, for the second term  $I_2$ , note that on each fixed element  $\Omega_{i,j,k}$ , we have

$$e_h(\mathbf{x}, t_m) = \sum_{l=i-1}^{i+1} \sum_{r=j-1}^{j+1} \sum_{s=k-1}^{k+1} e_{l,r,s}^m \phi_l^x(x) \phi_r^y(y) \phi_s^z(z) \tag{3.21}$$

and therefore

$$\begin{aligned}
 I_2 &= 2L^2 \sum_{i \in \mathbb{I}_x} \sum_{j \in \mathbb{I}_y} \sum_{k \in \mathbb{I}_z} \int_{\Omega_{i,j,k}} \left( \sum_{l=i-1}^{i+1} \sum_{r=j-1}^{j+1} \sum_{s=k-1}^{k+1} (2e_{l,r,s}^{m-1} - e_{l,r,s}^{m-2}) \phi_l^x(x) \phi_r^y(y) \phi_s^z(z) \right)^2 dx \\
 &\leq 54L^2 \sum_{i \in \mathbb{I}_x} \sum_{j \in \mathbb{I}_y} \sum_{k \in \mathbb{I}_z} \left[ \sum_{l=i-1}^{i+1} \sum_{r=j-1}^{j+1} \sum_{s=k-1}^{k+1} (2e_{l,r,s}^{m-1} - e_{l,r,s}^{m-2})^2 \right] \\
 &\quad \times \int_{\Omega_{i,j,k}} (\phi_l^x(x))^2 (\phi_r^y(y))^2 (\phi_s^z(z))^2 dx \\
 &\leq 16L^2 \|2\mathbf{e}^{m-1} - \mathbf{e}^{m-2}\|^2,
 \end{aligned} \tag{3.22}$$

where we have used the facts [41] that

$$\begin{aligned}
 \int_{x_{i-1/2}}^{x_{i+1/2}} (\phi_i^x(x))^2 dx &= \frac{7h_x}{12}, \\
 \int_{x_{i-1/2}}^{x_{i+1/2}} (\phi_{i+1}^x(x))^2 dx &= \int_{x_{i-1/2}}^{x_{i+1/2}} (\phi_{i-1}^x(x))^2 dx = \frac{h_x}{24}.
 \end{aligned}$$

Now substituting (3.20)-(3.22) into (3.19) and utilizing Lemma 3.3, we have

$$\|\widetilde{\mathcal{N}}^m - \mathcal{N}^m\|^2 \leq 16L^2 \|2\mathbf{e}^{m-1} - \mathbf{e}^{m-2}\|^2 + C(h_x^2 + h_y^2 + h_z^2)^2,$$

which proves the lemma. □

**Theorem 3.1.** *Suppose that model (1.1a)–(1.1b) has a unique solution  $u(\mathbf{x}, t) \in C^3([0, T]; C^2(\Omega))$  and the condition in Lemma 3.4 holds. Moreover, assume that  $f(u) \in C^1(\mathbb{R})$  and (3.8) is satisfied. If the stepsizes  $\tau, h_x, h_y, h_z$  and  $\frac{\tau^2}{\sqrt{h_x h_y h_z}}$  are sufficiently small, the BDF-FV scheme (3.7) admits a unique solution  $u_h(\mathbf{x}, t_m)$  satisfying*

$$\max_{\mathbf{x} \in \Omega} |u_h(\mathbf{x}, t_m)| \leq K + 1, \quad m \in \mathbb{I}_t. \tag{3.23}$$

Moreover, there exists a constant  $\hat{\tau} > 0$  such that the following error estimate holds for  $\tau < \hat{\tau}$

$$\|\mathbf{u}^m - \mathbf{U}^m\| + \|\mathbf{u}^m - \mathbf{U}^m\|_E \leq C(\tau^2 + h_x^2 + h_y^2 + h_z^2), \quad m \in \mathbb{I}_t, \tag{3.24}$$

where the constant  $C$  is independent of the mesh parameters  $h_x, h_y, h_z$  and  $\tau$ .

*Proof.* First, the existence and uniqueness of the BDF-FV solution follows immediately from the fact that the coefficient matrix of (3.7) is symmetric positive definite.

Next, we start to prove the boundedness result (3.23) and error estimate (3.24) by the mathematical induction method. Taking the discrete inner product of (3.17) with  $\mathbf{e}^m$ , by notations (3.10)–(3.11) we have

$$(\hat{D}_t \mathbf{e}^m, \mathbf{e}^m)_A + \|\mathbf{e}^m\|_E^2 = \tau (\widetilde{\mathcal{N}}^m - \mathcal{N}^m + \mathbf{R}^m, \mathbf{e}^m). \tag{3.25}$$

Firstly, we verify (3.23)–(3.24) for the case  $m = 1$  from the above equation. Note that  $\mathbf{e}^0 = \mathbf{0}$  and in this case the following inequality holds

$$\left(\hat{D}_t \mathbf{e}^1, \mathbf{e}^1\right)_A \geq \frac{1}{2} \left(\|\mathbf{e}^1\|_A^2 - \|\mathbf{e}^0\|_A^2\right) = \frac{1}{2} \|\mathbf{e}^1\|_A^2. \tag{3.26}$$

Now inserting (3.26) and Lemma 3.5 into (3.25) for  $m = 1$ , and then the norm equivalence in Lemma 3.3 implies

$$\|\mathbf{e}^1\|_A^2 + \|\mathbf{e}^1\|_E^2 \leq 2\tau \|\mathbf{R}^1\| \|\mathbf{e}^1\| \leq 4\sqrt{2}\tau \|\mathbf{R}^1\| \|\mathbf{e}^1\|_A \Rightarrow \|\mathbf{e}^1\|_A \leq 4\sqrt{2}\tau \|\mathbf{R}^1\|. \tag{3.27}$$

Thus, we can derive from Lemmas 2.1–2.2 and (3.16) that

$$\begin{aligned} & \|\mathbf{e}^1\|_A + \|\mathbf{e}^1\|_E \leq 8\tau \|\mathbf{R}^1\| \\ & \leq 8\sqrt{(x_R - x_L)(y_R - y_L)(z_R - z_L)} C\tau \left(\tau + h_x^2 + h_y^2 + h_z^2\right) \\ & \leq C \left(\tau^2 + h_x^2 + h_y^2 + h_z^2\right), \end{aligned} \tag{3.28}$$

for sufficiently small  $\tau < 1$ .

Therefore, by the norm equivalence in Lemma 3.3, the error inequality (3.24) holds for  $m = 1$ . Furthermore, using the triangle inequality and inverse inequality, we can easily get the boundedness of the numerical solution  $u_h(\mathbf{x}, t_1)$ , i.e.,

$$\begin{aligned} \max_{\mathbf{x} \in \Omega} |u_h(\mathbf{x}, t_1)| &= \|\mathbf{U}^1\|_\infty \leq \|\mathbf{u}^1\|_\infty + \|\mathbf{e}^1\|_\infty \leq \|\mathbf{u}^1\|_\infty + C(h_x h_y h_z)^{-\frac{1}{2}} \|\mathbf{e}^1\| \\ &\leq \|\mathbf{u}^1\|_\infty + C(h_x h_y h_z)^{-\frac{1}{2}} \left(\tau^2 + h_x^2 + h_y^2 + h_z^2\right) \leq K + 1, \end{aligned} \tag{3.29}$$

whenever  $\frac{\tau^2}{\sqrt{h_x h_y h_z}}$ ,  $h_x$ ,  $h_y$  and  $h_z$  are sufficiently small.

Next, we assume (3.23) holds for  $k \leq m - 1$  with  $m \geq 2$ . We need to prove that (3.23)–(3.24) also hold for  $k = m$ . Since for  $\forall a, b, c \in \mathbb{R}$ ,

$$(3a - 4b + c)a = \frac{1}{2} [a^2 + (2a - b)^2] - \frac{1}{2} [b^2 + (2b - c)^2] + \frac{1}{2} (a - 2b + c)^2. \tag{3.30}$$

Then, we conclude for  $m \geq 2$

$$\begin{aligned} & \left(\hat{D}_t \mathbf{e}^m, \mathbf{e}^m\right)_A \\ & \geq \frac{1}{4} \left[ \left(\|\mathbf{e}^m\|_A^2 + \|2\mathbf{e}^m - \mathbf{e}^{m-1}\|_A^2\right) - \left(\|\mathbf{e}^{m-1}\|_A^2 + \|2\mathbf{e}^{m-1} - \mathbf{e}^{m-2}\|_A^2\right) \right]. \end{aligned} \tag{3.31}$$

Now inserting (3.31) into (3.25), and then utilizing the Cauchy-Schwarz inequality and

the norm equivalence in Lemma 3.3, we have

$$\begin{aligned}
 & \| \mathbf{e}^m \|_A^2 + \| 2\mathbf{e}^m - \mathbf{e}^{m-1} \|_A^2 + \| \mathbf{e}^m \|_E^2 \\
 & \leq \| \mathbf{e}^{m-1} \|_A^2 + \| 2\mathbf{e}^{m-1} - \mathbf{e}^{m-2} \|_A^2 + 8\sqrt{2}\tau \| \widetilde{\mathcal{N}}^m - \mathcal{N}^m \| \| \mathbf{e}^m \|_A + 8\sqrt{2}\tau \| \mathbf{R}^m \| \| \mathbf{e}^m \|_A \\
 & \leq \| \mathbf{e}^{m-1} \|_A^2 + \| 2\mathbf{e}^{m-1} - \mathbf{e}^{m-2} \|_A^2 + 4\sqrt{2}\tau \left( \| \widetilde{\mathcal{N}}^m - \mathcal{N}^m \|^2 + \| \mathbf{R}^m \|^2 \right) + 8\sqrt{2}\tau \| \mathbf{e}^m \|_A^2 \\
 & \leq \| \mathbf{e}^{m-1} \|_A^2 + \left( 1 + 512\sqrt{2}L^2\tau \right) \| 2\mathbf{e}^{m-1} - \mathbf{e}^{m-2} \|_A^2 + 8\sqrt{2}\tau \| \mathbf{e}^m \|_A^2 + 4\sqrt{2}\tau \| \mathbf{R}^m \|^2 \\
 & \quad + C\tau \left( h_x^2 + h_y^2 + h_z^2 \right)^2, \tag{3.32}
 \end{aligned}$$

where we have used the estimate for  $\| \widetilde{\mathcal{N}}^m - \mathcal{N}^m \|$  via Lemma 3.5 based on the boundedness of the finite volume solutions  $u_h(\mathbf{x}, t_{m-1})$  and  $u_h(\mathbf{x}, t_{m-2})$ .

Denote

$$\Theta(\mathbf{e}^m) = \| \mathbf{e}^m \|_A^2 + \| 2\mathbf{e}^m - \mathbf{e}^{m-1} \|_A^2.$$

We can rewrite the inequality (3.32) as

$$\begin{aligned}
 & \Theta(\mathbf{e}^m) + \| \mathbf{e}^m \|_E^2 \\
 & \leq \frac{1 + 512\sqrt{2}L^2\tau}{1 - 8\sqrt{2}\tau} \Theta(\mathbf{e}^{m-1}) + \frac{4\sqrt{2}\tau}{1 - 8\sqrt{2}\tau} \| \mathbf{R}^m \|^2 + C\tau \left( h_x^2 + h_y^2 + h_z^2 \right)^2, \tag{3.33}
 \end{aligned}$$

for  $\tau < \frac{\sqrt{2}}{16}$ , which further implies

$$\begin{aligned}
 \Theta(\mathbf{e}^m) + \| \mathbf{e}^m \|_E^2 & \leq \frac{1 + 512\sqrt{2}L^2\tau}{1 - 8\sqrt{2}\tau} \left[ \frac{1 + 512\sqrt{2}L^2\tau}{1 - 8\sqrt{2}\tau} \Theta(\mathbf{e}^{m-2}) + \frac{4\sqrt{2}\tau}{1 - 8\sqrt{2}\tau} \| \mathbf{R}^{m-1} \|^2 \right. \\
 & \quad \left. + C\tau \left( h_x^2 + h_y^2 + h_z^2 \right)^2 \right] + \frac{4\sqrt{2}\tau}{1 - 8\sqrt{2}\tau} \| \mathbf{R}^m \|^2 + C\tau \left( h_x^2 + h_y^2 + h_z^2 \right)^2 \\
 & \leq \left( \frac{1 + 512\sqrt{2}L^2\tau}{1 - 8\sqrt{2}\tau} \right)^{m-1} \Theta(\mathbf{e}^1) + \frac{4\sqrt{2}\tau}{1 - 8\sqrt{2}\tau} \sum_{k=2}^m \left( \frac{1 + 512\sqrt{2}L^2\tau}{1 - 8\sqrt{2}\tau} \right)^{m-k} \| \mathbf{R}^k \|^2 \\
 & \quad + C\tau \sum_{k=2}^m \left( \frac{1 + 512\sqrt{2}L^2\tau}{1 - 8\sqrt{2}\tau} \right)^{m-k} \left( h_x^2 + h_y^2 + h_z^2 \right)^2. \tag{3.34}
 \end{aligned}$$

Noting the definition of  $\Theta(\mathbf{e}^m)$ , we know

$$\Theta(\mathbf{e}^1) = \| \mathbf{e}^1 \|_A^2 + \| 2\mathbf{e}^1 - \mathbf{e}^0 \|_A^2 = 5 \| \mathbf{e}^1 \|_A^2 \leq C \left( \tau^2 + h_x^2 + h_y^2 + h_z^2 \right)^2. \tag{3.35}$$



Also, noting the fact for  $\tau < \frac{\sqrt{2}}{16}$

$$\begin{aligned} \left(\frac{1+512\sqrt{2}L^2\tau}{1-8\sqrt{2}\tau}\right)^k &\leq \left(\frac{1+512\sqrt{2}L^2\tau}{1-8\sqrt{2}\tau}\right)^{T/\tau} \\ &\leq \left(1+\frac{(8+512L^2)\sqrt{2}\tau}{1-8\sqrt{2}\tau}\right)^{T/\tau} \leq e^{\frac{(8+512L^2)\sqrt{2}T}{1-8\sqrt{2}\tau}}. \end{aligned} \tag{3.36}$$

Then, we plug (3.35)–(3.36) into (3.34) to directly obtain

$$\Theta(\mathbf{e}^m) + \|\mathbf{e}^m\|_E^2 \leq C\left(\tau^2 + h_x^2 + h_y^2 + h_z^2\right)^2. \tag{3.37}$$

Now, we can obtain from the inequality (3.37) that

$$\|\mathbf{e}^m\| + \|\mathbf{e}^m\|_E \leq 2\sqrt{2}\|\mathbf{e}^m\|_A + \|\mathbf{e}^m\|_E \leq 2\sqrt{2\Theta(\mathbf{e}^m) + \|\mathbf{e}^m\|_E} \leq C\left(\tau^2 + h_x^2 + h_y^2 + h_z^2\right),$$

which proves (3.24) for  $k = m$ .

Finally, analogous to the process (3.29), we can easily prove the boundedness of the finite volume solution  $u_h(\mathbf{x}, t_m)$ :

$$\begin{aligned} \max_{\mathbf{x} \in \Omega} |u_h(\mathbf{x}, t_m)| &= \|\mathbf{U}^m\|_\infty \leq \|\mathbf{u}^m\|_\infty + \|\mathbf{e}^m\|_\infty \\ &\leq \|\mathbf{u}^m\|_\infty + C(h_x h_y h_z)^{-\frac{1}{2}}\left(\tau^2 + h_x^2 + h_y^2 + h_z^2\right) \leq K + 1, \end{aligned} \tag{3.38}$$

for sufficiently small  $\frac{\tau^2}{\sqrt{h_x h_y h_z}}$ ,  $h_x$ ,  $h_y$  and  $h_z$ . This completes the proof of Theorem 3.1.  $\square$

**Remark 3.4.** The temporal-spatial stepsize constraint condition in Theorem 3.1 is not very stringent. It only demands  $\tau \approx h^{3/4}$  for  $h_x = h_y = h_z = h$ . In particular, if the nonlinear reaction term  $f(u)$  satisfies the Lipschitz continuous condition, i.e., there exists a positive constant  $L$  such that

$$|f(u_1) - f(u_2)| \leq L|u_1 - u_2|, \quad \forall u_1, u_2 \in \mathbb{R}, \tag{3.39}$$

the assumption (3.8) as well as the temporal-spatial stepsize constraint can be naturally canceled, see, for example, [13, 41]. However, the Lipschitz assumption (3.39) greatly limits the application of the nonlinear model. For example, it is easy to check that (3.39) is satisfied for  $f(u) = (\sin u)^4$  in Section 5.1, however, it is not fulfilled for  $f(u) = u - u^3$  in Example 5.2. Therefore, in this paper we assume a more general case  $f(u) \in C^1(\mathbb{R})$  and hence (3.8) is needed.

**Corollary 3.1.** *Theorem 3.1 further shows that the conclusion of Lemma 3.5 reduces to*

$$\|\widetilde{\mathcal{N}}^m - \mathcal{N}^m\| = \mathcal{O}\left(h_x^2 + h_y^2 + h_z^2\right), \quad m \in \mathbb{I}_t.$$

We end this section by giving an optimal-order error estimates for the BDF-FV scheme (3.3) in the continuous  $L^2$  norm. By the classical interpolation theory, we have

$$\|u(\mathbf{x}, t_m) - \Pi_h u(\mathbf{x}, t_m)\|_{L^2} \leq C_\Omega \left( h_x^2 + h_y^2 + h_z^2 \right) \|u\|_{H^2}, \tag{3.40}$$

for  $u \in H^2(\Omega) \cap H_0^1(\Omega)$ , where  $C_\Omega$  is a positive constant that only depends on the domain  $\Omega$ .

Considering the definitions of  $\Pi_h$  (see, (3.12)) and  $\|\cdot\|_{L^2}$ , we obtain by (3.21) that

$$\begin{aligned} & \|\Pi_h u(\mathbf{x}, t_m) - u_h(\mathbf{x}, t_m)\|_{L^2}^2 = \int_\Omega (\Pi_h u(\mathbf{x}, t_m) - u_h(\mathbf{x}, t_m))^2 d\mathbf{x} \\ & = \sum_{i \in \mathbb{I}_x} \sum_{j \in \mathbb{I}_y} \sum_{k \in \mathbb{I}_z} \int_{\Omega_{i,j,k}} \left( \sum_{l=i-1}^{i+1} \sum_{r=j-1}^{j+1} \sum_{s=k-1}^{k+1} e_{l,r,s}^m \phi_l^x(x) \phi_r^y(y) \phi_s^z(z) \right)^2 d\mathbf{x}. \end{aligned}$$

Applying a similar process to (3.22) and Theorem 3.1, we can easily obtain the following estimate:

$$\|\Pi_h u(\mathbf{x}, t_m) - u_h(\mathbf{x}, t_m)\|_{L^2} \leq 2\sqrt{2} \|\mathbf{e}^m\| \leq 2\sqrt{2} \left( \tau^2 + h_x^2 + h_y^2 + h_z^2 \right). \tag{3.41}$$

Therefore, combing (3.40) and (3.41) together, and using the triangle inequality, we immediately have:

**Corollary 3.2.** *Under the assumptions in Theorem 3.1, we further have*

$$\|u(\mathbf{x}, t_m) - u_h(\mathbf{x}, t_m)\|_{L^2} \leq C \left( \tau^2 + h_x^2 + h_y^2 + h_z^2 \right), \quad m \in \mathbb{I}_t. \tag{3.42}$$

## 4 Derivation and error estimate of the BDF-FV-ADI scheme

In the previous section, a second-order accuracy BDF-FV scheme is proposed and analyzed. As pointed out in Remark 3.3, a fast solution method can be developed for the efficient implementation of BDF-FV scheme. However, as the grid parameters getting smaller and smaller, the developed method shall also be CPU time consuming. In order to improve the computational efficiency, we further construct an efficient alternating direction implicit method, named BDF-FV-ADI, to reduce the large-scale three-dimensional modeling to a series of independent small-scale one-dimensional analogs, and meanwhile the method can be implemented in parallel.

### 4.1 Derivation of the BDF-FV-ADI scheme

Define two perturbation terms of order  $\mathcal{O}(\tau^3)$ :

$$\begin{aligned} \mathbf{p}^1 := & \left( \eta_\alpha \eta_\beta \mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x + \eta_\alpha \eta_\gamma \mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x + \eta_\beta \eta_\gamma \mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x \right. \\ & \left. + \eta_\alpha \eta_\beta \eta_\gamma \mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x \right) \left( \hat{D}_t \mathbf{U}^1 \right), \quad m = 1, \end{aligned} \tag{4.1}$$

and

$$\begin{aligned}
 \mathbf{p}^m := & \left( \frac{4}{9} \eta_\alpha \eta_\beta \mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x + \frac{4}{9} \eta_\alpha \eta_\gamma \mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x + \frac{4}{9} \eta_\beta \eta_\gamma \mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x \right. \\
 & \left. + \frac{8}{27} \eta_\alpha \eta_\beta \eta_\gamma \mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x \right) (\hat{D}_t \mathbf{U}^m), \quad m \geq 2.
 \end{aligned} \tag{4.2}$$

Then adding them to the left-hand side of the BDF-FV scheme (3.7) and distributing them appropriately to the left and right-hand side of the equations, we are left with

$$\begin{aligned}
 & (\mathbf{A}_z + \eta_\gamma \mathbf{B}_z) \otimes (\mathbf{A}_y + \eta_\beta \mathbf{B}_y) \otimes (\mathbf{A}_x + \eta_\alpha \mathbf{B}_x) (\hat{D}_t \mathbf{U}^1) \\
 & = - \left( \eta_\alpha \mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x + \eta_\beta \mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x + \eta_\gamma \mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x \right) \mathbf{U}^0 + \tau (\mathcal{N}^1 + \mathcal{L}^1) \\
 & := \mathbf{F}^1,
 \end{aligned} \tag{4.3}$$

for  $m = 1$ , and

$$\begin{aligned}
 & \left( \mathbf{A}_z + \frac{2\eta_\gamma}{3} \mathbf{B}_z \right) \otimes \left( \mathbf{A}_y + \frac{2\eta_\beta}{3} \mathbf{B}_y \right) \otimes \left( \mathbf{A}_x + \frac{2\eta_\alpha}{3} \mathbf{B}_x \right) (\hat{D}_t \mathbf{U}^m) \\
 & = - \frac{1}{3} \left( \eta_\alpha \mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x + \eta_\beta \mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x + \eta_\gamma \mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x \right) (4\mathbf{U}^{m-1} - \mathbf{U}^{m-2}) \\
 & \quad + \tau (\mathcal{N}^m + \mathcal{L}^m) \\
 & := \mathbf{F}^m,
 \end{aligned} \tag{4.4}$$

for  $m \geq 2$ .

**Algorithm 4.1. BDF-FV-ADI at time  $t_1$ .**

- (i) Solving the subproblem in  $z$ -direction for the intermediate solution  $\mathbf{U}^{1,***} := \{U_{i,j,k}^{1,***}\} \in \mathbb{R}^N$  that

$$\left( (\mathbf{A}_z + \eta_\gamma \mathbf{B}_z) \otimes \mathbf{I}_{N_y} \otimes \mathbf{I}_{N_x} \right) \mathbf{U}^{1,***} = \mathbf{F}^1; \tag{4.5}$$

- (ii) Solving the subproblem in  $y$ -direction for the intermediate solution  $\mathbf{U}^{1,**} := \{U_{i,j,k}^{1,**}\} \in \mathbb{R}^N$  that

$$\left( \mathbf{I}_{N_z} \otimes (\mathbf{A}_y + \eta_\beta \mathbf{B}_y) \otimes \mathbf{I}_{N_x} \right) \mathbf{U}^{1,**} = \mathbf{U}^{1,***}; \tag{4.6}$$

- (iii) Solving the subproblem in  $x$ -direction for the intermediate solution  $\mathbf{U}^{1,*} := \{U_{i,j,k}^{1,*}\} \in \mathbb{R}^N$  that

$$\left( \mathbf{I}_{N_z} \otimes \mathbf{I}_{N_y} \otimes (\mathbf{A}_x + \eta_\alpha \mathbf{B}_x) \right) \mathbf{U}^{1,*} = \mathbf{U}^{1,**}; \tag{4.7}$$

(iv) Updating the solution  $\mathbf{U}^1$  via  $\hat{D}_t \mathbf{U}^1 = \mathbf{U}^{1,*}$ , i.e.,

$$\mathbf{U}^1 = \mathbf{U}^{1,*} + \mathbf{U}^0. \tag{4.8}$$

Equivalently, by Lemma 2.5, we can rewrite (4.3) for  $m = 1$  as

$$\begin{aligned} & \left( (\mathbf{A}_z + \eta_\gamma \mathbf{B}_z) \otimes \mathbf{I}_{N_y} \otimes \mathbf{I}_{N_x} \right) \left( \mathbf{I}_{N_z} \otimes (\mathbf{A}_y + \eta_\beta \mathbf{B}_y) \otimes \mathbf{I}_{N_x} \right) \\ & \left( \mathbf{I}_{N_z} \otimes \mathbf{I}_{N_y} \otimes (\mathbf{A}_x + \eta_\alpha \mathbf{B}_x) \right) \left( \hat{D}_t \mathbf{U}^1 \right) = \mathbf{F}^1, \end{aligned} \tag{4.9}$$

and from which the BDF-FV-ADI scheme at the first time level can be formulated as Algorithm 4.1.

Similarly, Eq. (4.4) is equivalent to

$$\begin{aligned} & \left( \left( \mathbf{A}_z + \frac{2\eta_\gamma}{3} \mathbf{B}_z \right) \otimes \mathbf{I}_{N_y} \otimes \mathbf{I}_{N_x} \right) \left( \mathbf{I}_{N_z} \otimes \left( \mathbf{A}_y + \frac{2\eta_\beta}{3} \mathbf{B}_y \right) \otimes \mathbf{I}_{N_x} \right) \\ & \left( \mathbf{I}_{N_z} \otimes \mathbf{I}_{N_y} \otimes \left( \mathbf{A}_x + \frac{2\eta_\alpha}{3} \mathbf{B}_x \right) \right) \left( \hat{D}_t \mathbf{U}^m \right) = \mathbf{F}^m. \end{aligned} \tag{4.10}$$

Once the solution  $\mathbf{U}^1$  is obtained via Algorithm 4.1, then from (4.10) we can get  $\mathbf{U}^m$  via the following Algorithm 4.2 for  $m = 2, 3, \dots, M$ .

**Algorithm 4.2. BDF-FV-ADI at time  $t_m$  ( $m \geq 2$ ).**

(i) Solving the subproblem in  $z$ -direction for the intermediate solution  $\mathbf{U}^{m,***} := \{U_{i,j,k}^{m,***}\} \in \mathbb{R}^N$  that

$$\left( \left( \mathbf{A}_z + \frac{2\eta_\gamma}{3} \mathbf{B}_z \right) \otimes \mathbf{I}_{N_y} \otimes \mathbf{I}_{N_x} \right) \mathbf{U}^{m,***} = \mathbf{F}^m; \tag{4.11}$$

(ii) Solving the subproblem in  $y$ -direction for the intermediate solution  $\mathbf{U}^{m,**} := \{U_{i,j,k}^{m,**}\} \in \mathbb{R}^N$  that

$$\left( \mathbf{I}_{N_z} \otimes \left( \mathbf{A}_y + \frac{2\eta_\beta}{3} \mathbf{B}_y \right) \otimes \mathbf{I}_{N_x} \right) \mathbf{U}^{m,**} = \mathbf{U}^{m,***}; \tag{4.12}$$

(iii) Solving the subproblem in  $x$ -direction for the intermediate solution  $\mathbf{U}^{m,*} := \{U_{i,j,k}^{m,*}\} \in \mathbb{R}^N$  that

$$\left( \mathbf{I}_{N_z} \otimes \mathbf{I}_{N_y} \otimes \left( \mathbf{A}_x + \frac{2\eta_\alpha}{3} \mathbf{B}_x \right) \right) \mathbf{U}^{m,*} = \mathbf{U}^{m,**}; \tag{4.13}$$

(iv) Updating the solution  $\mathbf{U}^m$  via  $\hat{D}_t \mathbf{U}^m = \mathbf{U}^{m,*}$ , i.e.,

$$\mathbf{U}^m = \frac{2}{3} \mathbf{U}^{m,*} + \frac{4}{3} \mathbf{U}^{m-1} - \frac{1}{3} \mathbf{U}^{m-2}. \tag{4.14}$$

### 4.2 Practical efficient implementation of the BDF-FV-ADI scheme

In this subsection, we briefly discuss the efficient implementation of the BDF-FV-ADI scheme described in Algorithms 4.1–4.2. As they only have a bit difference, we just take Algorithm 4.1 as a brief illustration.

For any  $N$ -dimensional vector  $\mathbf{v} = \{v_{i,j,k}\} \in \mathcal{V}_h$  defined in the form of (3.5), we denote its column vectors along each spatial direction by

$$\begin{aligned} \mathbf{v}_{:,j,k} &:= [v_{1,j,k}, v_{2,j,k}, \dots, v_{N_x,j,k}]^\top \in \mathbb{R}^{N_x}, & j \in \mathbb{I}_y, & k \in \mathbb{I}_z, \\ \mathbf{v}_{i,:k} &:= [v_{i,1,k}, v_{i,2,k}, \dots, v_{i,N_y,k}]^\top \in \mathbb{R}^{N_y}, & i \in \mathbb{I}_x, & k \in \mathbb{I}_z, \\ \mathbf{v}_{i,j,:} &:= [v_{i,j,1}, v_{i,j,2}, \dots, v_{i,j,N_z}]^\top \in \mathbb{R}^{N_z}, & i \in \mathbb{I}_x, & j \in \mathbb{I}_y, \end{aligned}$$

such that  $\mathbf{v}$  can be represented by block vectors, i.e.,

$$\mathbf{v} = \{\mathbf{v}_{:,j,k}\}_{j \in \mathbb{I}_y, k \in \mathbb{I}_z}, \quad \mathbf{v} = \{\mathbf{v}_{i,:k}\}_{i \in \mathbb{I}_x, k \in \mathbb{I}_z}, \quad \mathbf{v} = \{\mathbf{v}_{i,j,:}\}_{i \in \mathbb{I}_x, j \in \mathbb{I}_y}.$$

Actually, in practical computation, (4.5)–(4.7) reduce to solve a series of small-scale linear algebraic systems.

◇ First, the solution of (4.5) is equivalent to solve a series of  $N_z$ -by- $N_z$  linear system

$$(\mathbf{A}_z + \eta_\gamma \mathbf{B}_z) \mathbf{U}_{i,j,:}^{1,***} = \mathbf{F}_{i,j,:}^1, \quad i \in \mathbb{I}_x, \quad j \in \mathbb{I}_y, \tag{4.15}$$

along the  $z$ -direction. As the special matrix structures (see (3.6)), the coefficient matrix of (4.15) can be computed only one time and stored in  $\mathcal{O}(N_z)$  memory. The main computational costs lie in two aspects:

- (i) The first one is the evaluation of the right-hand side  $N$ -dimensional vector  $\mathbf{F}^1$  (see (4.3)). Following the same idea of Ref. [41], it can be computed in

$$N_z N_y \mathcal{O}(N_x \log N_x) + N_z N_x \mathcal{O}(N_y \log N_y) + N_x N_y \mathcal{O}(N_z \log N_z) = \mathcal{O}(N \log N)$$

operations only one time.

- (ii) Another one is the solution of these linear systems. However, as the coefficient matrix is symmetric positive definite, we can employ the well-known conjugate gradient (CG) solver [1]. As we can see from Algorithm 4.3 below, the main computational cost in this algorithm is the matrix-vector multiplication  $(\mathbf{A}_z + \eta_\gamma \mathbf{B}_z) \mathbf{w}$  for any  $\mathbf{w} \in \mathbb{R}^{N_z}$ , which requires  $\mathcal{O}(N_z \log N_z)$  operations per iteration [8]. Thus the total computational cost for these systems is

$$N_x N_y \mathcal{O}(L_z N_z \log N_z) = \mathcal{O}(L_z N \log N_z),$$

where  $L_z$  is the average number of iterations for the solution of each (4.15). Actually, (4.15) can be solved in parallel on different processors. This will further improve the computational efficiency.

◇ Then, the solution of (4.6) is equivalent to solve a series of  $N_y$ -by- $N_y$  linear system

$$\left(\mathbf{A}_y + \eta_\beta \mathbf{B}_y\right) \mathbf{U}_{i:,k}^{1,**} = \mathbf{U}_{i:,k}^{1,***}, \quad i \in \mathbb{I}_x, \quad k \in \mathbb{I}_z, \quad (4.16)$$

along the  $y$ -direction, which requires

$$N_x N_z \mathcal{O}(L_y N_y \log N_y) = \mathcal{O}(L_y N \log N_y)$$

operations, where  $L_y$  is the average number of iterations for the solution of each (4.16).

◇ Finally, the solution of (4.7) is equivalent to solve a series of  $N_x$ -by- $N_x$  linear system

$$\left(\mathbf{A}_x + \eta_\alpha \mathbf{B}_x\right) \mathbf{U}_{:,j,k}^{1,*} = \mathbf{U}_{:,j,k}^{1,***}, \quad j \in \mathbb{I}_y, \quad k \in \mathbb{I}_z, \quad (4.17)$$

along the  $x$ -direction, which requires

$$N_y N_z \mathcal{O}(L_x N_x \log N_x) = \mathcal{O}(L_x N \log N_x)$$

operations, where  $L_x$  is the average number of iterations for the solution of each (4.17).

**Algorithm 4.3. Review of CG method for linear system  $\mathbf{Ax} = \mathbf{b}$ .**

For an initial guess vector  $\mathbf{x}^0$ , compute  $\mathbf{r}^{(0)} = \mathbf{b} - \mathbf{Ax}^0$ .

For  $i = 1, 2, \dots$

$$\rho_{i-1} = \mathbf{r}^{(i-1)\top} \mathbf{r}^{(i-1)}.$$

If  $i = 1$ , then set  $\mathbf{p}^{(1)} = \mathbf{r}^{(0)}$ .

Else

$$\beta_{i-1} = \rho_{i-1} / \rho_{i-2}, \quad \mathbf{p}^{(i)} = \mathbf{r}^{(i-1)} + \beta_{i-1} \mathbf{p}^{(i-1)}.$$

End if

$$\mathbf{q}^{(i)} = \mathbf{A} \mathbf{p}^{(i)}, \quad \alpha_i = \rho_{i-1} / \mathbf{p}^{(i)\top} \mathbf{q}^{(i)}, \quad \mathbf{x}^{(i)} = \mathbf{x}^{(i-1)} + \alpha_i \mathbf{p}^{(i)}, \quad \mathbf{r}^{(i)} = \mathbf{r}^{(i-1)} - \alpha_i \mathbf{q}^{(i)}.$$

Check convergence; continue if necessary

End

$$\mathbf{x} = \mathbf{x}^{(i)}.$$

**Remark 4.1.** Based on the above discussion, we can obtain a fast version of Algorithm 4.3, named fast conjugate gradient (FCG) solver. Similarly, in practical computation, (4.11)–(4.13) reduce to solve a series of small-scale linear algebraic systems along each spatial direction:

$$\left(\mathbf{A}_z + \frac{2\eta_\gamma}{3} \eta_\gamma \mathbf{B}_z\right) \mathbf{U}_{i,j,:}^{m,***} = \mathbf{F}_{i,j,:}^m, \quad i \in \mathbb{I}_x, \quad j \in \mathbb{I}_y; \quad (4.18a)$$

$$\left(\mathbf{A}_y + \frac{2\eta_\gamma}{3} \eta_\beta \mathbf{B}_y\right) \mathbf{U}_{i,:,k}^{m,**} = \mathbf{U}_{i,:,k}^{m,***}, \quad i \in \mathbb{I}_x, \quad k \in \mathbb{I}_z; \quad (4.18b)$$

$$\left(\mathbf{A}_x + \frac{2\eta_\gamma}{3} \eta_\alpha \mathbf{B}_x\right) \mathbf{U}_{:,j,k}^{m,*} = \mathbf{U}_{:,j,k}^{m,***}, \quad j \in \mathbb{I}_y, \quad k \in \mathbb{I}_z; \quad (4.18c)$$

and also these equations can be solved in parallel. Besides, the memory requirement and computational cost are similar as discussed above.

In summary, we have the following conclusion of the implementation of the BDF-FV-ADI scheme.

**Proposition 4.1.** *Let  $L := \max\{L_x, L_y, L_z\}$ . The total computational cost for the BDF-FV-ADI scheme (4.3)–(4.4) is of order  $\mathcal{O}(LMN \log N)$ , and the memory requirement is of order  $\mathcal{O}(N)$ .*

### 4.3 Corresponding error estimate of the BDF-FV-ADI scheme

In this subsection, we devote to prove the convergence of the BDF-FV-ADI scheme (4.3)–(4.4) via the discrete energy method. We define the following weighted discrete norms

$$\begin{aligned} \|\mathbf{v}\| := & \left( \|\mathbf{v}\|_A^2 + \eta_\beta \eta_\gamma \|\mathbf{v}\|_{\mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x}^2 + \eta_\alpha \eta_\gamma \|\mathbf{v}\|_{\mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x}^2 \right. \\ & \left. + \eta_\alpha \eta_\beta \|\mathbf{v}\|_{\mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x}^2 + \eta_\alpha \eta_\beta \eta_\gamma \|\mathbf{v}\|_{\mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x}^2 \right)^{1/2}, \end{aligned} \tag{4.19a}$$

$$\begin{aligned} \|\mathbf{v}\|_{BDF} := & \left( \|\mathbf{v}\|_A^2 + \frac{4}{9} \eta_\beta \eta_\gamma \|\mathbf{v}\|_{\mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x}^2 + \frac{4}{9} \eta_\alpha \eta_\gamma \|\mathbf{v}\|_{\mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x}^2 \right. \\ & \left. + \frac{4}{9} \eta_\alpha \eta_\beta \|\mathbf{v}\|_{\mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x}^2 + \frac{8}{27} \eta_\alpha \eta_\beta \eta_\gamma \|\mathbf{v}\|_{\mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x}^2 \right)^{1/2}, \end{aligned} \tag{4.19b}$$

by (3.10) and Remark 3.2.

The following equivalence conclusion about the two norms can be proved easily.

**Lemma 4.1.** *The norms  $\|\cdot\|$  and  $\|\cdot\|_{BDF}$  are equivalent with the following relation holds*

$$\frac{2\sqrt{6}}{9} \|\mathbf{v}\| \leq \|\mathbf{v}\|_{BDF} \leq \|\mathbf{v}\|, \quad \mathbf{v} \in \mathcal{V}_h.$$

**Theorem 4.1.** *Suppose that model (1.1a)–(1.1b) has a unique solution  $u(\mathbf{x}, t) \in C^3([0, T]; C^2(\Omega)) \cap C^1([0, T]; C^{\alpha+\beta+\gamma}(\Omega))$  and the condition in Lemma 3.4 holds. Moreover, assume that  $f(u) \in C^1(\mathbb{R})$  and (3.8) is satisfied. If the stepsizes  $\tau, h_x, h_y, h_z$  and  $\frac{\tau^2}{\sqrt{h_x h_y h_z}}$  are sufficiently small, the BDF-FV-ADI scheme defined in (4.3)–(4.4) admits a unique solution  $u_h(\mathbf{x}, t_m)$  satisfying*

$$\max_{\mathbf{x} \in \Omega} |u_h(\mathbf{x}, t_m)| \leq K + 1, \quad m \in \mathbb{I}_t. \tag{4.20}$$

Moreover, there exists a constant  $\hat{\tau} > 0$  such that the following error estimate holds for  $\tau < \hat{\tau}$

$$\|\mathbf{u}^m - \mathbf{U}^m\| + \|\mathbf{u}^m - \mathbf{U}^m\|_E \leq C \left( \tau^2 + h_x^2 + h_y^2 + h_z^2 \right), \quad m \in \mathbb{I}_t, \tag{4.21}$$

where the constant  $C$  is independent of the mesh parameters  $h_x, h_y, h_z$  and  $\tau$ .

*Proof.* Due to the positive definiteness of the coefficient matrix yielded by the BDF-FV-ADI scheme (4.3)-(4.4), the existence and uniqueness of the numerical solution follows immediately.

Similar to the proof of Theorem 3.1, we shall prove (4.20)–(4.21) by the mathematical induction method. Let  $\mathbf{e}^m := \mathbf{u}^m - \mathbf{U}^m$  with  $\mathbf{e}^0 = 0$ . Considering the added small perturbation terms  $\mathbf{p}^m$ , we conclude that  $\mathbf{e}^m$  satisfies the following error equations:

$$(\mathbf{A}_z + \eta_\gamma \mathbf{B}_z) \otimes (\mathbf{A}_y + \eta_\beta \mathbf{B}_y) \otimes (\mathbf{A}_x + \eta_\alpha \mathbf{B}_x) (\hat{D}_t \mathbf{e}^1) = \tau (\tilde{\mathcal{N}}^1 - \mathcal{N}^1 + \mathbf{R}_{BDF}^1), \tag{4.22}$$

for  $m = 1$ , and

$$\begin{aligned} & (\mathbf{A}_z + \frac{2\eta_\gamma}{3} \mathbf{B}_z) \otimes (\mathbf{A}_y + \frac{2\eta_\beta}{3} \mathbf{B}_y) \otimes (\mathbf{A}_x + \frac{2\eta_\alpha}{3} \mathbf{B}_x) (\hat{D}_t \mathbf{e}^m) \\ &= -\frac{1}{3} (\eta_\alpha \mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x + \eta_\beta \mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x + \eta_\gamma \mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x) (4\mathbf{e}^{m-1} - \mathbf{e}^{m-2}) \\ & \quad + \tau (\tilde{\mathcal{N}}^m - \mathcal{N}^m + \mathbf{R}_{BDF}^m), \end{aligned} \tag{4.23}$$

for  $m \geq 2$ , where from Lemmas 2.1–2.2, (3.16) and (4.1)–(4.2) that

$$\mathbf{R}_{BDF}^m = (r_t^m + r_n^m + r_s^m + \mathbf{p}^m / \tau) \mathbf{E} = \begin{cases} \mathcal{O}(\tau + h_x^2 + h_y^2 + h_z^2) \mathbf{E}, & m = 1, \\ \mathcal{O}(\tau^2 + h_x^2 + h_y^2 + h_z^2) \mathbf{E}, & m \geq 2. \end{cases} \tag{4.24}$$

Next, we firstly prove (4.20)–(4.21) for the case  $m = 1$ . Note that (4.22) is equivalent to the following form:

$$\begin{aligned} & (\mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x + \eta_\alpha \eta_\beta \mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x + \eta_\alpha \eta_\gamma \mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x + \eta_\beta \eta_\gamma \mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x \\ & + \eta_\alpha \eta_\beta \eta_\gamma \mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x) (\hat{D}_t \mathbf{e}^1) + (\eta_\alpha \mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x + \eta_\beta \mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x + \eta_\gamma \mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x) \mathbf{e}^1 \\ &= \tau (\tilde{\mathcal{N}}^1 - \mathcal{N}^1 + \mathbf{R}_{BDF}^1). \end{aligned} \tag{4.25}$$

Then, taking the discrete inner product of (4.25) with  $\mathbf{e}^1$ , and following a similar treatment as (3.26)–(3.29), we derive

$$\|\|\| \mathbf{e}^1 \|\|\| + \|\mathbf{e}^1\|_E \leq C (\tau^2 + h_x^2 + h_y^2 + h_z^2), \tag{4.26}$$

for sufficiently small  $\tau < 1$ , and thus by Lemma 3.3 and definition (4.19a), this immediately yields the estimate (4.21) for  $m = 1$ . Moreover, the boundedness of the finite volume solution  $u_h(\mathbf{x}, t_1)$  in (4.20) can be proved similarly as (3.29) for sufficiently small  $\frac{\tau^2}{\sqrt{h_x h_y h_z}}$ ,  $h_x$ ,  $h_y$  and  $h_z$ .



Secondly, we assume that (4.20) holds for  $k \leq m - 1$  with  $m \geq 2$ . To prove (4.20)–(4.21) at the time instant  $t_m$ , we start from the following equivalent form of (4.23):

$$\begin{aligned} & \left( \mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x + \frac{4}{9} \eta_\alpha \eta_\beta \mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x + \frac{4}{9} \eta_\alpha \eta_\gamma \mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x + \frac{4}{9} \eta_\beta \eta_\gamma \mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x \right. \\ & \quad \left. + \frac{8}{27} \eta_\alpha \eta_\beta \eta_\gamma \mathbf{B}_z \otimes \mathbf{B}_y \otimes \mathbf{B}_x \right) (\hat{D}_t \mathbf{e}^m) \\ & \quad + (\eta_\alpha \mathbf{A}_z \otimes \mathbf{A}_y \otimes \mathbf{B}_x + \eta_\beta \mathbf{A}_z \otimes \mathbf{B}_y \otimes \mathbf{A}_x + \eta_\gamma \mathbf{B}_z \otimes \mathbf{A}_y \otimes \mathbf{A}_x) \mathbf{e}^m \\ = & \tau (\tilde{\mathcal{N}}^m - \mathcal{N}^m + \mathbf{R}_{BDF}^m), \quad m \geq 2. \end{aligned} \tag{4.27}$$

Then, similar as the proof of Theorem 3.1, by taking the discrete inner product of (4.27) with  $\mathbf{e}^m$  and using a similar inequality (3.31) with  $\|\cdot\|_A$  norm replaced by  $\|\cdot\|_{BDF}$  norm, we can obtain

$$\begin{aligned} & \|\mathbf{e}^m\|_{BDF}^2 + \|\mathbf{2e}^m - \mathbf{e}^{m-1}\|_{BDF}^2 + \|\mathbf{e}^m\|_E^2 \\ & \leq \|\mathbf{e}^{m-1}\|_{BDF}^2 + \|\mathbf{2e}^{m-1} - \mathbf{e}^{m-2}\|_{BDF}^2 + 4\tau (\tilde{\mathcal{N}}^m - \mathcal{N}^m + \mathbf{R}_{BDF}^m, \mathbf{e}^m) \\ & \leq \|\mathbf{e}^{m-1}\|_{BDF}^2 + (1 + 512\sqrt{2}L^2\tau) \|\mathbf{2e}^{m-1} - \mathbf{e}^{m-2}\|_{BDF}^2 + 8\sqrt{2}\tau \|\mathbf{e}^m\|_{BDF}^2 \\ & \quad + 4\sqrt{2}\tau \|\mathbf{R}_{BDF}^m\|^2 + C\tau (h_x^2 + h_y^2 + h_z^2)^2, \end{aligned} \tag{4.28}$$

where Lemma 3.5 is utilized to estimate  $\|\tilde{\mathcal{N}}^m - \mathcal{N}^m\|$  due to the fact  $u_h(\mathbf{x}, t_{m-1})$  and  $u_h(\mathbf{x}, t_{m-2})$  are bounded.

Denote

$$\mathbf{Q}(\mathbf{e}^m) = \|\mathbf{e}^m\|_{BDF}^2 + \|\mathbf{2e}^m - \mathbf{e}^{m-1}\|_{BDF}^2.$$

We can further deduce from (4.28), (4.24) and (3.36) that

$$\begin{aligned} & \mathbf{Q}(\mathbf{e}^m) + \|\mathbf{e}^m\|_E^2 \\ & \leq \frac{1 + 512\sqrt{2}L^2\tau}{1 - 8\sqrt{2}\tau} \mathbf{Q}(\mathbf{e}^{m-1}) + \frac{4\sqrt{2}\tau}{1 - 8\sqrt{2}\tau} \|\mathbf{R}_{BDF}^m\|^2 + C\tau (h_x^2 + h_y^2 + h_z^2)^2 \\ & \leq \left( \frac{1 + 512\sqrt{2}L^2\tau}{1 - 8\sqrt{2}\tau} \right)^{m-1} \mathbf{Q}(\mathbf{e}^1) + \frac{4\sqrt{2}\tau}{1 - 8\sqrt{2}\tau} \sum_{k=2}^m \left( \frac{1 + 512\sqrt{2}L^2\tau}{1 - 8\sqrt{2}\tau} \right)^{m-k} \|\mathbf{R}_{BDF}^k\|^2 \\ & \quad + C\tau \sum_{k=2}^m \left( \frac{1 + 512\sqrt{2}L^2\tau}{1 - 8\sqrt{2}\tau} \right)^{m-k} (h_x^2 + h_y^2 + h_z^2)^2 \\ & \leq C \left[ \mathbf{Q}(\mathbf{e}^1) + (\tau^2 + h_x^2 + h_y^2 + h_z^2)^2 \right], \quad \tau \leq \frac{\sqrt{2}}{16}. \end{aligned} \tag{4.29}$$

Noting the definition of  $\mathbf{Q}(\mathbf{e}^m)$  and (4.26), and meanwhile using Lemma 4.1, we have

$$\mathbf{Q}(\mathbf{e}^1) = 5 \|\mathbf{e}^1\|_{BDF}^2 \leq 5 \|\mathbf{e}^1\|^2 \leq C (\tau^2 + h_x^2 + h_y^2 + h_z^2)^2, \tag{4.30}$$

and then, we substitute (4.30) into (4.29) to obtain

$$\mathbf{Q}(\mathbf{e}^m) + \|\mathbf{e}^m\|_E^2 \leq C \left( \tau^2 + h_x^2 + h_y^2 + h_z^2 \right)^2,$$

which proves (4.21) using Lemma 3.3 and definition (4.19b).

Finally, similar to the process (3.38), we can easily obtain the boundedness results (4.20) for the BDF-FV-ADI solution  $u_h(\mathbf{x}, t_m)$  for sufficiently small  $\frac{\tau^2}{\sqrt{h_x h_y h_z}}$ ,  $h_x$ ,  $h_y$  and  $h_z$ . Thus, Theorem 4.1 is proved.  $\square$

**Corollary 4.1.** *Assume the conditions in Theorem 4.1 hold. Analogous to Corollary 3.2, we can further derive the optimal-order error estimate of the BDF-FV-ADI scheme in the sense of continuous  $L^2$  norm:*

$$\|u(\mathbf{x}, t_m) - u_h(\mathbf{x}, t_m)\|_{L^2} \leq C \left( \tau^2 + h_x^2 + h_y^2 + h_z^2 \right). \tag{4.31}$$

## 5 Numerical experiments

In this section, we carry out several numerical experiments to investigate the convergence and efficiency of the proposed finite volume methods. Both the BDF-FV scheme (3.7) and the BDF-FV-ADI scheme (4.3)–(4.4) are implemented, which are solved by the traditional GE solver, the CG solver and the FCG solver. All numerical experiments below are carried out using MATLAB R2018b on a Windows server with Intel(R) Xeon(R) E5-2650 processor of 128GB RAM and 2.30GHz CPU. Besides, in all simulations, the convergence orders of the schemes are measured as follows:

$$Cov_d = \log_2 \left( \frac{Err_d(2h, 2\tau)}{Err_d(h, \tau)} \right), \quad Cov_c = \log_2 \left( \frac{Err_c(2h, 2\tau)}{Err_c(h, \tau)} \right),$$

where  $Err_d(h, \tau)$  and  $Err_c(h, \tau)$  respectively denote the discrete and continuous  $L^2$ -norm errors with  $h = h_x = h_y = h_z$ .

### 5.1 Accuracy of the BDF-FV and BDF-FV-ADI schemes

In this subsection, the analytical solution of (1.1a) is given by

$$u(\mathbf{x}, t) = 64e^{-t} x^2 (1-x)^2 y^2 (1-y)^2 z^2 (1-z)^2,$$

for  $(\mathbf{x}, t) \in [0, 1]^3 \times [0, 1]$ , where the nonlinear reaction term  $f(u) = (\sin u)^4$ , and the linear part  $g(\mathbf{x}, t)$  is computed accordingly.

We run two sets of numerical experiments to verify the convergence of the BDF-FV and BDF-FV-ADI schemes via GE solver with respect to various fractional orders  $\alpha$ ,  $\beta$ ,  $\gamma$  and various diffusion coefficients  $d_x$ ,  $d_y$ ,  $d_z$ . First, for fixed diffusion coefficients  $d_x = d_y = d_z = 1$ , we test the discrete and continuous  $L^2$ -norm errors and convergence orders of

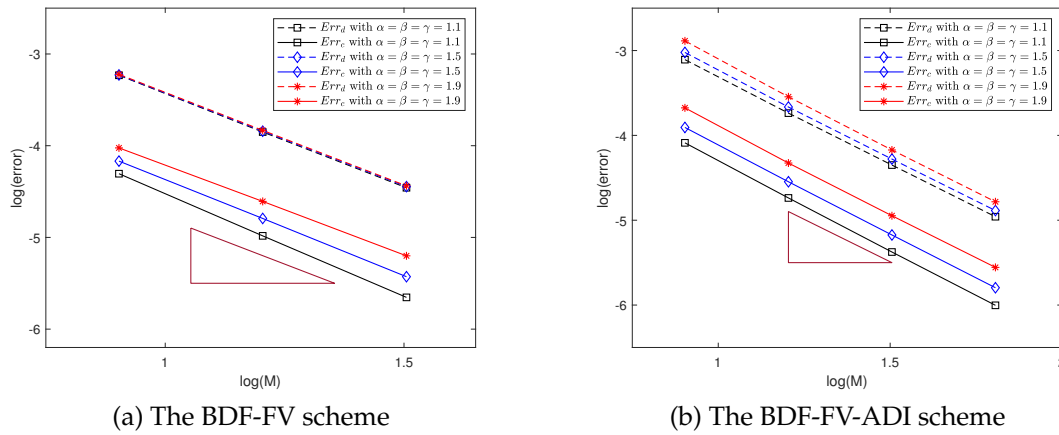


Figure 1: Errors and corresponding convergence orders, where the tangent of the triangle is 2.

the BDF-FV scheme and BDF-FV-ADI scheme, where different fractional orders  $\alpha = \beta = \gamma = 1.1, 1.5$  and  $1.9$  are selected. From the numerical results shown in Tables 1–2, we can observe that both the two numerical schemes generate the numerical solutions with the same magnitude accuracy, although an extra perturbation term is introduced in the ADI method. Meanwhile, second-order convergence in time and space is easily seen from Fig. 1, which is independent of the fractional orders.

Next, for fixed fractional orders  $\alpha=1.7, \beta=1.5$  and  $\gamma=1.3$ , we also test the convergence of the two schemes for various diffusion coefficients  $d_x=d_y=d_z=1; d_x=1.5, d_y=1, d_z=0.5$  and  $d_x=100, d_y=1, d_z=0.01$ . Similarly, numerical solutions with the same magnitude error accuracy and second-order convergence in the sense of discrete and continuous  $L^2$  norm errors are both observed from Tables 3–4 and Fig. 2. Moreover, we also see the error accuracy and convergence orders are independent of the diffusion coefficients.

Table 1: Results of the BDF-FV scheme for  $d_x=d_y=d_z=1$  and representative fractional orders.

$N_x=N_y=N_z=M$	$\alpha=\beta=\gamma=1.1$		$\alpha=\beta=\gamma=1.5$		$\alpha=\beta=\gamma=1.9$	
	$Err_d$	$Cov_d$	$Err_d$	$Cov_d$	$Err_d$	$Cov_d$
$2^3=8$	$5.86 \times 10^{-4}$	—	$5.91 \times 10^{-4}$	—	$6.00 \times 10^{-4}$	—
$2^4=16$	$1.41 \times 10^{-4}$	2.05	$1.44 \times 10^{-4}$	2.04	$1.47 \times 10^{-4}$	2.03
$2^5=32$	$3.48 \times 10^{-5}$	2.02	$3.58 \times 10^{-5}$	2.01	$3.65 \times 10^{-5}$	2.00
$2^6=64$	out of memory	—	out of memory	—	out of memory	—
	$Err_c$	$Cov_c$	$Err_c$	$Cov_c$	$Err_c$	$Cov_c$
$2^3=8$	$4.95 \times 10^{-5}$	—	$6.79 \times 10^{-5}$	—	$9.46 \times 10^{-5}$	—
$2^4=16$	$1.04 \times 10^{-5}$	2.25	$1.61 \times 10^{-5}$	2.08	$2.47 \times 10^{-5}$	1.94
$2^5=32$	$2.22 \times 10^{-6}$	2.24	$3.73 \times 10^{-6}$	2.11	$6.30 \times 10^{-6}$	1.97
$2^6=64$	out of memory	—	out of memory	—	out of memory	—

Table 2: Results of the BDF-FV-ADI scheme for  $d_x=d_y=d_z=1$  and representative fractional orders.

$N_x=N_y=N_z=M$	$\alpha=\beta=\gamma=1.1$		$\alpha=\beta=\gamma=1.5$		$\alpha=\beta=\gamma=1.9$	
	$Err_d$	$Cov_d$	$Err_d$	$Cov_d$	$Err_d$	$Cov_d$
$2^3=8$	$7.81 \times 10^{-4}$	—	$9.50 \times 10^{-4}$	—	$1.30 \times 10^{-3}$	—
$2^4=16$	$1.83 \times 10^{-4}$	2.10	$2.16 \times 10^{-4}$	2.14	$2.85 \times 10^{-4}$	2.19
$2^5=32$	$4.47 \times 10^{-5}$	2.03	$5.26 \times 10^{-5}$	2.04	$6.73 \times 10^{-5}$	2.08
$2^6=64$	$1.10 \times 10^{-5}$	2.02	$1.30 \times 10^{-5}$	2.02	$1.65 \times 10^{-5}$	2.03
	$Err_c$	$Cov_c$	$Err_c$	$Cov_c$	$Err_c$	$Cov_c$
$2^3=8$	$8.17 \times 10^{-5}$	—	$1.24 \times 10^{-4}$	—	$2.11 \times 10^{-4}$	—
$2^4=16$	$1.83 \times 10^{-5}$	2.16	$2.84 \times 10^{-5}$	2.13	$4.72 \times 10^{-5}$	2.16
$2^5=32$	$4.22 \times 10^{-6}$	2.11	$6.70 \times 10^{-6}$	2.08	$1.13 \times 10^{-5}$	2.06
$2^6=64$	$9.93 \times 10^{-7}$	2.09	$1.60 \times 10^{-6}$	2.07	$2.78 \times 10^{-6}$	2.03

Table 3: Results of the BDF-FV scheme for  $\alpha=1.7, \beta=1.5, \gamma=1.3$  and representative diffusion coefficients.

$N_x=N_y=N_z=M$	$d_x=d_y=d_z=1$		$d_x=1.5, d_y=1, d_z=0.5$		$d_x=100, d_y=1, d_z=0.01$	
	$Err_d$	$Cov_d$	$Err_d$	$Cov_d$	$Err_d$	$Cov_d$
$2^3=8$	$5.97 \times 10^{-4}$	—	$6.17 \times 10^{-4}$	—	$6.95 \times 10^{-4}$	—
$2^4=16$	$1.46 \times 10^{-4}$	2.04	$1.50 \times 10^{-4}$	2.04	$1.67 \times 10^{-4}$	2.06
$2^5=32$	$3.62 \times 10^{-5}$	2.01	$3.73 \times 10^{-5}$	2.01	$4.12 \times 10^{-5}$	2.02
$2^6=64$	out of memory	—	out of memory	—	out of memory	—
	$Err_c$	$Cov_c$	$Err_c$	$Cov_c$	$Err_c$	$Cov_c$
$2^3=8$	$7.06 \times 10^{-5}$	—	$7.35 \times 10^{-5}$	—	$7.92 \times 10^{-5}$	—
$2^4=16$	$1.70 \times 10^{-5}$	2.05	$1.79 \times 10^{-5}$	2.04	$1.96 \times 10^{-5}$	2.01
$2^5=32$	$4.02 \times 10^{-6}$	2.08	$4.26 \times 10^{-6}$	2.07	$4.75 \times 10^{-6}$	2.05
$2^6=64$	out of memory	—	out of memory	—	out of memory	—

Table 4: Results of the BDF-FV-ADI scheme for  $\alpha=1.7, \beta=1.5, \gamma=1.3$  and representative diffusion coefficients.

$N_x=N_y=N_z=M$	$d_x=d_y=d_z=1$		$d_x=1.5, d_y=1, d_z=0.5$		$d_x=100, d_y=1, d_z=0.01$	
	$Err_d$	$Cov_d$	$Err_d$	$Cov_d$	$Err_d$	$Cov_d$
$2^3=8$	$9.56 \times 10^{-4}$	—	$9.36 \times 10^{-4}$	—	$1.10 \times 10^{-3}$	—
$2^4=16$	$2.18 \times 10^{-4}$	2.13	$2.16 \times 10^{-4}$	2.12	$2.43 \times 10^{-4}$	2.18
$2^5=32$	$5.30 \times 10^{-5}$	2.04	$5.27 \times 10^{-5}$	2.03	$5.93 \times 10^{-5}$	2.03
$2^6=64$	$1.31 \times 10^{-5}$	2.02	$1.30 \times 10^{-5}$	2.01	$1.47 \times 10^{-5}$	2.01
	$Err_c$	$Cov_c$	$Err_c$	$Cov_c$	$Err_c$	$Cov_c$
$2^3=8$	$1.27 \times 10^{-4}$	—	$1.25 \times 10^{-4}$	—	$1.50 \times 10^{-4}$	—
$2^4=16$	$2.93 \times 10^{-5}$	2.12	$3.62 \times 10^{-5}$	2.09	$3.62 \times 10^{-5}$	2.05
$2^5=32$	$6.98 \times 10^{-6}$	2.07	$8.83 \times 10^{-6}$	2.06	$8.83 \times 10^{-6}$	2.04
$2^6=64$	$1.68 \times 10^{-6}$	2.06	$2.16 \times 10^{-6}$	2.05	$2.16 \times 10^{-6}$	2.03

In addition, it is observed that the BDF-FV-ADI scheme (4.3)-(4.4) is more memory saving than the BDF-FV scheme (3.7). For example, when  $N_x=N_y=N_z=M=64$ , the former can still run, while the latter is out of memory, as at this moment there are 262,144

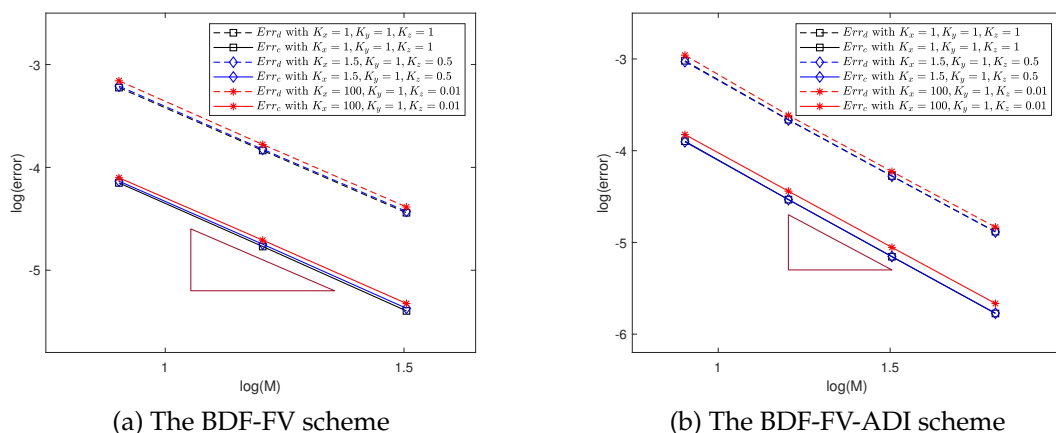


Figure 2: Errors and corresponding convergence orders, where the tangent of the triangle is 2.

unknowns at each time level. In the following test, we shall implement further experiments to corroborate the efficiency of proposed ADI method.

### 5.2 Performance of the BDF-FV and BDF-FV-ADI schemes via different solvers

In this test, we take  $f(u) = u - u^3$ , and in this case model (1.1a) reduces to the space-fractional Allen-Cahn equation with a polynomial double-well potential [12]. The linear part  $g(\mathbf{x}, t)$  is given such that the analytical solution is

$$u(\mathbf{x}, t) = 11134e^{-t}x^2(1-x)^2y^2(1-y)^2z^2(1-z)^2,$$

for  $(\mathbf{x}, t) \in [0, 1]^3 \times [0, 1]$ . We fix the fractional orders  $\alpha = 1.7, \beta = 1.5, \gamma = 1.3$  and diffusion coefficients  $d_x = d_y = d_z = 1$  to compare the performance of the BDF-FV scheme and the BDF-FV-ADI scheme via different solvers.

By testing this Allen-Cahn equation, we list the numerical errors and CPU times consumed by the GE, CG and FCG solvers for the two schemes in Tables 5–6, respectively. First, we observe that the proposed ADI method greatly reduces the CPU time and memory requirement compared with the BDF-FV scheme, no matter which solver is adopted. For example, when  $N_x = N_y = N_z = 2^4$ , it takes more than two hours for the BDF-FV scheme via the GE solver, and it is even out of memory for  $N_x = N_y = N_z = 2^6$ , while the BDF-FV-ADI scheme with the GE solver consumes only about six minutes for the latter case! What we have to mention more is that there is not enough memory for the BDF-FV scheme to run this numerical experiment when  $N_x = N_y = N_z \geq 2^6$ , while the BDF-FV-ADI scheme can still run even for  $N_x = N_y = N_z = 2^8$ . This confirms that the proposed ADI method can significantly reduce the memory requirement for the BDF-FV scheme.

Table 5: Results of the BDF-FV scheme for Allen-Cahn equation with  $\alpha = 1.7, \beta = 1.5, \gamma = 1.3$ .

$N_x = N_y = N_z = M$	CPU times (GE)	CPU times (CG)	CPU times (FCG)	$Err_d$	$Cov_d$
$2^3 = 8$	0.74 s	0.14 s	0.56 s	$9.82 \times 10^{-2}$	—
$2^4 = 16$	2 h 7 m 17 s	30.31 s	4.19 s	$2.42 \times 10^{-2}$	2.02
$2^5 = 32$	> 10 d	2 h 35 m 7 s	1 m 5 s	$6.00 \times 10^{-3}$	2.01
$2^6 = 64$	out of memory	out of memory	16 m 59 s	$1.50 \times 10^{-3}$	2.00

Table 6: Results of the BDF-FV-ADI scheme for Allen-Cahn equation with  $\alpha = 1.7, \beta = 1.5, \gamma = 1.3$ .

$N_x = N_y = N_z = M$	CPU times (GE)	CPU times (CG)	CPU times (FCG)	$Err_d$	$Cov_d$
$2^6 = 64$	6 m 17 s	2 m 18 s	3 m 55 s	$2.20 \times 10^{-3}$	—
$2^7 = 128$	6 h 32 m 15 s	3 h 7 m 10 s	1 h 37 m 59 s	$5.41 \times 10^{-4}$	2.02
$2^8 = 256$	> 10 d	8 d 13 h 37 m	1 d 8 h 48 m	$1.35 \times 10^{-4}$	2.01

Thus, the developed BDF-FV-ADI method is more suitable for large-scale modeling and simulations of three-dimensional problems.

Next, we see that all solvers basically generate the same error results, but the FCG solver for both schemes has clear advantages in computational efficiency and storage over the other two solvers. For example, when  $N_x = N_y = N_z = 2^7$  (about 2.1 millions of unknowns each time level), it takes more than six and a half hours for the implementation of the BDF-FV-ADI scheme via the GE solver, while the CG solver consumes about three hours. What is even more amazing is that the developed FCG solver takes only about one and a half hours! The contrasts shall be more obvious for even fine temporal/spatial meshes. Besides, when  $N_x = N_y = N_z = 2^6$ , both the traditional GE and CG solvers are running out of memory for the BDF-FV scheme, but the FCG solver with efficient computational strategy and storage solution (see Remark 3.3 and [41]) can still run. It is deemed that for fine temporal/spatial meshes, even the BDF-FV-ADI scheme with GE and CG solvers shall be out of memory, but the FCG solver can still run. In conclusion, numerical results show that the BDF-FV-ADI scheme via the FCG solver can greatly reduce the CPU time and storage, which is consistent with our analysis in subsection 4.2.

## 6 Conclusions

In this paper, by using the linear extrapolation technique to deal with the nonlinear reaction term, two linearized implicit finite volume schemes combined with the second-order BDF time discretization are developed for the three-dimensional nonlinear Riesz s-FRDEs. Second-order convergence of the proposed methods are strictly proved with respect to discrete and continuous  $L^2$  norms via the discrete energy method. Compared with the BDF-FV scheme, the BDF-FV-ADI method reduces the solution of a large-scale three-dimensional problem into a series of independent small-scale one-dimensional sub-problems, which greatly reduce the computational complexity and memory requirement. Moreover, practical efficient implementation of the ADI method is briefly discussed based

on the CG solver. Finally, numerical experiments are given to verify the theoretical analysis results.

## Acknowledgements

The authors would like to express their most sincere thanks to the referees for their very helpful comments and suggestions, which greatly improved the quality of this paper. This work was supported in part by the National Natural Science Foundation of China (Nos. 11971482 and 12131014), by the Natural Science Foundation of Shandong Province (Nos. ZR2017MA006, ZR2019MA015 and ZR2021MA020) and by the OUC Scientific Research Program for Young Talented Professionals.

## References

- [1] R. BARRETT, M. BERRY, T. CHAN, J. DEMMEL, J. DONATO, J. DONGARRA, V. EIJKHOUT, R. POZO, C. ROMINE AND H. VAN DER VORST, *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*, SIAM, Philadelphia, 1994.
- [2] K. BURRAGE, N. HALE AND D. KAY, *An efficient implicit FEM scheme for fractional-in-space reaction-diffusion equations*, *SIAM J. Sci. Comput.*, 34 (2012), pp. A2145–A2172.
- [3] A. BUENO-OROVIO, D. KAY AND K. BURRAGE, *Fourier spectral methods for fractional-in-space reaction-diffusion equations*, *BIT. Numer. Math.*, 54 (2014), pp. 937–954.
- [4] C. CELIK AND M. DUMAN, *Crank-Nicolson method for the fractional diffusion equation with the Riesz fractional derivative*, *J. Comput. Phys.*, 231 (2012), pp. 1743–1750.
- [5] H. CHEN, S. GAN, D. XU AND Q. LIU, *A second-order BDF compact difference scheme for fractional-order Volterra equation*, *Int. J. Comput. Math.*, 93 (2016), pp. 1140–1154.
- [6] X. CHENG, J. DUAN AND D. LI, *A novel compact ADI scheme for two-dimensional Riesz space fractional nonlinear reaction-diffusion equations*, *Appl. Math. Comput.*, 346 (2019), pp. 452–464.
- [7] H. FU, H. LIU AND H. WANG, *A finite volume method for two-dimensional Riemann-Liouville space-fractional diffusion equation and its efficient implementation*, *J. Comput. Phys.*, 388 (2019), pp. 316–334.
- [8] H. FU, Y. SUN, H. WANG AND X. ZHENG, *Stability and convergence of a Crank-Nicolson finite volume method for space fractional diffusion equations*, *Appl. Numer. Math.*, 139 (2019), pp. 38–51.
- [9] R. GRAY, *Toeplitz and circulant matrices: a review*, *Found. Trends Commun. Inf. Theory.*, 2 (2006), pp. 155–239.
- [10] H. HEJAZI, T. MORONEY AND F. LIU, *A finite volume method for solving the two-sided time-space fractional advection-dispersion equation*, *Cent. Euro. J. Phys.*, 11 (2013), pp. 1275–1283.
- [11] R. HORN AND C. JOHNSON, *Topics in Matrix Analysis*, Cambridge University Press, Cambridge, 1994.
- [12] T. HOU, T. TANG AND J. YANG, *Numerical analysis of fully discretized Crank-Nicolson scheme for fractional-in-space Allen-Cahn equations*, *J. Sci. Comput.*, 72 (2017), pp. 1–18.
- [13] D. HU AND X. CAO, *A fourth-order compact ADI scheme for two-dimensional Riesz space fractional nonlinear reaction-diffusion equation*, *Int. J. Comput. Math.*, 97 (2020), pp. 1928–1948.
- [14] J. JIA AND H. WANG, *A preconditioned fast finite volume scheme for a fractional differential equation discretized on a locally refined composite mesh*, *J. Comput. Phys.*, 299 (2015), pp. 842–862.

- [15] H. JIANG, F. LIU, I. TURNER AND K. BURRAGE, *Analytical solutions for the multi-term time-space Caputo-Riesz fractional advection-diffusion equations on a finite domain*, J. Math. Anal. Appl., 389 (2012), pp. 1117–1127.
- [16] B. JIN, R. LAZARO, J. PASCIAK AND Z. ZHOU, *Error analysis of a finite element method for the space-fractional parabolic equation*, SIAM J. Numer. Anal., 52 (2014), pp. 2272–2294.
- [17] A. LAUB, *Matrix Analysis for Scientists and Engineers*, SIAM, Philadelphia, 2005.
- [18] H. LIU, X. ZHENG, H. FU AND H. WANG, *Analysis and efficient implementation of ADI finite volume method for Riesz space-fractional diffusion equations in two space dimensions*, Numer. Math. Partial Differential Equations, 37 (2021), pp. 818–835.
- [19] J. LIU, C. ZHU, Y. CHEN AND H. FU, *A Crank-Nicolson ADI quadratic spline collocation method for two-dimensional Riemann-Liouville space-fractional diffusion equations*, Appl. Numer. Math., 160 (2021), pp. 331–348.
- [20] F. LIU, P. ZHUANG, I. TURNER, K. BURRAGE AND V. ANH, *A new fractional finite volume method for solving the fractional diffusion equation*, Appl. Math. Model., 38 (2014), pp. 3871–3878.
- [21] R. MAGIN, O. ABDULLAH, D. BALEANU AND X. ZHOU, *Anomalous diffusion expressed through fractional order differential operators in the Bloch-Torrey equation*, J. Magn. Reson., 190 (2008), pp. 255–270.
- [22] M. MEERSCHAERT AND C. TADJERAN, *Finite difference approximations for two sided space-fractional partial differential equations*, Appl. Numer. Math., 56 (2006), pp. 80–90.
- [23] K. MUSTAPHA AND W. MCLEAN, *Superconvergence of a discontinuous Galerkin method for fractional diffusion and wave equations*, SIAM J. Numer. Anal., 51 (2013), pp. 491–515.
- [24] J. PAN, R. KE, M. NG AND H. SUN, *Preconditioning techniques for diagonal-times-Toeplitz matrices in fractional diffusion equations*, SIAM J. Sci. Comput., 36 (2014), pp. A2698–A2719.
- [25] I. PODLUBNY, *Fractional Differential Equations*, Academic Press, New York, 1999.
- [26] A. QUARTERONI, R. SACCO AND F. SALERI, *Numerical Mathematics*, Springer, New York, 2007.
- [27] A. SIMMONS, Y. YANG AND T. MORONEY, *A finite volume method for two-sided fractional diffusion equations on non-uniform meshes*, J. Comput. Phys., 335 (2017), pp. 747–759.
- [28] T. TANG, L. WANG, H. YUAN AND T. ZHOU, *Rational spectral methods for PDEs involving fractional Laplacian in unbounded domains*, SIAM J. Sci. Comput., 42 (2020), pp. A585–A611.
- [29] C. TADJERAN AND M. MEERSCHAERT, *A second-order accurate numerical method for the two-dimensional fractional diffusion equation*, J. Comput. Phys., 220 (2007), pp. 813–823.
- [30] V. THOMÉE, *Galerkin Finite Element Methods for Parabolic Problems (2nd Ed.)*, Springer Series in Computational Mathematics, Springer, Berlin, 2006.
- [31] W. TIAN, H. ZHOU AND W. DENG, *A class of second order difference approximations for solving space fractional diffusion equations*, Math. Comput., 84 (2015), pp. 1703–1727.
- [32] P. VERMA AND M. KUMAR, *An analytical solution of multi-dimensional space fractional diffusion equations with variable coefficients*, Int. J. Model. Simulate. Sci. Comput., 12 (2021), 2150006.
- [33] H. WANG AND K. WANG, *An  $\mathcal{O}(N \log^2 N)$  alternating-direction finite difference method for two-dimensional fractional diffusion equations*, J. Comput. Phys., 230 (2011), pp. 7830–7839.
- [34] H. WANG AND N. DU, *Fast alternating-direction finite difference methods for three-dimensional space-fractional diffusion equations*, J. Comput. Phys., 258 (2014), pp. 305–318.
- [35] H. WANG, Y. CHEN, Y. HUANG AND W. MAO, *A posteriori error estimates of the Galerkin spectral methods for space-time fractional diffusion equations*, Adv. Appl. Math. Mech., 12 (2020), pp. 87–100.
- [36] Q. YANG, I. TURNER, T. MORONEY AND F. LIU, *A finite volume scheme with preconditioned*



- Lanczos method for two-dimensional space-fractional reaction-diffusion equations*, Appl. Math. Model., 38 (2014), pp. 3755–3762.
- [37] M. ZAKY, A. HENDY AND J. MACIAS-DIAZ, *Semi-implicit Galerkin-Legendre spectral schemes for nonlinear time-space fractional diffusion-reaction equations with smooth and nonsmooth solutions*, J. Sci. Comput., 82 (2020), 13.
- [38] F. ZENG, F. LIU, C. LI, K. BURRAGE, I. TURNER AND V. ANH, *A Crank-Nicolson ADI spectral method for a two-dimensional Riesz space fractional nonlinear reaction-diffusion equation*, SIAM J. Numer. Anal., 52 (2014), pp. 2599–2622.
- [39] H. ZHANG, F. LIU, X. JIANG, F. ZENG AND I. TURNER, *A Crank-Nicolson ADI Galerkin-Legendre spectral method for the two-dimensional Riesz space distributed-order advection-diffusion equation*, Comput. Math. Appl., 76 (2018), pp. 2460–2476.
- [40] X. ZHAO, Z. SUN AND Z. HAO, *A fourth-order compact ADI scheme for two-dimensional nonlinear space fractional Schrödinger equation*, SIAM J. Sci. Comput., 36 (2014), pp. A2865–A2886.
- [41] X. ZHENG, H. LIU, H. WANG AND H. FU, *An efficient finite volume method for nonlinear distributed-order space-fractional diffusion equations in three space dimensions*, J. Sci. Comput., 80 (2019), pp. 1395–1418.