

Numerical algorithm for three-dimensional space fractional advection diffusion equation

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Abstract. Space fractional advection diffusion equations are better to describe anomalous diffusion phenomena because of non-locality of fractional derivatives, which causes people to confront great trouble in problem solving while enjoying the convenience from mathematical modelling, especially in high dimensional cases. In this paper, we solve the three-dimensional problem by the process of dimension by dimension, which can be achieved through a predictor-corrector algorithm. In time discretization, Crank-Nicolson scheme is adopted to match second-order difference operator of the space direction. Then, the efficiency of this method is demonstrated by some numerical examples finally.

1 Introduction

In recent decades, anomalous diffusion has been widely recognized in the scientific fields. Thus the fractional partial differential equations, as models, are used to describe the corresponding phenomena. The space fractional advection diffusion equation (SFADE) is especially important in describing and understanding the dispersion phenomena involving two physical processes: advection and superdiffusion, where a particle plume spreads at a rate inconsistent with the classical Brownian motion model. In form, SFADE is derived by replacing the second-order derivative by a fractional derivative in the classical advection diffusion equation. By far, there have already been some important progresses for solving the fractional PDEs. The analytical methods having been proposed include the Fourier transform method, the Green function method [8], and the methods presented in [5]. However, in most cases, obtaining the exact solutions is very difficult because of the non-local property of the fractional derivative. Thus reliable and efficient numerical techniques have been developed, such as finite difference methods [9,13], finite element methods [6,14], finite volume methods [7] and spectral methods [1], etc.

Because of the extensive use of the three-dimensional models in research, this paper focuses on the three-dimensional SFADE in finite domain with zero Dirichlet boundary conditions. The fractional derivative is non-local operator, which causes the stiffness matrix of the discrete linear system is a Toeplitz type, and makes fractional partial differential equations more difficult to solve, especially in high-dimensional cases. To our knowledge, the numerical methods for solving the three-dimensional



problems are relatively sparse. Deng et al. extended the alternating direction implicit (ADI) schemes to the three-dimensional fractional PDEs, and improved their efficiency [4]. Chen et al. proposed a fractional ADI scheme for the three-dimensional fractional sub-diffusion equation [3]. Wang et al. developed a fast iterative ADI finite difference method for solving three-dimensional space fractional diffusion equations [11]. Here, we extend the predictor-corrector algorithm [12] to solve the fractional problem, i.e., the three-dimensional SFADE. The method adopted in this paper is of good stability properties, reasonable computational cost and ease of implementation for the three-dimensional problems. The idea behind the algorithm is to use a suitable combination of an explicit and implicit technique to obtain a method with better convergence characteristics, and solve the high-dimensional problems by the process of dimension by dimension. Abundant numerical examples are provided to verify the theoretical results afterwards.

The remainder of this paper is organized as follows. In section 2, we outline the three-dimensional SFADE and its fully discrete scheme by finite difference approximation. The numerical experiments are carried out in section 3 to verify the theoretical analysis, and the conclusions are summarized in the last section.

2 The predictor-corrector scheme for the three-dimensional SFADE

In this paper, we consider the following problem named as SFADE of order $1 < \alpha, \beta, \gamma < 2$

$$\begin{aligned} \frac{\partial u(x, y, z, t)}{\partial t} = & a_1 {}_{x_L} D_x^\alpha u(x, y, z, t) + a_2 {}_{x_R} D_x^\alpha u(x, y, z, t) \\ & + b_1 {}_{y_L} D_y^\beta u(x, y, z, t) + b_2 {}_{y_R} D_y^\beta u(x, y, z, t) \\ & + c_1 {}_{z_L} D_z^\gamma u(x, y, z, t) + c_2 {}_{z_R} D_z^\gamma u(x, y, z, t) \\ & + k_1 \frac{\partial u(x, y, z, t)}{\partial x} + k_2 \frac{\partial u(x, y, z, t)}{\partial y} + k_3 \frac{\partial u(x, y, z, t)}{\partial z} + f(x, y, z, t), \end{aligned} \quad (1)$$

with boundary and initial conditions

$$u(x, y, z, t) = 0, \quad (x, y, z, t) \in \partial\Omega \times (0, T], \quad (2)$$

$$u(x, y, z, 0) = u_0(x, y, z), \quad (x, y, z) \in \Omega, \quad (3)$$

where $\Omega = (x_L, x_R) \times (y_L, y_R) \times (z_L, z_R) \subset \mathbb{R}^3$.

a_1, b_1, c_1 and a_2, b_2, c_2 are the left and right diffusivity coefficients in the x, y , and z directions, which are non-negative constants. k_1, k_2 , and k_3 are advection coefficients in these three directions respectively, and $f(x, y, z, t)$ is a forcing function. The advection term in the SFADE is first-order classical derivative, and the fractional derivatives are Riemann-Liouville type defined as

$${}_{x_L} D_x^\alpha u(x) = \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_{x_L}^x (x-\xi)^{1-\alpha} u(\xi) d\xi, \quad (4)$$

and

$${}_x D_{x_R}^\alpha u(x) = \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_x^{x_R} (\xi-x)^{1-\alpha} u(\xi) d\xi. \quad (5)$$

Equations (4) and (5) are called the left and right Riemann-Liouville fractional derivatives in x direction. The left and right Riemann-Liouville fractional derivatives in y and z directions can be defined in similar way. When $a_1 = a_2$, $b_1 = b_2$, $c_1 = c_2$, and $k_1 = k_2 = k_3 = 0$, the Riesz fractional diffusion equation is obtained as a special case of (1).

2.1 Discretizations of Riemann-Liouville fractional derivatives

Let N_1, N_2, N_3 and M be positive integers, $h_1 = (x_R - x_L)/N_1$, $h_2 = (y_R - y_L)/N_2$, $h_3 = (z_R - z_L)/N_3$ and $\tau = T/M$ be the uniform step sizes of space and time respectively, by which we define a spatial and temporal partition $x_i = x_L + ih_1$ for $i = 0, 1, \dots, N_1$, $y_j = y_L + jh_2$ for $j = 0, 1, \dots, N_2$, $z_m = z_L + mh_3$

for $m=0,1,\dots,N_3$, and $t_n = n\tau$ for $n=0,1,\dots,M$. $u_{i,j,m}^n$ denotes the approximated value of $u(x_i, y_j, z_m, t_n)$, and $f_{i,j,m}^n = f(x_i, y_j, z_m, t_n)$. We use the second-order approximation operators given in [2,10] to discretize the left and right Riemann-Liouville fractional derivatives (4) and (5), i.e.,

$$\begin{aligned} {}_{x_L}D_x^\alpha u(x, y_j, z_m, t_n) \Big|_{x=x_i} &= \delta_{\alpha,x}^+ u(x_i, y_j, z_m, t_n) + O(h_1^2), \\ {}_xD_{x_R}^\alpha u(x, y_j, z_m, t_n) \Big|_{x=x_i} &= \delta_{\alpha,x}^- u(x_i, y_j, z_m, t_n) + O(h_1^2), \end{aligned}$$

where

$$\begin{aligned} \delta_{\alpha,x}^+ u(x_i, y_j, z_m, t_n) &:= \frac{1}{\Gamma(4-\alpha)h_1^\alpha} \sum_{l=0}^{i+1} g_l^\alpha u(x_{i-l+1}, y_j, z_m, t_n), \\ \delta_{\alpha,x}^- u(x_i, y_j, z_m, t_n) &:= \frac{1}{\Gamma(4-\alpha)h_1^\alpha} \sum_{l=0}^{N_1-i+1} g_l^\alpha u(x_{i+l-1}, y_j, z_m, t_n), \end{aligned}$$

and

$$g_l^\alpha = \begin{cases} 1, & l=0 \\ -4+2^{3-\alpha}, & l=1, \\ 6-2^{5-\alpha}+3^{3-\alpha}, & l=2, \\ (l+1)^{3-\alpha}-4l^{3-\alpha}+6(l-1)^{3-\alpha}-4(l-2)^{3-\alpha}+(l-3)^{3-\alpha}, & l \geq 3. \end{cases}$$

Moreover, we use the centered difference formula to approximate the classical first-order space derivative in advection term. Denote both classical and fractional approximation operators related to variable x as follows

$$D_x u_{i,j,m}^n = \frac{u_{i+1,j,m}^n - u_{i-1,j,m}^n}{2h_1}, \quad (6)$$

$$\delta_{\alpha,x}^+ u_{i,j,m}^n = \frac{1}{\Gamma(4-\alpha)h_1^\alpha} \sum_{l=0}^{i+1} g_l^\alpha u_{i-l+1,j,m}^n, \quad (7)$$

$$\delta_{\alpha,x}^- u_{i,j,m}^n = \frac{1}{\Gamma(4-\alpha)h_1^\alpha} \sum_{l=0}^{N_1-i+1} g_l^\alpha u_{i+l-1,j,m}^n. \quad (8)$$

Notations

$$D_x u_{i,j,m}^n = k_1 D_x u_{i,j,m}^n,$$

$$\delta_{\alpha,x}^+ u_{i,j,m}^n = a_1 \delta_{\alpha,x}^+ u_{i,j,m}^n,$$

$$\delta_{\alpha,x}^- u_{i,j,m}^n = a_2 \delta_{\alpha,x}^- u_{i,j,m}^n,$$

are introduced for simplicity.

Analogously, the discrete operators and notations corresponding to variables y and z can be described.

2.2 Numerical scheme for the three-dimensional SFADE

We use the strategies (6)-(8) to discrete the space derivatives in the three directions, and the Crank-Nicolson scheme is used in time direction. Then equation (1) can be written in the following form

$$\begin{aligned} &\left(1 - \frac{\tau}{2} \delta_{\alpha,x} - \frac{\tau}{2} \delta_{\beta,y} - \frac{\tau}{2} \delta_{\gamma,z}\right) u(x_i, y_j, z_m, t_{n+1}) \\ &= \left(1 + \frac{\tau}{2} \delta_{\alpha,x} + \frac{\tau}{2} \delta_{\beta,y} + \frac{\tau}{2} \delta_{\gamma,z}\right) u(x_i, y_j, z_m, t_n) + \tau f(x_i, y_j, z_m, t_{n+1/2}) + R_{i,j,m}^{n+1}, \end{aligned}$$

where

$$\delta_{\alpha,x} := \delta_{\alpha,x}^+ + \delta_{\alpha,x}^- + D_x,$$

$$\delta_{\beta,y} := \delta_{\beta,y}^+ + \delta_{\beta,y}^- + D_y,$$

$$\delta_{\gamma,z} := \delta_{\gamma,z}^+ + \delta_{\gamma,z}^- + D_z,$$

$$t_{n+1/2} = (t_n + t_{n+1})/2,$$

and the local truncation error

$$|R_{i,j,m}^{n+1}| \leq C\tau(\tau^2 + h_1^2 + h_2^2 + h_3^2),$$

with C being some positive constant.

Subsequently, taking $f_{i,j,m}^{n+1/2} = f(x_i, y_j, z_m, t_{n+1/2})$, we derive the full discretization scheme of (1) as

$$\begin{aligned} & \left(1 - \frac{\tau}{2}\delta_{\alpha,x} - \frac{\tau}{2}\delta_{\beta,y} - \frac{\tau}{2}\delta_{\gamma,z}\right) u_{i,j,m}^{n+1} \\ &= \left(1 + \frac{\tau}{2}\delta_{\alpha,x} + \frac{\tau}{2}\delta_{\beta,y} + \frac{\tau}{2}\delta_{\gamma,z}\right) u_{i,j,m}^n + \tau f_{i,j,m}^{n+1/2}. \end{aligned} \quad (9)$$

We add

$$\begin{aligned} & \left(\frac{\tau^2}{4}\delta_{\alpha,x}\delta_{\beta,y} + \frac{\tau^2}{4}\delta_{\alpha,x}\delta_{\gamma,z} + \frac{\tau^2}{4}\delta_{\beta,y}\delta_{\gamma,z}\right)(u_{i,j,m}^{n+1} - u_{i,j,m}^n) \\ & - \frac{\tau^3}{8}\delta_{\alpha,x}\delta_{\beta,y}\delta_{\gamma,z}(u_{i,j,m}^{n+1} + u_{i,j,m}^n) \end{aligned}$$

to the left hand side of equation (9) and distribute the appropriate half of the above term to the right hand side, then we are left with

$$\begin{aligned} & \left(1 - \frac{\tau}{2}\delta_{\alpha,x}\right)\left(1 - \frac{\tau}{2}\delta_{\beta,y}\right)\left(1 - \frac{\tau}{2}\delta_{\gamma,z}\right) u_{i,j,m}^{n+1} \\ &= \left(1 + \frac{\tau}{2}\delta_{\alpha,x}\right)\left(1 + \frac{\tau}{2}\delta_{\beta,y}\right)\left(1 + \frac{\tau}{2}\delta_{\gamma,z}\right) u_{i,j,m}^n + \tau f_{i,j,m}^{n+1/2}. \end{aligned} \quad (10)$$

We adopt the predictor-corrector scheme [12] to solve the system of equations (10). It can be proved rigorously that the numerical scheme is unconditionally stable and second-order convergent in both time and space directions by the matrix method, though we omit them here.

$$\left(1 - \frac{\tau}{2}\delta_{\alpha,x}\right) u_{i,j,m}^{n+1/6} = u_{i,j,m}^n + \frac{\tau}{2} f_{i,j,m}^{n+1/2}; \quad (11)$$

$$\left(1 - \frac{\tau}{2}\delta_{\beta,y}\right) u_{i,j,m}^{n+2/6} = u_{i,j,m}^{n+1/6}; \quad (12)$$

$$\left(1 - \frac{\tau}{2}\delta_{\gamma,z}\right) u_{i,j,m}^{n+3/6} = u_{i,j,m}^{n+2/6}; \quad (13)$$

$$u_{i,j,m}^{n+1} = u_{i,j,m}^n + \tau(\delta_{\alpha,x} u_{i,j,m}^{n+3/6} + \delta_{\beta,y} u_{i,j,m}^{n+3/6} + \delta_{\gamma,z} u_{i,j,m}^{n+3/6}) + \tau f_{i,j,m}^{n+1/2}. \quad (14)$$

Equations (11)-(13) represent the predictor, which determine $u_{i,j,m}^t$ at $t = (n+1/2)\tau$ by splitting scheme. Equation (14) is the corrector.

3 Numerical examples

In this section, some numerical experiments are carried out to verify the convergent orders and stability of our method. Let U_h and U denote the numerical solution and exact solution respectively, and in the numerical experiments we compute the global truncation error of $U_h - U$ in the following discrete L^∞ and L^2 norms

$$\begin{aligned} \|U_h - U\|_{L^\infty} &:= \max_{1 \leq m \leq N_3-1, 1 \leq j \leq N_2-1, 1 \leq i \leq N_1-1} |u_{i,j,m}^M - u(x_i, y_j, z_m, T)| \\ \|U_h - U\|_{L^2} &:= \left(\sum_{m=1}^{N_3-1} \sum_{j=1}^{N_2-1} \sum_{i=1}^{N_1-1} |u_{i,j,m}^M - u(x_i, y_j, z_m, T)|^2 h_1 h_2 h_3 \right)^{1/2}. \end{aligned}$$

Example 3.1. Consider equation (1) on $\Omega \times T = (0,1)^3 \times [0,1]$ with zero Dirichlet boundary conditions on the cube for all $t > 0$

$$\begin{aligned} & \frac{\partial u(x, y, z, t)}{\partial t} + \frac{\partial u(x, y, z, t)}{\partial x} + \frac{\partial u(x, y, z, t)}{\partial y} + \frac{\partial u(x, y, z, t)}{\partial z} \\ &= \left({}_0D_x^\alpha + {}_xD_1^\alpha \right) u(x, y, z, t) + \left({}_0D_y^\beta + {}_yD_1^\beta \right) u(x, y, z, t) \\ &+ \left({}_0D_z^\gamma + {}_zD_1^\gamma \right) u(x, y, z, t) + f(x, y, z, t). \end{aligned}$$

The exact solution is

$$u(x, y, z, t) = e^{-t} x^3 (1-x)^3 y^3 (1-y)^3 z^3 (1-z)^3$$

with the initial data $u_0(x, y, z) = u(x, y, z, 0)$. The forcing function $f(x, y, z, t)$ can be easily obtained.

Table 1: The L^∞ and L^2 errors and convergent orders for example 3.1 at $t=1$ with $\tau = h_1 = h_2 = h_3$.

	τ	$\ U_h - U\ _{L^\infty}$	Rate	$\ U_h - U\ _{L^2}$	Rate
$\alpha=1.2 \quad \beta=1.2$ $\gamma=1.2$	1/10	3.2536e-007	-	5.4273e-008	-
	1/20	7.9892e-008	2.0259	1.3476e-008	2.0098
	1/40	2.0205e-008	1.9833	3.3392e-009	2.0128
	1/80	5.0166e-009	2.0099	8.3033e-010	2.0077
	1/160	1.2497e-009	2.0051	2.0700e-010	2.0041
$\alpha=1.4 \quad \beta=1.5$ $\gamma=1.6$	1/10	2.4730e-006	-	4.3714e-007	-
	1/20	5.9312e-007	2.0599	1.0108e-007	2.1126
	1/40	1.4392e-007	2.0431	2.4131e-008	2.0665
	1/80	3.5184e-008	2.0323	5.8858e-009	2.0356
	1/160	8.6882e-009	2.0178	1.4529e-009	2.0183
$\alpha=1.9$ $\beta=1.9 \quad \gamma=1.9$	1/10	3.0171e-005	-	5.5585e-006	-
	1/20	5.6971e-006	2.4049	1.0826e-006	2.3602
	1/40	1.2066e-006	2.2393	2.1857e-007	2.3083
	1/80	2.8059e-007	2.1044	4.9724e-008	2.1316
	1/160	6.7409e-008	2.0575	1.1871e-008	2.0665

Example 3.2. Consider equation (1) on $\Omega \times T = (0,1)^3 \times [0,1]$ with zero Dirichlet boundary conditions on the cube for all $t > 0$. The convection and diffusion coefficients are given as

$$\begin{aligned} k_1 &= 0.25x, & k_2 &= 0.25y, & k_3 &= 0.25z, \\ a_1 &= x^\alpha, & a_2 &= (1-x)^\alpha, & b_1 &= y^\beta, \\ b_2 &= (1-y)^\beta, & c_1 &= z^\gamma, & c_2 &= (1-z)^\gamma. \end{aligned} \quad (15)$$

The exact solution is

$$u(x, y, z, t) = e^{-t} x^3 (1-x)^3 y^3 (1-y)^3 z^3 (1-z)^3$$

with the initial data $u_0(x, y, z) = u(x, y, z, 0)$. The forcing function $f(x, y, z, t)$ can be easily obtained.

Table 2: The L^∞ and L^2 errors and convergent orders for example 3.2 at $t=1$ with coefficients given in (15) and $\tau = h_1 = h_2 = h_3$.

	τ	$\ U_h - U\ _{L^\infty}$	Rate	$\ U_h - U\ _{L^2}$	Rate
$\alpha=1.2 \quad \beta=1.2$ $\gamma=1.2$	1/10	1.3401e-007	-	3.6232e-008	-
	1/20	3.2549e-008	2.0417	8.6020e-009	2.0745
	1/40	8.1374e-009	2.0000	2.1119e-009	2.0261
	1/80	2.0315e-009	2.0020	5.2465e-010	2.0091
	1/160	5.0803e-010	1.9996	1.3085e-010	2.0034

$\alpha=1.4 \quad \beta=1.5$ $\gamma=1.6$	1/10	3.5712e-007	-	9.1509e-008	-
	1/20	8.8817e-008	2.0075	2.3259e-008	1.9761
	1/40	2.2122e-008	2.0054	5.7916e-009	2.0058
	1/80	5.5125e-009	2.0047	1.4417e-009	2.0062
	1/160	1.3760e-009	2.0022	3.5954e-010	2.0035
$\alpha=1.9$ $\beta=1.9 \quad \gamma=1.9$	1/10	1.4596e-006	-	3.8000e-007	-
	1/20	3.4108e-007	2.0974	8.8657e-008	2.0997
	1/40	8.2214e-008	2.0527	2.1091e-008	2.0716
	1/80	2.0175e-008	2.0268	5.1381e-009	2.0373
	1/160	5.0072e-009	2.0105	1.2680e-009	2.0187

4 Conclusion

In this paper, an efficient numerical scheme for solving the three-dimensional SFADE is provided. The idea behind the predictor-corrector algorithm is to combine an explicit technique with an implicit one properly to obtain a method with better convergence characteristics, and dispose the high-dimensional problem by the process of dimension by dimension. Enough numerical experiments are carried out to verify the effectiveness of the algorithm, illustrating that the method is unconditionally stable, and is second-order convergent in both time and space directions, in discrete L^∞ and L^2 norms, respectively. Actually, the algorithm in this work is still efficient for other high dimensional space fractional PDEs.

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