Research Article

A Fast Implicit Finite Difference Method for Fractional Advection-Dispersion Equations with Fractional Derivative Boundary Conditions

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Received 4 June 2017; Revised 16 August 2017; Accepted 22 August 2017; Published 24 September 2017

Academic Editor: Mariano Torrisi

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Fractional advection-dispersion equations, as generalizations of classical integer-order advection-dispersion equations, are used to model the transport of passive tracers carried by fluid flow in a porous medium. In this paper, we develop an implicit finite difference method for fractional advection-dispersion equations with fractional derivative boundary conditions. First-order consistency, solvability, unconditional stability, and first-order convergence of the method are proven. Then, we present a fast iterative method for the implicit finite difference scheme, which only requires storage of $O(K)$ and computational cost of $O(K \log K)$. Traditionally, the Gaussian elimination method requires storage of $O(K^2)$ and computational cost of $O(K^3)$. Finally, the accuracy and efficiency of the method are checked with a numerical example.

1. Introduction

Fractional derivatives are almost as old as their more familiar integer-order counterparts [1, 2]. Fractional advection-dispersion equations are used to model many problems in physics, biology, and finance [3–5]. Fractional differential equations have attracted fantastic attention of many authors in recent years [6–11].

The fractional space derivatives are used to establish anomalous diffusion and dispersion models, where the propagation velocity of the particle beam is different from the classical Brown motion model. When the space second derivative in a diffusion or dispersion model is replaced with a fractional space derivative, it leads to superdiffusion. In this paper, we consider a one-dimensional fractional advection-dispersion equation with fractional derivative boundary conditions:

$$\frac{\partial p(r, t)}{\partial t} = -v(r) \frac{\partial p(r, t)}{\partial r} + d(r) \frac{\partial^\alpha p(r, t)}{\partial r^\alpha} + f(r, t), \quad (1)$$

$$0 < r < R, \quad 0 < t,$$

$$p(0, t) = 0,$$

$$\beta p(R, t) + \left(d(r) \frac{\partial^{\alpha-1} p(r, t)}{\partial r^{\alpha-1}} \right) \Big|_{r=R} = w(t), \quad (2)$$

$$0 < t,$$

$$p(r, 0) = u(r), \quad 0 \leq r \leq R, \quad (3)$$

where $1 < \alpha \leq 2$; $p(r, t)$ is the distribution function of the diffusion quantity; $v(r)$ is flow velocity; $d(r)$ is diffusion coefficient; $f(r, t)$ is the source term. We assume $v(r) \geq 0$ and $d(r) \geq 0$, so that the flow is from left to right. The space fractional partial derivatives in (1) and (2) are left-sided Riemann-Liouville fractional derivatives over the x domain. For a function $g(x)$ over the interval $L < x < R$, the left-sided Riemann-Liouville fractional derivative of order μ is defined by

$$\frac{d^\mu g(x)}{dx^\mu} = \frac{1}{\Gamma(n-\mu)} \frac{d^n}{dx^n} \int_L^x \frac{g(\xi)}{(x-\xi)^{\mu+1-n}} d\xi, \quad (4)$$

where n is an integer, such that $n - 1 < \mu \leq n$. See [12] for details. If μ is an integer, then (4) gives the standard integer derivative. $\beta = 0$ corresponds to a fractional Neumann boundary condition and $\beta > 0$ corresponds to a fractional Robin boundary condition. In this paper, we only discuss $\beta > 0$.

For a one-dimensional advection-dispersion equation with constant coefficients, Benson et al. [13] got available analytical solutions using Fourier transform method. However, many problems require a model with variable coefficients. Meerschaert and Tadjeran [14] developed finite difference approximations for one-dimensional fractional advection-dispersion equations with Dirichlet boundary conditions. And, recently, some authors have discussed numerical method for fractional equations with fractional derivative boundary conditions. Jia and Wang [15] developed fast implicit finite difference methods for two-sided space fractional diffusion equations with fractional derivative boundary conditions. Guo et al. [16] developed implicit finite difference method for fractional percolation equation with Dirichlet and fractional boundary conditions. As far as we know, the study on numerical method for one-dimensional advection-dispersion equations with fractional derivative boundary conditions is still limited. This motivates us to examine a fast implicit finite difference method for fractional advection-dispersion equations with fractional derivative boundary conditions in this paper.

The rest of the paper is organized as follows. In Section 2, we develop an implicit finite difference method and analyze its consistency. In Section 3, the solvability, unconditional stability, and convergence of the method are proven. In Section 4, we present a fast iterative method for the implicit finite difference scheme, which only requires storage of $O(K)$ and computational cost of $O(K \log K)$. In Section 5, a numerical experiment is presented to verify the accuracy and efficiency of the proposed scheme.

2. The Implicit Finite Difference Method for the Advection-Dispersion Equations with Fractional Derivative Boundary Conditions and Its Consistency

First, let $h = R/K$ and Δt be the spatial mesh width and the time step, where K is a positive integer. We define a spatial partition by $r_i = ih$ for $i = 0, 1, \dots, K$ and a temporal partition by $t_n = n\Delta t$ for $n = 0, 1, \dots, N$. Let $v_i = v(r_i)$, $d_i = d(r_i)$, $f_i^n = f(r_i, t_n)$, $w^n = w(t_n)$, $u_i = u(r_i)$. Denote the exact and numerical solutions at the mesh point (r_i, t_n) by $P_i^n = p(r_i, t_n)$ and p_i^n , respectively. $P_i^0 = u_0(r_i)$ and $p_0^n = 0$.

Then, we employ the backward Euler scheme to approximate the first-order time derivative; a right-shifted Grünwald formula to approximate left-sided α -order Riemann-Liouville fractional derivative and standard Grünwald formula to approximate $\alpha - 1$ -order Riemann-Liouville fractional derivative are defined as follows [12]:

$$\begin{aligned} \frac{\partial p}{\partial t} \Big|_{(r_i, t_{n+1})} &= \frac{P_i^{n+1} - P_i^n}{\Delta t} + O(\Delta t), \\ \frac{\partial p}{\partial r} \Big|_{(r_i, t_{n+1})} &= \frac{P_i^{n+1} - P_{i-1}^{n+1}}{h} + O(h), \end{aligned}$$

$$\frac{\partial^\alpha p}{\partial r^\alpha} \Big|_{(r_i, t_{n+1})} = \frac{1}{h^\alpha} \sum_{j=0}^{i+1} g_{\alpha,j} P_{i-j+1}^{n+1} + O(h),$$

$$\frac{\partial^{\alpha-1} p}{\partial r^{\alpha-1}} \Big|_{(R, t_{n+1})} = \frac{1}{h^{\alpha-1}} \sum_{j=0}^K g_{\alpha-1,j} P_{K-j}^{n+1} + O(h), \quad (5)$$

where $g_{\delta,l}$, ($\delta = \alpha - 1; \alpha$) is normalized Grünwald weights:

$$g_{\delta,l} = \frac{\Gamma(l - \delta)}{\Gamma(-\delta) \Gamma(l + 1)}. \quad (6)$$

Moreover, the normalized Grünwald weights satisfy the properties in the following Lemma 1.

Lemma 1. Let μ be a positive real number and the integer $n \geq 1$. We have

- (i) $g_{\mu,0} = 1$, $g_{\mu,j} = (1 - (\mu + 1)/j)g_{\mu,j-1}$ for $j \geq 1$;
- (ii) $g_{\mu,1} < g_{\mu,2} < \dots < 0$, $\sum_{j=0}^n g_{\mu,j} > 0$ for $0 < \mu < 1$;
- (iii) $g_{\mu,2} > g_{\mu,3} > \dots > 0$, $\sum_{j=0}^n g_{\mu,j} < 0$ for $1 < \mu < 2$.

Therefore implicit finite difference method for the advection-dispersion equations with fractional derivative boundary conditions (1)–(3) can be written as follows:

$$\begin{aligned} \frac{p_i^{n+1} - p_i^n}{\Delta t} &= \left(-v_i \frac{p_i^{n+1} - p_{i-1}^{n+1}}{h} + \frac{d_i}{h^\alpha} \sum_{j=0}^{i+1} g_{\alpha,k} p_{i-j+1}^{n+1} \right) + f_i^n, \\ &\text{for } i = 1, 2, \dots, K-1, \end{aligned} \quad (7)$$

$$p_0^n = 0,$$

$$\beta p_K^{n+1} + \left(\frac{d_K}{h^{\alpha-1}} \sum_{j=0}^K g_{\alpha-1,j} p_{K-j}^{n+1} \right) = w^{n+1},$$

$$p_i^0 = u_i.$$

Denote the local truncation error by R_i^{n+1} for $1 \leq i \leq K$. Then, from (7), we have

$$\begin{aligned} R_i^{n+1} &= \frac{P_i^{n+1} - P_i^n}{\Delta t} \\ &\quad - \left(-v_i \frac{P_i^{n+1} - P_{i-1}^{n+1}}{h} + \frac{d_i}{h^\alpha} \sum_{k=0}^{i+1} g_{\alpha,k} P_{i-k+1}^{n+1} \right) - f_i^n \\ &= O(\Delta t) + O(h), \quad 1 \leq i \leq K-1, \end{aligned} \quad (8)$$

$$\begin{aligned} R_N^{n+1} &= \beta P_K^{n+1} - \left(\frac{d_K}{h^{\alpha-1}} \sum_{j=0}^K g_{\alpha-1,j} P_{K-j}^{n+1} \right) - w^{n+1} \\ &= O(h). \end{aligned}$$

From (8), this implicit finite difference scheme is consistent. Equations (7) may be rearranged as follows:

$$\begin{aligned}
 & -g_{\alpha,0}B_i p_{i+1}^{n+1} + (1 + E_i - g_{\alpha,1}B_i) p_i^{n+1} \\
 & - (E_i + g_{\alpha,2}B_i) p_{i-1}^{n+1} - B_i \sum_{k=3}^{i+1} g_{\alpha,k} p_{i-k+1}^{n+1} = p_i^n \\
 & + \Delta t f_i^{n+1}, \\
 & (\beta h^{\alpha-1} + d_K g_{\alpha-1,0}) p_K^{n+1} \\
 & + \left(d_K \sum_{j=1}^{K-1} g_{\alpha-1,j} p_{K-j}^{n+1} \right) = h^{\alpha-1} w^{n+1},
 \end{aligned} \tag{9}$$

where $B_i = d_i \Delta t / h^\alpha$, $E_i = v_i \Delta t / h$. Equations (9) can be written in matrix form:

$$\mathbf{A} \mathbf{p}^{n+1} = \mathbf{q}^n + \mathbf{f}^{n+1}, \tag{10}$$

where

$$\begin{aligned}
 \mathbf{p}^{n+1} &= (p_1^{n+1}, p_2^{n+1}, \dots, p_K^{n+1})^T, \\
 \mathbf{q}^n &= (p_1^n, p_2^n, \dots, p_{K-1}^n, 0)^T, \\
 \mathbf{f}^{n+1} &= (\Delta t f_1^{n+1}, \Delta t f_2^{n+1}, \dots, \Delta t f_{K-1}^{n+1}, h^{\alpha-1} w^{n+1})^T,
 \end{aligned} \tag{11}$$

where the coefficient matrix $\mathbf{A} = [a_{i,j}]_{K \times K}$ and its entries are

$$\begin{aligned}
 & a_{i,j} \\
 & \begin{cases} -g_{\alpha,i+1-j}B_i, & \text{for } 1 \leq j \leq i-2, 1 \leq i \leq K-1; \\ -E_i - g_{\alpha,2}B_i, & \text{for } 1 \leq j = i-1 \leq K-1; \\ 1 + E_i - g_{\alpha,1}B_i, & \text{for } j = i, 1 \leq i \leq K-1; \\ -g_{\alpha,0}B_i, & \text{for } j = i+1, 1 \leq i \leq K-1; \\ 0, & \text{for } j = i+2, 1 \leq i \leq K-1; \\ g_{\alpha-1,K-j}d_K, & \text{for } 1 \leq j \leq K-1, i = K; \\ \beta h^{\alpha-1} + d_K g_{\alpha-1,0}, & \text{for } i = j = K. \end{cases}
 \end{aligned} \tag{12}$$

3. Solvability, Stability, and Convergence Analysis

Having developed a numerical scheme and shown that it is consistent, in the following theorems, we show this method is solvable, unconditionally stable, and convergent.

Theorem 2 (solvability). *If $\beta > 0$, (10) is uniquely solvable.*

Proof. Let r_i be the sum of absolute values of elements along the i th row excluding the diagonal elements $A_{i,i}$. According to Lemma 1, we can get

$$\begin{aligned}
 r_i &= \sum_{j=1, j \neq i}^K |A_{i,j}| \\
 &= \sum_{j=1}^{i-2} |-B_i g_{\alpha,i+1-j}^{(\alpha)}| + |E_i + B_i g_2^{(\alpha)}| + |B_i g_0^{(\alpha)}| \\
 &= \left(\sum_{j=0}^i g_j^{(\alpha)} - g_1^{(\alpha)} \right) B_i + E_i < -g_1^{(\alpha)} B_i < A_{i,i} \\
 &\quad (1 \leq i \leq K-1),
 \end{aligned} \tag{13}$$

$$\begin{aligned}
 r_K &= \sum_{j=1}^{K-1} |A_{K,j}| = \sum_{j=1}^{K-1} |d_K g_{K-j}^{(\alpha-1)}| = -\sum_{j=1}^{K-1} d_K g_j^{(\alpha-1)} \\
 &= -d_K \left(\sum_{j=0}^{K-1} g_j^{(\alpha-1)} - g_0^{(\alpha-1)} \right) < d_K g_0^{(\alpha-1)} < A_{K,K}.
 \end{aligned}$$

Matrix A is strictly diagonal, which guarantees the invertibility of matrix A . Hence, (10) is uniquely solvable. $\square$

To discuss the stability of the numerical method, we denote by $\tilde{p}_i^n$ ($1 \leq i \leq K$) the approximate solution of the difference scheme with the initial condition $\tilde{p}_i^0$ ($1 \leq i \leq K$) and define $\epsilon_i^n = p_i^n - \tilde{p}_i^n$, $\epsilon^n = (\epsilon_1^n, \epsilon_2^n, \dots, \epsilon_K^n)^T$, $\|\epsilon^n\|_\infty = \max_{1 \leq i \leq K} |\epsilon_i^n|$.

Theorem 3. *The implicit finite difference method for the advection-dispersion equations with fractional derivative boundary conditions defined by (7) is unconditionally stable.*

Proof. From (9) and the definition of ϵ_i^n , we have

$$\begin{aligned}
 & -g_{\alpha,0}B_i \epsilon_{i+1}^{n+1} + (1 + E_i - g_{\alpha,1}B_i) \epsilon_i^{n+1} \\
 & - (E_i + g_{\alpha,2}B_i) \epsilon_{i-1}^{n+1} - B_i \sum_{k=3}^{i+1} g_{\alpha,k} \epsilon_{i-k+1}^{n+1} = \epsilon_i^n,
 \end{aligned} \tag{14}$$

$$(\beta h^{\alpha-1} + d_K g_{\alpha-1,0}) \epsilon_K^{n+1} + \left(d_K \sum_{j=1}^{K-1} g_{\alpha-1,j} \epsilon_{K-j}^{n+1} \right) = 0. \tag{15}$$

By Lemma 1, we have

$$\sum_{j=1}^{K-1} |g_{\alpha-1,j}| = -\sum_{j=1}^{K-1} g_{\alpha-1,j} < g_{\alpha-1,0}. \tag{16}$$

It follows from (15) that

$$\begin{aligned}
 |\epsilon_K^{n+1}| &= \frac{|d_K \sum_{j=1}^{K-1} g_{\alpha-1,j} \epsilon_{K-j}^{n+1}|}{|\beta h^{\alpha-1} + g_{\alpha-1,0} d_K|} \\
 &\leq \frac{d_K \sum_{j=1}^{K-1} |g_{\alpha-1,j}| |\epsilon_{K-j}^{n+1}|}{h^{\alpha-1} \beta + g_{\alpha-1,0} d_K} < \max_{1 \leq i \leq K-1} |\epsilon_i^n|.
 \end{aligned} \tag{17}$$

Therefore, we suppose that $\|\varepsilon^n\|_\infty = |\varepsilon_{i_0}^n|$, where $1 \leq i_0 \leq N-1$. By Lemmas 1(i) and (iii), then

$$\begin{aligned}
\|\varepsilon^{n+1}\|_\infty &= |\varepsilon_{i_0}^{n+1}| < \left(1 + E_{i_0} - E_{i_0} - \sum_{k=0}^{i_0+1} g_{\alpha,k} B_{i_0}\right) |\varepsilon_{i_0}^{n+1}| \\
&= (1 + E_{i_0} - g_{\alpha,1} B_{i_0}) |\varepsilon_{i_0}^{n+1}| - (g_{\alpha,0} B_{i_0}) |\varepsilon_{i_0}^{n+1}| - (E_{i_0} \\
&\quad + g_{\alpha,2} B_{i_0}) |\varepsilon_{i_0}^{n+1}| - \left(\sum_{k=3}^{i_0+1} g_{\alpha,k} B_{i_0}\right) |\varepsilon_{i_0}^{n+1}| \leq (1 + E_{i_0} \\
&\quad - g_{\alpha,1} B_{i_0}) |\varepsilon_{i_0}^{n+1}| - (g_{\alpha,0} B_{i_0}) |\varepsilon_{i_0+1}^{n+1}| - (E_{i_0} + g_{\alpha,2} B_{i_0}) \\
&\quad \cdot |\varepsilon_{i_0-1}^{n+1}| - \left(\sum_{k=3}^{i_0+1} g_{\alpha,k} B_{i_0}\right) |\varepsilon_{i_0-k+1}^{n+1}| \\
&\leq \left| (1 + E_{i_0} - g_{\alpha,1} B_{i_0}) \varepsilon_{i_0}^{n+1} - (g_{\alpha,0} B_{i_0}) \varepsilon_{i_0+1}^{n+1} \right. \\
&\quad \left. - (E_{i_0} + g_{\alpha,2} B_{i_0}) \varepsilon_{i_0-1}^{n+1} - \left(\sum_{k=3}^{i_0+1} g_{\alpha,k} B_{i_0}\right) \varepsilon_{i_0-k+1}^{n+1} \right| \\
&= |\varepsilon_{i_0}^n| \leq \|\varepsilon^n\|_\infty,
\end{aligned} \tag{18}$$

which implies that $\|\varepsilon^n\|_\infty < \|\varepsilon^0\|_\infty$.

Thus, the implicit finite difference method defined by (7) is unconditionally stable. $\square$

For the convergence analysis, we define $e_i^n = P_i^n - p_i^n$ ($1 \leq i \leq K$) and $\mathbf{e}^n = (e_1^n, e_2^n, \dots, e_K^n)^T$, $\|\mathbf{e}^n\|_\infty = \max_{1 \leq i \leq K} |e_i^n|$.

Theorem 4. *There exists a positive constant C , independent of h and Δt , such that*

$$\|\mathbf{e}^{n+1}\|_\infty \leq C(\Delta t + h), \quad 1 \leq n \leq N. \tag{19}$$

Proof. From (9), we have

$$\begin{aligned}
&-g_{\alpha,0} B_i e_{i+1}^{n+1} + (1 + E_i - g_{\alpha,1} B_i) e_i^{n+1} \\
&- (E_i + g_{\alpha,2} B_i) e_{i-1}^{n+1} - B_i \sum_{k=3}^{i+1} g_{\alpha,k} e_{i-k+1}^{n+1} = e_i^n \\
&+ \Delta t R_i^{n+1}, \\
&(\beta h^{\alpha-1} + d_K g_{\alpha-1,0}) e_K^{n+1} \\
&+ \left(d_K \sum_{j=0}^{K-1} g_{\alpha-1,j} e_{K-j}^{n+1} \right) = h^{\alpha-1} R_K^{n+1},
\end{aligned} \tag{20}$$

with $e_0^{n+1} = 0$, and $e_i^0 = 0, i = 0, 1, \dots, K$. If $\|\mathbf{e}^{n+1}\|_\infty = |e_K^{n+1}| \geq \max_{1 \leq i \leq K-1} |e_i^{n+1}|$, we have

$$\begin{aligned}
&(\beta h^{\alpha-1} + d_K g_{\alpha-1,0}) e_K^{n+1} + \left(d_K \sum_{j=0}^{K-1} g_{\alpha-1,j} e_{K-j}^{n+1} \right) \\
&= h^{\alpha-1} R_K^{n+1}.
\end{aligned} \tag{21}$$

By Lemma 1(ii), then

$$\begin{aligned}
&\beta h^{\alpha-1} + d_K \sum_{j=0}^{K-1} g_{\alpha-1,j} |e_K^{n+1}| \\
&= (\beta h^{\alpha-1} + d_K g_{\alpha-1,0}) |e_K^{n+1}| - d_K \sum_{j=1}^{K-1} |g_{\alpha-1,j}| |e_K^{n+1}| \\
&\leq (\beta h^{\alpha-1} + d_K g_{\alpha-1,0}) |e_K^{n+1}| - d_K \sum_{j=1}^{K-1} |g_{\alpha-1,j}| |e_{K-j}^{n+1}| \\
&\leq (\beta h^{\alpha-1} + d_K g_{\alpha-1,0}) |e_K^{n+1}| - d_K \sum_{j=1}^{K-1} |g_{\alpha-1,j} e_{K-j}^{n+1}| \\
&\leq \left| (\beta h^{\alpha-1} + d_K g_{\alpha-1,0}) e_K^{n+1} + d_K \sum_{j=1}^{K-1} g_{\alpha-1,j} e_{K-j}^{n+1} \right| \\
&= h^{\alpha-1} |R_K^{n+1}|.
\end{aligned} \tag{22}$$

With Lemma 1 and the Stirling formula for the Gamma function [17], we have

$$\begin{aligned}
\left(\sum_{j=0}^{K-1} g_{\alpha-1,j} \right)^{-1} &= (-1)^{K-1} \binom{\alpha-2}{K-1}^{-1} \\
&= \frac{\Gamma(K)}{\Gamma(2-\alpha) \Gamma(K-\alpha+1)} \\
&= O(K^{\alpha-1}),
\end{aligned} \tag{23}$$

as $K \rightarrow \infty$. Combining (22) and (23), we get

$$|e_K^{n+1}| \leq \left(d_K \sum_{j=0}^{K-1} g_{\alpha-1,j} \right)^{-1} h^{\alpha-1} |R_K^{n+1}| \leq C_1 h. \tag{24}$$

If $\|\mathbf{e}^{n+1}\|_\infty = |e_{i_0}^{n+1}| > |e_K^{n+1}|, 1 \leq i_0 \leq K-1$, then

$$\begin{aligned}
\|\mathbf{e}^{n+1}\|_\infty &= |e_{i_0}^{n+1}| < \left(1 + E_{i_0} - E_{i_0} - \sum_{k=0}^{i_0+1} g_{\alpha,k} B_{i_0}\right) \\
&\cdot |e_{i_0}^{n+1}| = (1 + E_{i_0} - g_{\alpha,1} B_{i_0}) |e_{i_0}^{n+1}| - (g_{\alpha,0} B_{i_0}) \\
&\cdot |e_{i_0}^{n+1}| - (E_{i_0} + g_{\alpha,2} B_{i_0}) |e_{i_0}^{n+1}| - \left(\sum_{k=3}^{i_0+1} g_{\alpha,k} B_{i_0}\right) \\
&\cdot |e_{i_0}^{n+1}| \leq (1 + E_{i_0} - g_{\alpha,1} B_{i_0}) |e_{i_0}^{n+1}| - (g_{\alpha,0} B_{i_0}) \\
&\cdot |e_{i_0+1}^{n+1}| - (E_{i_0} + g_{\alpha,2} B_{i_0}) |e_{i_0-1}^{n+1}| - \left(\sum_{k=3}^{i_0+1} g_{\alpha,k} B_{i_0}\right) \\
&\cdot |e_{i_0-k+1}^{n+1}| \leq \left| (1 + E_{i_0} - g_{\alpha,1} B_{i_0}) e_{i_0}^{n+1} \right.
\end{aligned}$$

$$\begin{aligned}
& - (g_{\alpha,0} B_{i_0}) e_{i_0+1}^{n+1} - (E_{i_0} + g_{\alpha,2} B_{i_0}) e_{i_0-1}^{n+1} \\
& - \left(\sum_{k=3}^{i_0+1} g_{\alpha,k} B_{i_0} \right) e_{i_0-k+1}^{n+1} \Big| = |e_{i_0}^n + \Delta t R_{i_0}^{n+1}| \\
& \leq \max_{1 \leq i \leq K-1} |e_i^n| + \Delta t C_2 (\Delta t + h).
\end{aligned} \tag{25}$$

By induction, we can finally obtain

$$\|e^n\|_\infty \leq C_1 h + n \Delta t C_2 (\Delta t + h) \leq C (\Delta t + h). \tag{26}$$

This completes the proof. $\square$

4. Storage and Fast Krylov Subspace Method of the Coefficient Matrix

The following theorem shows that the storage of matrix A can be stored in $O(K)$ memories, instead of $O(K^2)$ memories.

Theorem 5. *Coefficient matrix A can be stored in $4K + 1$ memories.*

Proof. We express coefficient matrix A defined by (12) in block form as follows:

$$A = \begin{bmatrix} A_{K-1,K-1} & A_{K-1,K} \\ A_{K,K-1}^T & a_{K,K} \end{bmatrix}, \tag{27}$$

where $A_{K-1,K-1}$ is the $(K-1) \times (K-1)$ matrix that consists of the first $K-1$ rows and the first $K-1$ columns. $A_{K,K-1}^T$ is an $(K-1)$ -dimensional row vector that consists of the first $K-1$ entries in the K th row of matrix A , and $A_{K-1,K}$ is an $(K-1)$ -dimensional column vector that consists of the first $K-1$ entries in the K th column of matrix A . Matrix $A_{K-1,K-1}$ has the similar form as that in the finite difference method for (1)–(3) with the fractional derivative boundary conditions [15]. $A_{K-1,K-1}$ can be shown to have the following decomposition:

$$\begin{aligned}
A_{K-1,K-1} &= I - \text{diag}(\{B_i\}_{i=1}^{K-1}) \cdot A^{(\alpha)} \\
&\quad + \text{diag}(\{E_i\}_{i=1}^{K-1}) \cdot A^{(\beta)},
\end{aligned} \tag{28}$$

where I is the identity matrix of the order $K-1$. And $A^{(\alpha)}$ and $A^{(\beta)}$ are $(N-1)$ th-order Toeplitz matrix given as follows:

$$A^{(\alpha)} = \begin{bmatrix} g_{\alpha,1} & g_{\alpha,0} & 0 & \cdots & 0 & 0 \\ g_{\alpha,2} & g_{\alpha,1} & g_{\alpha,0} & \ddots & 0 & 0 \\ g_{\alpha,3} & g_{\alpha,2} & g_{\alpha,1} & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ g_{\alpha,K-2} & g_{\alpha,K-3} & g_{\alpha,K-4} & \ddots & g_{\alpha,1} & g_{\alpha,0} \\ g_{\alpha,K-1} & g_{\alpha,K-2} & g_{\alpha,K-3} & \cdots & g_{\alpha,2} & g_{\alpha,1} \end{bmatrix},$$

$$A^{(\beta)} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ -1 & 1 & 0 & \ddots & 0 & 0 \\ 0 & -1 & 1 & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \ddots & 1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{bmatrix}. \tag{29}$$

According to the definition of (12), we can write $A_{K-1,K}$ and $A_{K,K-1}^T$ as follows:

$$\begin{aligned}
A_{K-1,K} &= -B_{K-1} \cdot g_{\alpha,0} \cdot I_{K-1}, \\
A_{K,K-1}^T &= d_K \cdot g^{(\alpha)},
\end{aligned} \tag{30}$$

where $g^{(\alpha)} = (g_{\alpha,K-1}, g_{\alpha,K-2}, \dots, g_{\alpha,1})$, and I_{K-1} is the $(K-1)$ th column of I . $\square$

Thus, in order to store A , we need only to store $(B_1, B_2, \dots, B_{K-1})^T, (E_1, E_2, \dots, E_{K-1})^T, (g_{\alpha,0}, g_{\alpha,1}, \dots, g_{\alpha,K-1})^T, g^{(\beta)} = (1, -1, \dots, 0)^T, A_{K,K-1} = (a_{K,1}, a_{K,2}, \dots, a_{K,K-1})^T, I$, and $a_{K,K}$, which totally have $4K + 1$ parameters, instead of storing the super triangular matrix A in a straightforward but naive way that required K^2 memories.

Theorem 6. *For any vector $\mu_K \in R^K$ and T_K to be a Toeplitz matrix of order K , the matrix-vector multiplication $T_K \mu_K$ can be carried out in $O(K \log K)$ operations without any lossy compression.*

Proof. A Toeplitz matrix is a matrix in which each descending diagonal from left to right is constant. Let T_K be a Toeplitz matrix of order K of the following form:

$$T_K = \begin{bmatrix} t_0 & t_{-1} & t_{-2} & \cdots & t_{2-K} & t_{1-K} \\ t_1 & t_0 & t_{-1} & \ddots & t_{3-K} & t_{2-K} \\ t_2 & t_1 & t_0 & \ddots & \ddots & t_{3-K} \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ t_{K-2} & t_{K-3} & \ddots & \ddots & t_0 & t_{-1} \\ t_{K-1} & t_{K-2} & t_{K-3} & \cdots & t_1 & t_0 \end{bmatrix}. \tag{31}$$

The matrix-vector multiplication $T_K \mu_K$ can be carried out via the fast Fourier transform (FFT). First, we embed Toeplitz matrix T_K into a $2K \times 2K$ circulant matrix C_{2N} as follows [18, 19]:

$$C_{2K} = \begin{bmatrix} T_K & B_K \\ B_K & T_K \end{bmatrix},$$

TABLE 1: Error behavior for the implicit finite difference scheme (7), for example, at time $T = 1$ and $\beta = 1.0$.

$\Delta t = h$	$\alpha = 1.9$		$\alpha = 1.8$		$\alpha = 1.6$	
	$\ e_h^N\ _\infty$	Error – rate	$\ e_h^N\ _\infty$	Error – rate	$\ e_h^N\ _\infty$	Error – rate
2^{-4}	0.0299	—	0.0351	—	0.0565	—
2^{-5}	0.0155	1.9290	0.0185	1.8973	0.0308	1.8344
2^{-6}	0.0079	1.9620	0.0096	1.9271	0.0164	1.8781
2^{-7}	0.0040	1.9750	0.0049	1.9592	0.0087	1.8851
2^{-8}	0.0020	2.0000	0.0025	1.9600	0.0047	1.8510

$$B_K = \begin{bmatrix} 0 & t_{1-K} & \cdots & t_{-2} & t_{-1} \\ t_{K-1} & 0 & t_{1-K} & \ddots & t_{-2} \\ \vdots & t_{K-1} & 0 & \ddots & \cdots \\ t_2 & \ddots & \ddots & \ddots & t_{1-K} \\ t_1 & t_2 & \cdots & t_{K-1} & 0 \end{bmatrix}. \quad (32)$$

It is known that a circulant matrix C_{2K} can be decomposed as follows [19, 20]:

$$C_{2K} = F_{2K}^{-1} \text{diag}(F_{(2K)} c_{2K}) F_{2K}, \quad (33)$$

where c_{2K} is the first column vector of C_{2K} . F_{2K} is the $2K \times 2K$ discrete Fourier transform matrix in which (j, k) -entry $(F_{2K})_{j,k}$ of the matrix F_{2K} is given by

$$(F_{2K})_{j,k} = \frac{1}{2K} \exp\left(\frac{2\pi i j k}{2K}\right), \quad (34)$$

$$i = \sqrt{-1}, \quad 0 \leq j, k \leq 2K - 2.$$

For any vector $\mu_K \in R^K$, we extend the vector by 0 to a $2K$ -dimensional vector $\mu_{2K} = \begin{pmatrix} \mu_K \\ 0 \end{pmatrix}$. It is well known that the matrix-vector multiplication $F_{2K} \mu_{2K}$ can be carried out in $O(2K \log 2K) = O(K \log K)$ operations via the fast Fourier transform. Equation (33) shows that $F_{2K} \mu_{2K}$ can be evaluated in $O(K \log K)$ operations. We observe

$$C_{2K} \begin{pmatrix} \mu_K \\ 0 \end{pmatrix} = F_{2K}^{-1} \text{diag}(F_{2K} c_{2K}) F_{2K} \begin{pmatrix} \mu_K \\ 0 \end{pmatrix}. \quad (35)$$

At the same time,

$$C_{2K} \begin{pmatrix} \mu_K \\ 0 \end{pmatrix} = \begin{pmatrix} T_K & B_K \\ B_K & T_K \end{pmatrix} \begin{pmatrix} \mu_K \\ 0 \end{pmatrix} = \begin{pmatrix} T_K \mu_K \\ B_K \mu_K \end{pmatrix}. \quad (36)$$

Thus, the upper half of the vector multiplication $F_{2K} \mu_{2K}$ gives the matrix-vector multiplication $T_K \mu_K$. So we can evaluate $T_K \mu_K$ in $O(K \log K)$ operations. Then, by (28) we evaluate $A_{K-1, K-1} \mu_{K-1}$ in $O(K \log K)$ operations. Then, from (27), for any vector $\mu_K \in R^K$, the matrix-vector multiplication $T_K \mu_K$ is evaluated in $O(K \log K)$ operations without any lossy compression. $\square$

Remark 7. If the system matrix A from (10) is a dense and full coefficient matrix, the Gaussian elimination method

FIGURE 1: The behavior solution at $T = 1$ with $\Delta t = h = 2^{-6}$, $\alpha = 1.9$.

requires storage of $O(K^2)$ and computational cost of $O(K^3)$. In this paper, the system matrix A is supertriangular; the traditional Gaussian elimination method requires storage of $O(K^2)$ and computational cost of $O(K^2)$. We present a fast iterative method for the implicit finite difference scheme, which only requires storage of $O(K)$ and computational cost of $O(K \log K)$.

5. A Numerical Example

The following fractional differential equation was considered:

$$\frac{\partial p(r, t)}{\partial t} = -v(r) \frac{\partial p(r, t)}{\partial r} + d(r) \frac{\partial^\alpha p(r, t)}{\partial r^\alpha} + f(r, t) \quad (37)$$

On a finite domain $[0, 1]$. The flow velocity is $v(r) = \alpha/(4 - 2\alpha)$. Diffusion coefficient is $d(r) = \Gamma(2 - \alpha) \cdot r^{\alpha-1}$. The source term is $f(r, t) = 5e^{-t}(r^2 + (3\alpha - 4)/(4 - 2\alpha))$. The initial function is $u(r) = 5r(1 - r)$. And the boundary conditions are $w(t) = 5e^{-t}(1/(2 - \alpha) - 2/(3 - \alpha)(2 - \alpha))$.

Note that the exact solution to this problem is $p(r, t) = 5e^{-t}r(1 - r)$. In the numerical experiments, we consider three different α in the case, respectively. Table 1 shows $\|e_h^N\|_\infty$ the maximum error of the numerical solution of at the time $T = 1$ and $\beta = 1.0$. The stability and its order $O(\Delta t + h)$ of convergence are proved.

Figures 1–3 show the numerical solutions obtained by applying the Euler method (10) discussed above, with $\alpha = 1.9$,

FIGURE 2: The behavior solution at $T = 1$ with $\Delta t = h = 2^{-6}$, $\alpha = 1.8$.

FIGURE 3: The behavior solution at $T = 1$ with $\Delta t = h = 2^{-6}$, $\alpha = 1.6$.

$\alpha = 1.8$, and $\alpha = 1.6$ respectively, with $T = 1$, $\beta = 1.0$ and $\Delta t = h = 2^{-6}$. The numerical solution compares well with the exact analytic solution to the fractional partial differential equation in these test cases.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

Acknowledgments

This work was supported by the National Science Foundation of China under Grants 61375063, 61271355, 11301549, and 11271378.

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