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A Finite Difference Method for Boundary Value Problems of a Caputo Fractional Differential Equation

Pin Lyu[1], Seakweng Vong[1] and Zhibo Wang[2,*]

[1] *Department of Mathematics, University of Macau, Avenida da Universidade, Taipa, Macau, China.*
[2] *School of Applied Mathematics, Guangdong University of Technology, Guangzhou 510520, Guangdong, China.*

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Abstract. In this paper, we consider a two-point boundary value problem with Caputo fractional derivative, where the second order derivative of the exact solution is unbounded. Based on the equivalent form of the main equation, a finite difference scheme is derived. The L_∞ convergence of the difference system is discussed rigorously. The convergence rate in general improves previous results. Numerical examples are provided to demonstrate the theoretical results.

AMS subject classifications: 65L10, 65L12, 65L20

Key words: Boundary value problem, Caputo fractional derivative, Finite difference method, Convergence, Derivative bound.

1. Introduction

Study on fractional derivatives has attracted lots of attentions in recent years due to its variety in applications. Significant progress on numerical analysis of differential equations with fractional-order derivatives have been made by many researchers [1, 3–6, 9–18, 20, 21, 24–29]. Study of efficient numerical methods for time-fractional differential equations grows to be a popular research topic in the past decade, interested readers can refer to some typical articles [1,16,17,24,28] where equations with Caputo derivative are considered. For space-fractional differential equations, approaches such as the Grünwald-Letnikov formula, shifted Grünwald-Letnikov formula, weighted and shifted Grünwald-Letnikov formula and compact operator were successfully applied to obtain numerical schemes for solving the Riemann-Liouville fractional differential equations, see also [3, 10, 18, 21, 25, 29] for more details. However, many of these works were done under the special restriction that the

*Corresponding author. *Email addresses:* lyupin1991@163.com (P. Lyu), swvongcumac.mo (S. Vong), wzbmath@gdut.edu.cn (Z. Wang)

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exact solutions are smooth on the domain where they are posed and this assumption may not hold in some practical applications. Therefore singular behavior, which may be the true behavior [19], of solutions near boundaries deserves further investigation and this is the main concern of our current study.

In this paper, we consider the following two-point boundary value problem

$$-{}_0^C D^\gamma u(x) + b(x)u'(x) + c(x)u(x) = f(x), \quad x \in (0,1), \tag{1.1}$$

subject to

$$u(0) - \alpha_0 u'(0) = g_0, \quad u(1) + \alpha_1 u'(1) = g_1, \tag{1.2}$$

where $\gamma \in (1,2)$ and ${}_0^C D^\gamma u(x)$ is the Caputo fractional derivative of $u(x)$ defined as

$${}_0^C D^\gamma u(x) = \frac{1}{\Gamma(2-\gamma)} \int_0^x u''(s)(x-s)^{1-\gamma} ds,$$

with $\Gamma(\cdot)$ being the gamma function. The constants $\alpha_0, \alpha_1, g_0, g_1$ and the functions b, c, f are given, and α_0, α_1 satisfy

$$\alpha_0 \geq \frac{1}{\gamma - 1}, \quad \alpha_1 \geq 0. \tag{1.3}$$

We note that the condition was proposed in [2]. Very recently, finite difference methods for (1.1)–(1.3) were studied in [7,23], where rigorous analysis under reasonably general and realistic hypotheses on the behavior of the solution near the boundaries were given. It was showed that proposed finite difference schemes converge with order $h^{\gamma-1}$, where h is the grid size. The Caputo fractional derivative in these two references is approximated by the widely-used first order discretisation formula introduced in [22]. In [23], the convection term is approximated by upwind scheme, while the standard central difference is discussed in [7]. Numerical results in [7] showed that the central approximation is a little bit more accurate than the upwind approximation, but it will be restrictive when γ is close to 1. Further discussions on the numerical behavior of several finite difference schemes for some Riemann-Liouville and Caputo boundary value problems were given in [8]. In this paper, we focus on the Caputo fractional boundary value problem. One may note that the numerical experiments in [7,23] showed that the schemes preform much better in practise and there may be rooms for improvement of the theoretical analysis. Inspired by these results, this paper continues the study in this direction. We propose to solve an equivalent form of (1.1)-(1.3). Following the delicate estimates established in [7,23], we obtain improved convergence under an additional condition. We remark that the central and upwind difference approximations of the convection term make no essential difference to our proof. However, more routine arguments will be needed for the discussion of the central difference approximation. Therefore, for simplicity of presentation, we only discuss the upwind scheme in this paper.

Based on an equivalent form of the considered model, a finite difference scheme will be proposed in the next section. Error analysis of the proposed scheme will be studied in Section 3. In Section 4, numerical experiments are carried out to support the theoretical results, the paper ends with a brief conclusion.

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2. The Proposed Finite Difference Scheme

2.1. An equivalent equation

In order to derive a higher order scheme than that in [23], we first introduce an equivalent form of the problem (1.1) and (1.2).

Denote $\phi = {}_0^C D^\gamma u$. From [23], we have the formula

$$u(x) = u(0) + u'(0)x + \frac{\phi(0)}{\gamma\Gamma(\gamma)}x^\gamma + \frac{1}{\gamma\Gamma(\gamma)}\int_0^x (x-s)^\gamma \phi'(s)ds \tag{2.1}$$

for $u \in \mathbb{C}[0,1]$. Taking limitation of equation (1.1), we get

$$\phi(0) = b(0)u'(0) + c(0)u(0) - f(0) = \frac{u(0)-g_0}{\alpha_0}b(0) + c(0)u(0) - f(0).$$

Now, for the solution of (1.1) and (1.2), consider the function

$$v(x) = u(x) - \frac{\phi(0)}{\gamma\Gamma(\gamma)}x^\gamma. \tag{2.2}$$

We have $v(0) = u(0)$, $v'(0) = u'(0)$ and v satisfies

$$\begin{aligned}
&-{}_0^C D^\gamma v(x) + b(x)v'(x) + c(x)v(x)\\
&= -{}_0^C D^\gamma u(x) + b(x)u'(x) + c(x)u(x) + \Big[1 - \frac{x^{\gamma-1}b(x)}{\Gamma(\gamma)} - \frac{x^\gamma c(x)}{\gamma\Gamma(\gamma)}\Big]\phi(0)\\
&= f(x) + \Big[1 - \frac{x^{\gamma-1}b(x)}{\Gamma(\gamma)} - \frac{x^\gamma c(x)}{\gamma\Gamma(\gamma)}\Big]\Big[\frac{u(0)-g_0}{\alpha_0}b(0) + c(0)u(0) - f(0)\Big]\\
&= \Big[1 - \frac{x^{\gamma-1}b(x)}{\Gamma(\gamma)} - \frac{x^\gamma c(x)}{\gamma\Gamma(\gamma)}\Big]\Big[\frac{b(0)}{\alpha_0} + c(0)\Big]v(0)\\
&\quad - \Big[1 - \frac{x^{\gamma-1}b(x)}{\Gamma(\gamma)} - \frac{x^\gamma c(x)}{\gamma\Gamma(\gamma)}\Big]\Big[\frac{b(0)g_0}{\alpha_0} + f(0)\Big] + f(x).
\end{aligned}$$

Denote

$$\psi(x) = 1 - \frac{x^{\gamma-1}b(x)}{\Gamma(\gamma)} - \frac{x^\gamma c(x)}{\gamma\Gamma(\gamma)}, \quad \kappa_1 = \frac{b(0)}{\alpha_0} + c(0), \quad \kappa_2 = \frac{b(0)g_0}{\alpha_0} + f(0).$$

Then the equation (1.1) can be rewritten as

$$-{}_0^C D^\gamma v(x) + b(x)v'(x) + c(x)v(x) = \kappa_1\psi(x)v(0) - \kappa_2\psi(x) + f(x), \quad x \in (0,1). \tag{2.3}$$

The boundary condition for the left end point is the same as the first equation of (1.2). For the right boundary, noticing (2.2), we have

$$v(1) = u(1) - \frac{\phi(0)}{\gamma\Gamma(\gamma)}, \qquad v'(1) = u'(1) - \frac{\phi(0)}{\Gamma(\gamma)}.$$

Then, with the second equation of (1.2), the right boundary condition is given as

$$v(1) + \alpha_1 v'(1) = g_1 - \frac{1+\alpha_1\gamma}{\Gamma(\gamma+1)}\phi(0) = g_1 + \frac{1+\alpha_1\gamma}{\Gamma(\gamma+1)}\big[\kappa_2 - \kappa_1 v(0)\big].$$

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2.2. The finite difference scheme

After developing the equivalent form (2.3) of (1.1), and noting that the corresponding boundary conditions take similar forms as (1.2), we propose finite central difference scheme as that in [23] to solve for $v(x)$ in (2.3).

Let $h = 1/N$ be the step size with N is a given integer. For $j = 0, 1, \cdots, N$, denotes $x_j = jh$, and $s_j = s(x_j)$, where s can be the functions b, c or f. Suppose v_k be the numerical approximation of $v(x_k)$, and define

$$\tilde{f}_j = \begin{cases} g_0, & j = 0, \\ (\kappa_1 v_0 - \kappa_2)\psi(x_j) + f_j, & 1 \le j \le N-1, \\ g_1 + \frac{1+\alpha_1\gamma}{\Gamma(\gamma+1)}\big[\kappa_2 - \kappa_1 v_0\big], & j = N. \end{cases}$$

Similar to (4.5) in [23], we obtain the following finite difference scheme for (2.3):

$$-\frac{1}{h^\gamma \Gamma(3-\gamma)} \sum_{k=0}^{j-1} d_{j-k}(v_{k+2} - 2v_{k+1} + v_k) + b_j D^{\aleph} v_j + c_j v_j = \tilde{f}_j, \quad 1 \le j \le N-1, \tag{2.4}$$

where the first term on the left hand side of (2.4) comes from the discretisation formula in [22] for the fractional derivative $-{}_0^C D^\gamma v(x_j)$, with the coefficients

$$d_k = \begin{cases} k^{2-\gamma} - (k-1)^{2-\gamma}, & k \ge 1, \\ 0, & k = 0. \end{cases}$$

Here we use the upwind approximation $b_j D^{\aleph} v_j$ for $b(x_j)v'(x_j)$, which is given as

$$b_j D^{\aleph} v_j = -\frac{(b_j + |b_j|)v_{j-1}}{2h} + \frac{|b_j| v_j}{h} + \frac{(b_j - |b_j|)v_{j+1}}{2h}.$$

The derivatives $v'(0)$ and $v'(1)$ in the boundary conditions are approximated by $(v_1 - v_0)/h$ and $(v_N - v_{N-1})/h$, respectively.

Let $\vec{v} = (v_0\ v_1\ \cdots\ v_N)^T$ and $\vec{\tilde{f}} = (\tilde{f}_0\ \tilde{f}_1\ \cdots\ \tilde{f}_N)^T$. We consider the matrix form of (2.4) and the related boundary discretisation:

$$A\vec{v} = \vec{\tilde{f}}, \tag{2.5}$$

where $A \triangleq (a_{jk})_{j,k=0}^N$ has the following structure:
the 0th row is

$$\big((1 + \alpha_0 h^{-1})\ -\alpha_0 h^{-1}\ 0\ 0\ \cdots\ 0\big),$$

the Nth row is

$$\big(0\ 0\ \cdots\ 0\ -\alpha_1 h^{-1}\ (1 + \alpha_1 h^{-1})\big),$$

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and the jth ($j=1,2,\cdots,N-1$) row satisfies

$$\begin{aligned}
a_{j0} &= \frac{-d_j}{h^\gamma\Gamma(3-\gamma)} - \delta_{j1}\frac{b_1+|b_1|}{2h},\\
a_{j1} &= \frac{-d_{j-1}+2d_j}{h^\gamma\Gamma(3-\gamma)} - \delta_{j2}\frac{b_2+|b_2|}{2h} + \delta_{j1}\left(\frac{|b_1|}{h}+c_1\right),\\
a_{jk} &= \frac{-d_{j-k}+2d_{j-k+1}-d_{j-k+2}}{h^\gamma\Gamma(3-\gamma)} - \delta_{j,k+1}\frac{b_j+|b_j|}{2h} + \delta_{jk}\left(\frac{|b_j|}{h}+c_j\right)\\
&\quad + \delta_{j,k-1}\frac{b_j-|b_j|}{2h}, \quad \text{for} \quad k=2,3,\cdots,N,
\end{aligned}$$

in which

$$\delta_{jk} = \begin{cases} 1, & \text{if } j=k,\\ 0, & \text{otherwise.}\end{cases}$$

Theorem 4.4 in [23] has proved that A is invertible with $A^{-1}\geq 0$. Once $\vec{v}$ is solved from the scheme (2.5), $\vec{u}=(u_0\ u_1\ \cdots\ u_N)^T$ can be obtained by equation (2.2).

3. Error Analysis

Denote the error $\vec{e}=(e_0\ e_1\ \cdots\ e_N)^T = v-\vec{v}$, where v is the vector with each component takes value from the exact solution $v(x)$. Define $\vec{\tau}=(\tau_0\ \tau_1\ \cdots\ \tau_N)^T$ to be the truncation error of system (2.5). It holds that

$$A\vec{e} = e_0\vec{\eta} + \vec{\tau}, \tag{3.1}$$

where $\vec{\eta}=(0\ \kappa_1\psi(x_1)\ \cdots\ \kappa_1\psi(x_{N-1})\ -\kappa_1\frac{1+\alpha_1\gamma}{\Gamma(\gamma+1)})^T$, and

$$\begin{aligned}
\tau_0 &= (Av)_0 - \tilde{f}_0 = \alpha_0 v'(x_0) - \frac{\alpha_0}{h}\big[v(x_1)-v(x_0)\big], \qquad (3.2)\\
\tau_N &= (Av)_N - \tilde{f}_N - (e_0\vec{\eta})_N = -\alpha_1 v'(x_N) + \frac{\alpha_1}{h}\big[v(x_N)-v(x_{N-1})\big],\\
\tau_j &= (Av)_j - \tilde{f}_j - (e_0\vec{\eta})_j = (Av)_j - b(x_j)v'(x_j) - c(x_j)v(x_j), \quad 1\leq j\leq N-1.
\end{aligned}$$

To study the convergence, we need to study the truncation error. The following Notation and Theorem are given in [23], which is important to bound the truncation error.

Notation. For integer $q\geq 1$ and $\nu\in(-\infty,1)$, define $C^{q,\nu}(0,1]$ to be the set of continuous functions $y:[0,1]\to\mathbb{R}$ that are q times continuously differentiable in $(0,1]$ and satisfy the bounds

$$|y^{(i)}(x)| \leq \begin{cases} C, & \text{if } i<1-\nu,\\ C(1+|\ln x|), & \text{if } i=1-\nu,\\ Cx^{1-\nu-i}, & \text{if } i>1-\nu,\end{cases}$$

for $0<x\leq 1$ and $i=1,2,\cdots,q$, where C is a constant.

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Theorem 3.1. *Let $b,c,f \in C^{q,\mu}(0,1]$ for some integer $q \geq 2$ and $\mu \leq 2-\gamma$. Assume that $c \geq 0$ and the condition (1.3) is satisfied. Then, (1.1)–(1.2) has a unique solution u with $u \in C^1[0,1] \cap C^{q+1}(0,1]$, and ${}_0^C D^\gamma u \in C^{q,2-\gamma}(0,1]$.*

In the remaining of this paper, we always assume that $b,c,f \in C^{q,\mu}(0,1]$, and the constant C stands for a generic positive constant which is independent of the step size h. Then by Theorem 3.1, we have

$$\left|\phi^{(i)}(x)\right| \leq Cx^{\gamma-1-i}. \tag{3.3}$$

Denote

$$w(x) = \frac{1}{\Gamma(\gamma+1)} \int_0^x (x-s)^\gamma \phi'(s)ds,$$

then

$$\begin{aligned}
\left|w(x)\right| &= \left|\frac{1}{\Gamma(\gamma+1)} \int_0^x (x-s)^\gamma \phi'(s)ds\right| \leq Cx^{2\gamma-1} \int_0^1 (1-s)^\gamma s^{\gamma-2}ds \leq Cx^{2\gamma-1}, \qquad (3.4)\\
\left|w'(x)\right| &= \left|\frac{1}{\Gamma(\gamma)} \int_0^x (x-s)^{\gamma-1} \phi'(s)ds\right| \leq Cx^{2\gamma-2} \int_0^1 (1-s)^{\gamma-1} s^{\gamma-2}ds \leq Cx^{2\gamma-2},\\
\left|w''(x)\right| &= \left|\frac{1}{\Gamma(\gamma-1)} \int_0^x (x-s)^{\gamma-2} \phi'(s)ds\right| \leq Cx^{2\gamma-3} \int_0^1 (1-s)^{\gamma-2} s^{\gamma-2}ds \leq Cx^{2\gamma-3},
\end{aligned}$$

in which we have used (3.3) and the property of the beta function

$$\int_0^1 (1-s)^{\gamma-k} s^{\gamma-2}ds = B(\gamma-k+1,\gamma-1) \leq C, \quad k = 0,1,2.$$

Noticing (2.1) and (2.2), we have

$$\begin{aligned}
&v(jh) = u(0) + u'(0)jh + w(jh), \quad 0 \leq j \leq N, && (3.5)\\
&v'(jh) = u'(0) + w'(jh), \quad 0 \leq j \leq N, && (3.6)\\
&v''(x) = w''(x).
\end{aligned}$$

To analyze the truncation errors, we list the following lemma firstly, which will be used in Lemma 3.2.

Lemma 3.1. *For any given small $\epsilon > 0$, there exists a constant C, which is independent of h and j, such that*

$$h^{\gamma-1} \sum_{k=1}^{j-1} d_{j-k} k^{2\gamma-4} \leq \begin{cases} C(j-1)^{1-\gamma} h^{\gamma-1}, & \gamma < 1.5, \\ C(j-1)^{1-\gamma} h^{2-\gamma-\varepsilon}, & \gamma \geq 1.5. \end{cases}$$

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Proof. The main idea of the proof is similar to that for Lemma 4.5 in [23]. For $\gamma < 1.5$, we have $2\gamma - 3 < 0$, then

$$h^{\gamma-1}\sum_{k=1}^{j-1} d_{j-k}k^{2\gamma-4} \le Cj^{1-\gamma}h^{\gamma-1} \le C(j-1)^{1-\gamma}h^{\gamma-1}.$$

When $\gamma \ge 1.5$, we have

$$\begin{aligned}\sum_{k=1}^{j-1} d_{j-k}k^{2\gamma-4}h^{\gamma-1} &= \sum_{k=1}^{j-1} d_{j-k}k^{-1-\varepsilon}k^{2\gamma-3+\varepsilon}h^{2\gamma-3+\varepsilon}h^{2-\gamma-\varepsilon}\\ &\le C\sum_{k=1}^{j-1} d_{j-k}k^{-1-\varepsilon}h^{2-\gamma-\varepsilon}\\ &\le Cj^{1-\gamma}h^{2-\gamma-\varepsilon}\\ &\le C(j-1)^{1-\gamma}h^{2-\gamma-\varepsilon}.\end{aligned}$$

□

The following lemma is one of the main ingredients of this paper, which describes the bound of the truncation errors of the finite difference scheme (2.5).

Lemma 3.2. *For any given small $\epsilon > 0$, there exists a constant C such that the truncation errors in* (3.1) *satisfy*

$$|\tau_j| \le \begin{cases} Ch^{2\gamma-2}, & \text{if } j = 0,\\ Ch^{\gamma-1}, & \text{if } j = 1,\\ C\max\left\{h^{\gamma-1}(j-1)^{\gamma-2}, h^{\min\{\gamma-1,2-\gamma-\epsilon\}}(j-1)^{1-\gamma}\right\}, & \text{if } j = 2,\cdots,N-1,\\ Ch, & \text{if } j = N.\end{cases}$$

Proof. When $j = 0$, it follows from (3.2), (3.4), (3.5) and (3.6) that

$$|\tau_0| = \alpha_0\left|v'(0) - \frac{v(h)-v(0)}{h}\right| = \alpha_0 h^{-1}\left|w(h)\right| \le Ch^{2\gamma-2}.$$

When $j = N$, similar to the proof of Lemma 4.6 in [23],

$$|\tau_N| = \alpha_1\left|v'(1) - \frac{v(1)-v(1-h)}{h}\right| \le \alpha_1\int_{s=1-h}^{1} Cs^{\gamma-2}ds \le Ch.$$

When $1 < j < N$, we write $\tau_j = R_j + \sum_{k=0}^{j-1}\tau_{j,k}$, where

$$R_j = b_j D^{\aleph}v_j - (bu')(x_j),$$

and

$$\tau_{j,k} = \frac{1}{\Gamma(2-\gamma)}\int_{x_k}^{x_{k+1}} (x_j - s)^{1-\gamma}v''(s)ds - \frac{d_{j-k}}{h^{\gamma}\Gamma(3-\gamma)}\left[v(x_{k+2}) - 2v(x_{k+1}) + v(x_k)\right].$$

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From (4.21) in [23], we have

$$|R_j| \le Ch^{\gamma-1}(j-1)^{\gamma-2}. \tag{3.7}$$

On the other hand, note that $\int_{x_k}^{x_{k+1}}(x_j-s)^{1-\gamma}ds = h^{2-\gamma}d_{j-k}/(2-\gamma)$, by the integral mean value theorem,

$$\begin{aligned}\tau_{j,k} &= \frac{v''(\xi_1)}{\Gamma(2-\gamma)}\int_{x_k}^{x_{k+1}}(x_j-s)^{1-\gamma}ds - \frac{d_{j-k}}{h^{\gamma}\Gamma(3-\gamma)}\big[v(x_{k+2})-2v(x_{k+1})+v(x_k)\big]\\ &= \frac{h^{2-\gamma}d_{j-k}}{\Gamma(3-\gamma)}\big[w''(\xi_1)-w''(\xi_2)\big]\\ &= \frac{h^{2-\gamma}d_{j-k}}{\Gamma(3-\gamma)\Gamma(\gamma-1)}\left[\int_0^1 \xi_1^{\gamma-1}(1-s)^{\gamma-2}\phi'(\xi_1 s)ds - \int_0^1 \xi_2^{\gamma-1}(1-s)^{\gamma-2}\phi'(\xi_2 s)ds\right],\end{aligned}$$

where $\xi_1 \in (x_k, x_{k+1}),\ \xi_2 \in (x_k, x_{k+2})$.

Note that, when h is small, for $1 \le k \le j-1$,

$$\begin{aligned}\left|\xi_1^{\gamma-1}\phi'(\xi_1 s) - \xi_2^{\gamma-1}\phi'(\xi_2 s)\right| &\le \xi_1^{\gamma-1}\left|\phi'(\xi_1 s)-\phi'(\xi_2 s)\right| + \left|\xi_1^{\gamma-1}-\xi_2^{\gamma-1}\right|\left|\phi'(\xi_2 s)\right|\\ &\le Chx_{k+1}^{\gamma-1}x_k^{\gamma-3} + Chx_k^{\gamma-2}x_k^{\gamma-2}\\ &\le Chx_k^{\gamma-3}x_{k+1}^{\gamma-1},\end{aligned}$$

which implies that

$$|\tau_{j,k}| \le Cd_{j-k}h^{3-\gamma}x_k^{\gamma-3}x_{k+1}^{\gamma-1} = Cd_{j-k}h^{\gamma-1}k^{\gamma-3}(k+1)^{\gamma-1} \le 2^{\gamma-1}Cd_{j-k}h^{\gamma-1}k^{2\gamma-4}.$$

By Lemma 3.1, we then have

$$\sum_{k=1}^{j-1}|\tau_{j,k}| \le Ch^{\gamma-1}\sum_{k=1}^{j-1}d_{j-k}k^{2\gamma-4} \le Ch^{\min\{\gamma-1,2-\gamma-\epsilon\}}(j-1)^{1-\gamma}. \tag{3.8}$$

For $\tau_{j,0}$, we have

$$|\tau_{j,0}| \le \left|\frac{1}{\Gamma(2-\gamma)}\int_0^h (x_j-s)^{1-\gamma}v''(s)ds\right| + \left|\frac{d_j}{h^{\gamma}\Gamma(3-\gamma)}\big[v(x_2)-2v(x_1)+v(x_0)\big]\right|. \tag{3.9}$$

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For the first term on the right of (3.9), we have

$$\begin{aligned}\left|\frac{1}{\Gamma(2-\gamma)}\int_0^h (x_j-s)^{1-\gamma}v''(s)ds\right| &\le C\left|\int_0^h (x_j-s)^{1-\gamma}\int_0^s (s-\xi)^{\gamma-2}\phi'(\xi)d\xi ds\right| \\ &= C\left|\int_0^h \phi'(\xi)\int_\xi^h (x_j-s)^{1-\gamma}(s-\xi)^{\gamma-2}dsd\xi\right| \\ &\le C\left|\int_0^h \phi'(\xi)(x_j-h)^{1-\gamma}\int_\xi^h (s-\xi)^{\gamma-2}dsd\xi\right| \\ &\le C(j-1)^{1-\gamma}h^{1-\gamma}\left|\int_0^h \phi'(\xi)(h-\xi)^{\gamma-1}d\xi\right| \\ &= C(j-1)^{1-\gamma}h^{1-\gamma}\left|\Gamma(\gamma)w'(h)\right| \\ &\le C(j-1)^{1-\gamma}h^{\gamma-1}.\end{aligned}$$

For the second term, noticing that $d_j = 1/(2-\gamma)\int_{j-1}^{j} x^{1-\gamma}dx \le C(j-1)^{1-\gamma}$, then we get

$$\begin{aligned}\left|\frac{d_j}{h^\gamma\Gamma(3-\gamma)}\big[v(x_2)-2v(x_1)+v(x_0)\big]\right| &= \frac{d_j}{h^\gamma\Gamma(3-\gamma)}\left|w(2h)-2w(h)\right| \\ &\le C\frac{(j-1)^{1-\gamma}}{h^\gamma}h^{2\gamma-1} \\ &\le C(j-1)^{1-\gamma}h^{\gamma-1}.\end{aligned}$$

Therefore

$$|\tau_{j,0}| \le C(j-1)^{1-\gamma}h^{\gamma-1}. \tag{3.10}$$

With (3.7),(3.8) and (3.10), we get

$$|\tau_j| \le \sum_{k=0}^{j-1}|\tau_{j,k}| + |R_j| \le C\max\left\{h^{\gamma-1}(j-1)^{\gamma-2}, h^{\min\{\gamma-1,2-\gamma-\epsilon\}}(j-1)^{1-\gamma}\right\}, \quad 1<j<N.$$

When $j=1$, we need to estimate $\tau_{1,0}$. From arguments given above, we know that

$$\left|\frac{d_1}{h^\gamma\Gamma(3-\gamma)}\big[v(x_2)-2v(x_1)+v(x_0)\big]\right| \le Ch^{\gamma-1},$$

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and

$$\begin{aligned}
&\left|\frac{1}{\Gamma(2-\gamma)}\int_0^h (h-s)^{1-\gamma}v''(s)ds\right| \\
\le& C\int_0^h \left|\phi'(\xi)\right| \int_\xi^h (h-s)^{1-\gamma}(s-\xi)^{\gamma-2}dsd\xi \\
=& C\int_0^h \left|\phi'(\xi)\right| \left(\int_\xi^{\frac{h+\xi}{2}} (h-s)^{1-\gamma}(s-\xi)^{\gamma-2}ds + \int_{\frac{h+\xi}{2}}^h (h-s)^{1-\gamma}(s-\xi)^{\gamma-2}ds\right)d\xi \\
\le& C\int_0^h \xi^{\gamma-2}\left(\int_\xi^{\frac{h+\xi}{2}} (\frac{h-\xi}{2})^{1-\gamma}(s-\xi)^{\gamma-2}ds + \int_{\frac{h+\xi}{2}}^h (h-s)^{1-\gamma}(\frac{h-\xi}{2})^{\gamma-2}ds\right)d\xi \\
\le& C\int_0^h \xi^{\gamma-2}d\xi = Ch^{\gamma-1},
\end{aligned}$$

which imply that $|\tau_{1,0}| \le Ch^{\gamma-1}$.

On the other hand,

$$|R_1| = \left|b_1\left(\frac{v(2h)-v(h)}{h} - v'(h)\right)\right| = |b_1|\left|\left(\frac{w(2h)}{h} - w'(h)\right)\right| \le Ch^{2\gamma-2}, \quad \text{if } b_1 < 0,$$

$$|R_1| = \left|b_1\left(\frac{v(h)-v(0)}{h} - v'(h)\right)\right| = |b_1|\left|\left(\frac{w(h)}{h} - w'(h)\right)\right| \le Ch^{2\gamma-2}, \quad \text{if } b_1 \ge 0.$$

Hence

$$|\tau_1| \le |\tau_{1,0}| + |R_1| \le Ch^{\gamma-1}.$$

The whole proof is thus completed. □

Another critical step for proving the convergence of the scheme is some rescaling of A. We note that a rescaled matrix of A has very nice properties [7,23]. However, if the column $\vec{\eta}$ is combined with A, these properties will no longer hold. This is why $\vec{\eta}$ is considered separately. For the completeness of our presentation, we now recall the rescaling of A. Firstly we introduce $A' \triangleq (a'_{jk})_{j,k=0}^N$ by applying the same elementary transformation on A as subsection 4.2 in [7]. That is

$$A' = E^{(N-2)}E^{(N-1)}\cdots E^{(1)}A,$$

where the elementary matrix $E^{(k)} = (e_{ij}^{(k)})_{i,j=0}^N$ with

$$e_{ij}^{(k)} = \delta_{ij} - \frac{a_{k0}}{a_{00}}\delta_{ik}\delta_{j0}.$$

Then we have $a'_{11} > 0$ and $a'_{j1} < 0$ for $j = 2,3,\cdots,N-1$, see Lemma 4.3 in [7] for more details. As a result,

$$A'\vec{e} = e_0\vec{\eta} + \vec{\tau}', \tag{3.11}$$

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where $\tau_0' = \tau_0,\ \tau_N' = \tau_N$, and

$$\tau_j' = \tau_j + \frac{\tau_0}{1+\alpha_0 h^{-1}}\left[\frac{d_j}{h^\gamma\Gamma(3-\gamma)} + \delta_{j1}\frac{b_1+|b_1|}{2h}\right], \quad j = 1,2,\cdots,N-1.$$

We further rescale the system (3.11) by multiplying the jth equation by

$$\frac{(1+\alpha_0 h^{-1})h^\gamma\Gamma(3-\gamma)}{d_j}, \quad j = 1,\cdots,N-1,$$

to obtain

$$\tilde{A}\vec{e} = e_0\vec{\tilde{\eta}} + \vec{\tilde{\tau}},$$

where $\tilde{A}$ is the desired rescaled coefficient matrix of the system, $\vec{\tilde{\eta}} = (\tilde{\eta}_0\ \tilde{\eta}_1\ \cdots\ \tilde{\eta}_{N-1}\ \tilde{\eta}_N)^T$, $\vec{\tilde{\tau}} = (\tau_0\ \tilde{\tau}_1\ \cdots\ \tilde{\tau}_{N-1}\ \tau_N)^T$ are the corresponding rescaled vectors with

$$\begin{aligned}
\tilde{\eta}_0 =& \eta_0, \quad \tilde{\eta}_N = \eta_N,\\
\tilde{\eta}_j =& \frac{(1+\alpha_0 h^{-1})h^\gamma\Gamma(3-\gamma)}{d_j}\eta_j,\\
\tilde{\tau}_j =& \frac{(1+\alpha_0 h^{-1})h^\gamma\Gamma(3-\gamma)}{d_j}\tau_j'\\
=& \frac{(1+\alpha_0 h^{-1})h^\gamma\Gamma(3-\gamma)}{d_j}\tau_j + \left[1+\delta_{j1}\frac{b_1+|b_1|}{2h}\frac{h^\gamma\Gamma(3-\gamma)}{d_j}\right]\tau_0,
\end{aligned}$$

where $j = 1,\cdots,N-1$.

The proof of Theorem 4.7 in [7] showed that $\tilde{A}$ is an M matrix and $\|(\tilde{A})^{-1}\|_\infty \le 1$. Moreover, the entries $\tilde{b}_{jk}$ of $(\tilde{A})^{-1}$ are nonnegative, and $\sum_{k=0}^N b_{0k} \le 1$. With these properties of $\tilde{A}$, convergence of schemes can be established in [7, 23]. However, in our situation, we need additional arguments to tackle with the column $\vec{\tilde{\eta}}$. These are summarized in the following theorem.

Theorem 3.2. *Suppose that the conditions in Theorem* 3.1 *hold. Assume further that*

$$\max\left\{(2-\gamma)(\alpha_0+1)\eta^*, -\kappa_1\frac{1+\alpha_1\gamma}{\Gamma(\gamma+1)}\right\} < 1, \tag{3.12}$$

where $\eta^* = \sup_x\{\kappa_1\psi(x)\}$. *For any given small* $\epsilon > 0$, *there exists a constant* C *such that the error* $\vec{e}$ *in* (3.1) *satisfies*

$$\|\vec{e}\|_\infty \le Ch^{\min\{1-\epsilon,2\gamma-2\}},$$

where $\|\vec{e}\|_\infty = \max_{j=0,1,\cdots,N}|e_j|$.

Proof. Noticing that, for $j \ge 2$,

$$d_j \ge (2-\gamma)j^{1-\gamma} \ge (2-\gamma)2^{1-\gamma}(j-1)^{1-\gamma},$$

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and

$$\frac{h^{\gamma-1}(j-1)^{\gamma-2}}{d_j} \le C\frac{h^{\gamma-1}(j-1)^{\gamma-2}}{(j-1)^{1-\gamma}} = Ch^{2-\gamma}h^{2\gamma-3}(j-1)^{2\gamma-3} \le Ch^{2-\gamma},$$
$$\frac{h^{\min\{\gamma-1,2-\gamma-\epsilon\}}(j-1)^{1-\gamma}}{d_j} \le C\frac{h^{\min\{\gamma-1,2-\gamma-\epsilon\}}(j-1)^{1-\gamma}}{(j-1)^{1-\gamma}} = Ch^{\min\{\gamma-1,2-\gamma-\epsilon\}}.$$

Thus, by Lemma 3.2, we get

$$|\tilde{\tau}_j| \le Ch^{\min\{1-\epsilon,2\gamma-2\}}, \quad j = 1,2,\cdots,N-1.$$

Since $d_j = 1/(2-\gamma)\int_{j-1}^{j} x^{1-\gamma}dx \ge j^{1-\gamma}/(2-\gamma)$, then

$$\frac{h^{\gamma-1}}{d_j} \le \frac{(2-\gamma)h^{\gamma-1}}{j^{1-\gamma}} = (2-\gamma)h^{\gamma-1}j^{\gamma-1} \le 2-\gamma, \quad j = 1,\cdots,N-1,$$

and then

$$\max_{1\le j\le N-1}\{0,\tilde{\eta}_j\} \le \left(\frac{h^{\gamma}+\alpha_0 h^{\gamma-1}}{d_j}\right)\max_{1\le j\le N-1}\{0,\eta_j\} \le (2-\gamma)(\alpha_0+1)\max\{0,\eta^*\}.$$

With the assumption that the condition (3.12) holds, we have

$$\max_{0\le j\le N}\{0,\tilde{\eta}_j\} \le \max\left\{0,(2-\gamma)(\alpha_0+1)\eta^*,-\kappa_1\frac{1+\alpha_1\gamma}{\Gamma(\gamma+1)}\right\} < 1. \tag{3.13}$$

From the rescaled system,

$$e_0 = e_0\left[(\tilde{A})^{-1}\vec{\tilde{\eta}}\right]_0 + \left[(\tilde{A})^{-1}\vec{\tilde{\tau}}\right]_0 = e_0\sum_{k=0}^{N}\tilde{b}_{0k}\tilde{\eta}_k + \left[(\tilde{A})^{-1}\vec{\tilde{\tau}}\right]_0.$$

That is

$$e_0\left(1-\sum_{k=0}^{N}\tilde{b}_{0k}\min\{0,\tilde{\eta}_k\}\right) = e_0\sum_{k=0}^{N}\tilde{b}_{0k}\max\{0,\tilde{\eta}_k\} + \left[(\tilde{A})^{-1}\vec{\tilde{\tau}}\right]_0.$$

Thus we get

$$|e_0| \le \left|e_0\left(1-\sum_{k=0}^{N}\tilde{b}_{0k}\min\{0,\tilde{\eta}_k\}\right)\right| \le \max_{0\le j\le N}\{0,\tilde{\eta}_j\}|e_0|\sum_{k=0}^{N}\tilde{b}_{0k} + Ch^{2\gamma-2}$$
$$\le \max\left\{0,(2-\gamma)(\alpha_0+1)\eta^*,-\kappa_1\frac{1+\alpha_1\gamma}{\Gamma(\gamma+1)}\right\}|e_0| + Ch^{2\gamma-2}.$$

Therefore, with the inequality (3.13), we obtain $|e_0| \le Ch^{2\gamma-2}$, and consequently we get that $|e_j| \le Ch^{\min\{1-\epsilon,2\gamma-2\}}$ for all j by the equation $\vec{e} = e_0[(\tilde{A})^{-1}\vec{\tilde{\eta}}] + [(\tilde{A})^{-1}\vec{\tilde{\tau}}]$. □

Remark 3.1. From (2.2), we know that the error between the exact solution u and the approximate solution $\vec{u}$ satisfies $u-\vec{u} = v-\vec{v} = \vec{e}$. Thus we have

$$\|u-\vec{u}\|_\infty = \|\vec{e}\|_\infty \le Ch^{\min\{1-\epsilon,2\gamma-2\}},$$

if the assumptions in Theorem 3.2 are fulfilled.

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4. Numerical Experiments

In this section, we carry out numerical experiments for the proposed scheme (2.5) to illustrate our theoretical statements. All our tests were done in MATLAB R2014a with a desktop computer (Dell optiplex 7020) having the following configuration: Intel(R) Core(TM) i7-4790 CPU 3.60GHz and 16.00G RAM. The maximum norm errors between the exact and the numerical solutions

$$E_\infty(h) = \max_{0\le j\le N} |e_j|,$$

are shown in the following tables. Furthermore, the convergence order, denoted by

$$\text{Rate} = \log_2\left(\frac{E_\infty(2h)}{E_\infty(h)}\right),$$

is reported.

Example 4.1. ([23]) We consider the problem on $(0,1)$,

$$-{}_0^C D^\gamma u(x) + x^2 u'(x) + (1+x)u(x) = f(x),$$
$$u(0) - \frac{1}{\gamma-1}u'(0) = g_0, \quad u(1) + u'(1) = g_1,$$

where $f(x)$ and g_0, g_1 are chosen such that the exact solution is $u(x) = x^\gamma + x^{2\gamma-1} + 1 + 3x - 7x^2 + 4x^3 + x^4$.

Table 1 lists the numerical results of Example 4.1 for different γ with $N = 64, 128, \cdots, 2048$. We can see that the convergence order is always close to 1 which is better than $2\gamma-2$ when $\gamma < 1.5$, this can also be seen in Table 1 in [23].

5. Conclusion

In this paper, based on the equivalent form of the main equation, a high order finite difference scheme is proposed to solve a two-point boundary value problem with Caputo fractional derivative, where the second order derivative of the exact solution has singular behavior. The L_∞ convergence of the difference system is discussed rigorously. Numerical examples are also provided to demonstrate the theoretical results.

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Table 1: Numerical results of scheme (2.5) for Example 4.1.

		$N=64$	$N=128$	$N=256$	$N=512$	$N=1024$	$N=2048$
$\gamma=1.001$	$E_\infty(h)$	1.481e-01	7.735e-02	3.987e-02	2.037e-02	1.034e-02	5.227e-03
	Rate	0.938	0.956	0.969	0.978	0.985	$*$
$\gamma=1.1$	$E_\infty(h)$	1.458e-01	7.519e-02	3.829e-02	1.934e-02	9.727e-03	4.878e-03
	Rate	0.956	0.974	0.985	0.992	0.996	$*$
$\gamma=1.2$	$E_\infty(h)$	1.441e-01	7.376e-02	3.736e-02	1.881e-02	9.442e-03	4.730e-03
	Rate	0.966	0.981	0.990	0.995	0.997	$*$
$\gamma=1.3$	$E_\infty(h)$	1.433e-01	7.314e-02	3.698e-02	1.860e-02	9.335e-03	4.676e-03
	Rate	0.971	0.984	0.991	0.995	0.997	$*$
$\gamma=1.4$	$E_\infty(h)$	1.431e-01	7.301e-02	3.693e-02	1.859e-02	9.333e-03	4.678e-03
	Rate	0.971	0.983	0.990	0.994	0.997	$*$
$\gamma=1.5$	$E_\infty(h)$	1.428e-01	7.303e-02	3.702e-02	1.867e-02	9.390e-03	4.712e-03
	Rate	0.968	0.980	0.987	0.992	0.995	$*$
$\gamma=1.6$	$E_\infty(h)$	1.417e-01	7.272e-02	3.701e-02	1.873e-02	9.449e-03	4.754e-03
	Rate	0.963	0.975	0.982	0.987	0.991	$*$
$\gamma=1.7$	$E_\infty(h)$	1.382e-01	7.131e-02	3.649e-02	1.857e-02	9.413e-03	4.757e-03
	Rate	0.955	0.966	0.975	0.980	0.985	$*$
$\gamma=1.8$	$E_\infty(h)$	1.300e-01	6.745e-02	3.473e-02	1.779e-02	9.075e-03	4.615e-03
	Rate	0.947	0.958	0.965	0.971	0.976	$*$
$\gamma=1.9$	$E_\infty(h)$	1.133e-01	5.876e-02	3.030e-02	1.557e-02	7.981e-03	4.080e-03
	Rate	0.948	0.955	0.960	0.965	0.968	$*$

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