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Convergence analysis of a finite difference scheme for a two-point boundary value problem with a Riemann-Liouville-Caputo fractional derivative

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Abstract The Riemann-Liouville-Caputo (RLC) derivative is a new class of derivative that is motivated by modelling considerations; it lies between the more familiar Riemann-Liouville and Caputo derivatives. The present paper studies a two-point boundary value problem on the interval $[0,L]$ whose highest-order derivative is an RLC derivative of order $\alpha \in (1,2)$. It is shown that the choice of boundary condition at $x=0$ strongly influences the regularity of the solution. For the case where the solution lies in $C^1[0,L] \cap C^{q+1}(0,L]$ for some positive integer q, a finite difference scheme is used to solve the problem numerically on a uniform mesh. In the error analysis of the scheme, the weakly singular behaviour of the solution at $x=0$ is taken into account and it is shown that the method is almost first-order convergent. Numerical results are presented to illustrate the performance of the method.

Keywords Fractional differential equation · Riemann-Liouville-Caputo fractional derivative · weak singularity · maximum principle · finite difference scheme

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1 Introduction

1.1 Types of fractional derivative

Differential equations with fractional space derivatives have been used in the literature to model various physical processes (see [4, 11, 15] and the references therein). Two of the most widely studied fractional derivatives are the Riemann-Liouville fractional derivative $D^{\beta}_{RL}v$ and the Caputo fractional derivative $D^{\beta}_{C}v$ of order β, where $n-1<\beta<n$ and n is a positive integer. For all sufficiently regular functions, these derivatives are defined by (see, for example, [3]): For all $x\in(0,L]$,

$$D^{\beta}_{RL}v(x):=\frac{1}{\Gamma(n-\beta)}\left(\frac{d}{dx}\right)^{n}\int_{t=0}^{x}(x-t)^{n-1-\beta}v(t)\,dt,$$

$$D^{\beta}_{C}v(x):=\frac{1}{\Gamma(n-\beta)}\int_{t=0}^{x}(x-t)^{n-1-\beta}\,v^{(n)}(t)\,dt,\ \text{ where } v^{(n)}(t):=\frac{d^{n}v(t)}{dt^{n}}. \quad (1.1)$$

Recently, modellers of physical processes [1, 2, 5, 16] suggested an alternative definition of fractional derivative for $1<\beta<2$ that is intermediate to the above two definitions. Following [10] we call this new derivative a *Riemann-Liouville-Caputo* fractional derivative; it is also known as a Patie-Simon fractional derivative [1, 12, 16] and as a conservative Caputo derivative [22].

The Riemann-Liouville-Caputo (RLC) fractional derivative D^{α}_{RLC} of order $\alpha\in(1,2)$ is defined by

$$D^{\alpha}_{RLC}v(x):=\frac{d}{dx}D^{\alpha-1}_{C}v(x)=\frac{d}{dx}\left(\int_{t=0}^{x}\frac{(x-t)^{1-\alpha}v'(t)}{\Gamma(2-\alpha)}\,dt\right)\quad\text{for } x>0,$$

provided this derivative exists.

If v' is absolutely continuous on $[0,L]$, then $D^{\alpha}_{RL}v(x)$ and $D^{\alpha}_{C}v(x)$ exist for all $x\in(0,L]$, and integrations by parts show that $D^{\alpha}_{RLC}v(x)$ also exists with

$$D^{\alpha}_{RL}v(x)=D^{\alpha}_{RLC}v(x)+\frac{x^{-\alpha}}{\Gamma(1-\alpha)}v(0)$$

and

$$D^{\alpha}_{C}v(x)=D^{\alpha}_{RLC}v(x)-\frac{x^{1-\alpha}}{\Gamma(2-\alpha)}v'(0). \quad (1.2)$$

Observe from (1.2) that if $v'(0)=0$, then $D^{\alpha}_{C}v(x)=D^{\alpha}_{RLC}v(x)$. Note also that the RLC fractional derivative has $D^{\alpha}_{RLC}1=D^{\alpha}_{RLC}x^{\alpha-1}=0$, while it is well known that $D^{\alpha}_{C}1=D^{\alpha}_{C}x=0$ and $D^{\alpha}_{RL}x^{\alpha-1}=D^{\alpha}_{RL}x^{\alpha-2}=0$. These differences between the kernels of the various derivatives imply that the character of the solution of a fractional differential equation depends strongly on the choice of fractional derivative used.

1.2 Topics of the paper

In this paper we shall consider the differential equation

$$-D^{\alpha}_{RLC}u+b(x)u'+c(x)u=f(x) \ \text{ for } x\in(0,L), \tag{1.3}$$

where the given functions b,c and f are smooth. The formulation of our boundary value problem will be completed by the imposition of boundary conditions at $x=0$ and $x=L$ in addition to (1.3).

A careless choice of boundary condition at $x=0$ can yield a solution that lies in $C[0,L]$ but not in $C^1[0,L]$. For example, in the case $b\equiv c\equiv 0$ in (1.3), one wants a boundary condition that excludes the kernel function $x^{\alpha-1}$ of Section 1.1 from the solution. We shall show that a choice of boundary condition at $x=0$ that has been advocated by several modellers yields a solution $u\in C^1[0,L]$; nevertheless $u''(x)$ blows up as x approaches 0, so the solution is weakly singular at $x=0$. A standard (classical) Robin boundary condition is imposed at $x=L$, where the solution is smooth. The full description of the boundary value problem will be given in (2.3).

As well as discussing the correct formulation of the boundary value problem for (1.3), our paper investigates the approximate solution of the boundary value problem by a finite difference method on a uniform mesh, where our discretisation of the RLC derivative is based on (1.2) and the well-known L1 approximation of the Caputo fractional derivative. A standard central difference approximation is used for the convective term bu' in (1.3). The weakly singular behaviour of the solution at $x=0$ is taken into account in deriving truncation error estimates for the scheme. Error estimates are then deduced using a discrete comparison principle with a suitable barrier function; we prove first-order convergence (up to a logarithmic factor).

The structure of the paper is as follows. In Section 2 we discuss the choice of boundary condition at $x=0$ and the properties of the solution of the boundary value problem. Furthermore, a maximum principle for the differential operator is established. The finite difference scheme is presented in Section 3 and the finite difference operator is shown to satisfy a discrete maximum principle. We prove first-order convergence (up to a logarithmic factor) of the numerical method in Section 4 by a consistency and stability argument. Numerical results are presented in Section 5.

Notation: In this paper C denotes a generic constant that can depend on the data of the boundary value problem but it is independent of the mesh of the numerical method used for its approximation. Note that C can take different values in different places. We write $\|\cdot\|_\infty$ for the norm in the Lebesgue space $L_\infty[0,L]$.

2 Properties of the two-point boundary value problem

2.1 Choice of boundary condition at $x=0$

Modelling with variants of the differential equation (1.3) is discussed in [1, 2, 5], where the authors advocate the use of the boundary condition

$$0=D^{\alpha-1}_C u(0):=\lim_{x\to 0^+} D^{\alpha-1}_C u(x) \tag{2.1}$$

to avoid a troublesome singularity in the solution u at $x = 0$.

A related theoretical result appears when we examine a special case of (1.3) whose solution can be determined exactly:

$$-D^{\alpha}_{RLC} w + bw' = f \text{ on } (0, L), \tag{2.2}$$

where b and f are constants. Using Laplace transforms (see Appendix) one can show easily that the general solution of (2.2) is given by

$$w(x) = -f x^{\alpha} E_{\alpha-1,\alpha+1}(bx^{\alpha-1}) + \left[D^{\alpha-1}_C w(0)\right] x^{\alpha-1} E_{\alpha-1,\alpha}(bx^{\alpha-1}) + w(0)$$

for $0 < x \le L$, where $E_{\beta,\gamma}(\cdot)$ is the two-parameter Mittag-Leffler function defined by

$$E_{\beta,\gamma}(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k\beta + \gamma)} \text{ for } \beta, \gamma > 0 \text{ and all real numbers } z.$$

It follows that $w \in C^1[0, L]$ (in fact, w' is absolutely continuous on $[0, L]$) if and only if (2.1) is satisfied.

Furthermore, every function $v \in C^1[0, L]$ satisfies (2.1), by [3, Lemma 3.11].

All this evidence leads us to impose the boundary condition (2.1) at $x = 0$.

Remark 2.1 The wellposedness of the problem $-D^{\alpha}_{RLC} u = f$ with various boundary conditions and the regularity of its solution are considered in [10, 22]. In particular, different types of Neumann boundary conditions are considered in [22].

2.2 The two-point boundary value problem

The discussion of Section 2.1 leads us to consider the two-point boundary value problem

$$-D^{\alpha}_{RLC} u(x) + b(x)u'(x) + c(x)u(x) = f(x) \text{ for } x \in (0, L), \tag{2.3a}$$
$$D^{\alpha-1}_C u(0) = 0, \; u(L) + \beta_1 u'(L) = \gamma_1, \tag{2.3b}$$

where the constants $\beta_1 \ge 0$ and γ_1 and the functions $b, c, f \in C[0, L]$ are given. We seek solutions u of (2.3) such that u' is absolutely continuous on $[0, L]$ to ensure that $D^{\alpha}_{RLC} u(x)$ is defined; we say such solutions are *admissible solutions*. In (2.3b) we are able to permit a general classical boundary condition at $x = L$, as all the technical difficulties associated with (2.3a) are at $x = 0$.

To discuss existence and uniqueness of an admissible solution to (2.3), the next result will be helpful.

Lemma 2.1 *Suppose that u is an admissible solution of the two-point boundary value problem* (2.3). *Then* $u'(0) = 0$.

Proof The continuity of $bu' + cu - f$ on $[0,L]$ and (2.3a) imply that $D^{\alpha}_{RLC}u \in C[0,L]$. In particular, $D^{\alpha}_{RLC}u(0)$ exists. That is,

$$D^{\alpha}_{RLC}u(0) = \frac{d}{dx}\left(D^{\alpha-1}_{C}u\right)(x)\bigg|_{x=0} = \lim_{x\to 0^+}\frac{D^{\alpha-1}_{C}u(x) - D^{\alpha-1}_{C}u(0)}{x} \text{ exists.}$$

But $D^{\alpha-1}_{C}u(0) = 0$, so for existence of this limit one must have $|D^{\alpha-1}_{C}u(x)| \leq Cx$ for all $x \in [0,\delta_1]$ for some $\delta_1 > 0$, where C is some constant.

If $u'(0) \neq 0$, then there exists $\delta_2 > 0$ such that $u'(x)$ has constant sign with $|u'(x)| \geq \frac{1}{2}|u'(0)|$ for $0 \leq x \leq \delta_2$. Hence, for $0 < x < \min\{\delta_1,\delta_2\}$ one has

$$\begin{aligned}
|D^{\alpha-1}_{C}u(x)| &= \left|\frac{1}{\Gamma(2-\alpha)}\int_{s=0}^{x}(x-s)^{1-\alpha}u'(s)\,ds\right| \\
&\geq \frac{|u'(0)|}{2\Gamma(2-\alpha)}\int_{s=0}^{x}(x-s)^{1-\alpha}\,ds \\
&= \frac{|u'(0)|}{2\Gamma(3-\alpha)}x^{2-\alpha},
\end{aligned}$$

which contradicts $|D^{\alpha-1}_{C}u(x)| \leq Cx$ above. Consequently $u'(0) = 0$.

Lemma 2.1 and (1.2) yield $D^{\alpha}_{C}u(x) = D^{\alpha}_{RLC}u(x)$ for all $x \in (0,L)$, if u is any admissible solution of our problem (2.3).

2.3 Existence and uniqueness of a solution

We can now see that (2.3) is equivalent to the following Caputo boundary value problem:

$$-D^{\alpha}_{C}u(x) + b(x)u'(x) + c(x)u(x) = f(x) \quad \text{for } x \in (0,L), \tag{2.4a}$$

$$u'(0) = 0,\ u(L) + \beta_1 u'(L) = \gamma_1. \tag{2.4b}$$

For the arguments of Section 2.2 have shown that any admissible solution of (2.3) is also a solution of (2.4). Conversely, if u is a solution of (2.4) with u' absolutely continous on $[0,L]$, then by (1.2) one has $D^{\alpha}_{C}u(x) = D^{\alpha}_{RLC}u(x)$ for all $x \in (0,L)$, and by [3, Lemma 3.11] one has $D^{\alpha-1}_{C}u(0) = 0$.

This equivalence of (2.3) and (2.4) will enable us to obtain quickly an existence result for the solution of (2.3), since problems such as (2.4) have been studied previously in the literature; for example, see [13, 14, 17, 19].

For each positive integer q and $-\infty < \nu < 1$, let $C^{q,\nu}(0,L]$ be the space of all functions $y \in C[0,L]$ that are q-times continuously differentiable on $(0,L]$ with

$$\|y\|_{q,\nu} := \sup_{0<x\leq L}|y(x)| + \sum_{k=1}^{q}\sup_{0<x\leq L}\left[x^{k-(1-\nu)}|y^{(k)}(x)|\right] < \infty.$$

In other words, $C^{q,\nu}(0,L]$ is the space of functions $y \in C[0,L] \cap C^{q}(0,L]$ such that $|y(x)| \leq C$ and $|y^{(k)}(x)| \leq C'(1 + x^{(1-\nu)-k})$ for $k = 1,\ldots,q$ and $x \in (0,L)$, where C' is some constant. By [20], $C^{q,\nu}(0,L]$ is a Banach space. Note that $C^{q}[0,L] \subset C^{q,\nu}(0,L]$.

Invoking [17, Theorem 2.1] (alternatively, see [13]), one now obtains

Theorem 2.1 *Let $b, c, f \in C^{q,\mu}(0,L]$ for some positive integer q and some $\mu \in (-\infty, 1)$. Assume that the problem (2.3) (equivalently, the problem (2.4)) has only the trivial solution $u \equiv 0$ when $f \equiv 0$ and $\gamma_1 = 0$. Then (2.3) has a unique solution $u \in C^1[0,L]$ with $D^{\alpha}_{RLC}u \in C^{q,\nu}(0,L]$, where $\nu := \max\{\mu, 2-\alpha\}$.*

In the statement of Theorem 2.1 we omitted a further condition that appears in the general result of [17, Theorem 2.1] because it is evidently satisfied in our problem: the only polynomial of degree at most 1 that satisfies the boundary conditions (2.4b) when $\gamma_1 = 0$ is the polynomial 0.

Corollary 2.1 *Let $b, c, f \in C^{q,\mu}(0,L]$ for some positive integer q and some $\mu \in (-\infty, 1)$, with $\mu \le 2-\alpha$. Then the solution u of (2.3) that is guaranteed by Theorem 2.1 lies in $C^{q+1}(0,L]$ and satisfies*

$$|u^{(i)}(x)| \le \begin{cases} C & \textit{if } i = 0, \\ Cx^{\alpha-i} & \textit{if } i = 1, 2, 3, \ldots, q+1, \end{cases}$$

for $0 < x < L$ and some constant C.

Proof Combining Theorem 2.1 and [19, Theorem 3.4], one has

$$|u^{(i)}(x)| \le \begin{cases} C & \text{if } i = 0, 1, \\ Cx^{\alpha-i} & \text{if } i = 2, 3, \ldots, q+1. \end{cases}$$

These bounds and the condition $u'(0) = 0$ imply the improved bound

$$|u'(x)| = \left| \int_0^x u''(t)\,dt \right| \le C \int_0^x t^{\alpha-2}\,dt \le Cx^{\alpha-1}.$$

Corollary 2.1 provides derivative estimates that are useful for numerical analysis, and also shows that the solution u of Theorem 2.1 is admissible (i.e., that u' is absolutely continuous on $[0,L]$).

2.4 Comparison principle

In this subsection we discuss a comparison/maximum principle for the problem (2.3). As in the study of comparison principles for classical second-order boundary value problems, we assume from now on that

$$c(x) \ge 0 \quad \text{for } x \in [0,L]. \tag{2.5}$$

Lemma 2.2 (Comparison Principle) *Assume that $v \in C^1[0,L] \cap C^{2,\mu}(0,L]$ for some $\mu \in (-1,0)$, and that v satisfies*

$$-D^{\alpha}_{RLC}v(x) + b(x)v'(x) + c(x)v(x) = g(x) \quad \textit{for } x \in (0,L), \tag{2.6a}$$

$$D^{\alpha-1}_{C}v(0) \le 0, \; v(L) + \beta_1 v'(L) \ge 0, \tag{2.6b}$$

where $g \in C[0,L]$ with $g > 0$ on $[0,L]$. Assume also that (2.5) holds. Then $v(x) \ge 0$ for $x \in [0,L]$.

Proof By contradiction. Suppose that $v(x)$ achieves its absolute minimum at $x = x^* \in [0,L]$ with $v(x^*) < 0$. Clearly $x^* \neq L$, as it would imply $v(L) < 0$ and $v'(L) \leq 0$.

From (2.6a), $b,c,g \in C[0,L]$ and $v \in C^1[0,L]$, clearly $D^\alpha_{RLC}v \in C[0,L]$. One can easily modify the proof of Lemma 2.1 to show that our hypothesis $D^{\alpha-1}_C v(0) \leq 0$ implies that $v'(0) \leq 0$. Suppose $x^* = 0$. Then $v'(0) \geq 0$ and consequently $v'(0) = 0$. Furthermore, $v(0) = v(x^*) < 0$, and we recall that $c \geq 0$, so taking the limit as $x \to 0^+$ in (2.6a) yields $D^\alpha_{RLC}v(0) < 0$. Therefore, there exists $\delta_3 > 0$ such that $D^\alpha_{RLC}v < 0$ on $[0,\delta_3]$. But $D^\alpha_{RLC}v(x) = (d/dx)D^{\alpha-1}_C v(x)$ and $D^{\alpha-1}_C v(0) \leq 0$; it follows that $D^{\alpha-1}_C v(x) < 0$ on $(0,\delta_3]$. Now, invoking [3, Theorem 3.8] and (as in [3]) writing $J^{\alpha-1}$ for the Riemann-Liouville integral operator of order $\alpha - 1$, we get

$$v(\delta_3) - v(0) = J^{\alpha-1}D^{\alpha-1}_C v(\delta_3) < 0,$$

which contradicts our supposition that $v(x)$ has an absolute minimum at $x = 0$.

Thus one must have $x^* \in (0,L)$. As $v \in C^1[0,L] \cap C^{2,\mu}(0,L]$ with $-1 < \mu < 0$, by [19, p.700] one has

$$D^\alpha_C v(x^*) \geq \frac{(x^*)^{-\alpha}}{\Gamma(2-\alpha)}(\alpha-1)[v(0) - v(x^*)] - \frac{(x^*)^{1-\alpha}}{\Gamma(2-\alpha)}v'(0).$$

Hence (1.2) yields

$$D^\alpha_{RLC}v(x^*) \geq \frac{(x^*)^{-\alpha}}{\Gamma(2-\alpha)}(\alpha-1)[v(0) - v(x^*)] \geq 0,$$

by the definition of x^*. But this inequality and (2.5) give

$$(-D^\alpha_{RLC}v + bv' + cv)(x^*) = (-D^\alpha_{RLC}v + cv)(x^*) \leq 0,$$

which contradicts (2.6a).

Remark 2.2 In [14], the problem (2.4) with b constant, $c(x) \equiv 0$ for $x \in [0,L]$ and more general boundary conditions than in (2.4b) is considered. Using the associated Green's function, the authors deduce sufficient conditions that ensure a maximum principle.

Corollary 2.2 *Let* $b,c,f \in C^{q,\mu}(0,L]$ *for some positive integer* q *and some* $\mu \in (-\infty,1)$. *Assume that* (2.5) *holds. Then* (2.3) *has a unique solution* $u \in C^1[0,L]$ *with* $D^\alpha_{RLC}u \in C^{q,\nu}(0,L]$, *where* $\nu := \max\{\mu, 2-\alpha\}$.

Proof From Lemma 2.2 it follows that the problem (2.3) has in $C^1[0,L]$ only the trivial solution $u \equiv 0$ when $f \equiv 0$ and $\gamma_1 = 0$. Thus Theorem 2.1 can now be invoked to give the desired result.

3 Finite difference scheme

We use a uniform mesh on $[0,L]$. Let N be a positive integer. Set $h = L/N$. Set $x_j = jh$ for $j = 0,1,\ldots,N$. Define $\omega^N := \{x_j : j = 1,2,\ldots,N-1\}$ and $\bar{\omega}^N := \{x_j : j = 0,1,\ldots,N\}$.

Our discretisation of (2.3) is: Find $\{U_j\}_{j=0}^N$ such that

$$L_N U_j := -D^+(D_{C,L1}^{\alpha-1} U_j) + b_j D^0 U_j + c_j U_j = f_j \quad \text{for } j = 1,2,\ldots,N-1, \tag{3.1a}$$

$$-D^+ U_0 = 0, \quad U_N + \beta_1 D^+ U_{N-1} = \gamma_1, \tag{3.1b}$$

where $b_j := b(x_j)$ and similarly for c_j and f_j, while $D^+ Z_j := (Z_{j+1} - Z_j)/h$ and $D^0 Z_j := (Z_{j+1} - Z_{j-1})/(2h)$ denote the standard forward difference and central difference quotients.

In the remaining term $D^+(D_{C,L1}^{\alpha-1} U_j)$ in (3.1), $D_{C,L1}^{\alpha-1} U_j$ is the well-known L1 discretization of the Caputo fractional derivative $D_C^{\alpha-1} u(x_j)$, viz.,

$$D_{C,L1}^{\alpha-1} U_j := \frac{1}{\Gamma(2-\alpha)} \int_{t=0}^{x_j} (x-t)^{1-\alpha}\, \bar{U}'(t)\, dt \quad \text{for } x_j > 0 \tag{3.1c}$$

where $\bar{U}(x) := \sum_{k=0}^N \phi_k(x) U_k$ is the linear interpolant of the nodal values $\{(x_j, U_j)\}$, with each ϕ_k the piecewise linear "hat" function associated with the point x_k. A short calculation shows that

$$D_{C,L1}^{\alpha-1} Z_j = \frac{1}{h^{\alpha-1}\Gamma(3-\alpha)} \sum_{k=0}^{j-1} (Z_{k+1} - Z_k) d_{j-k} \quad \text{for } j = 1,2,\ldots,N, \tag{3.2}$$

with $d_k := (2-\alpha) \int_{s=k-1}^{k} s^{1-\alpha}\, ds$ for $k = 1,2,\ldots$. (For later use we also set $d_k = 0$ for $k \le 0$.) Thus,

$$\begin{aligned}
-D^+(D_{C,L1}^{\alpha-1} Z_j) &= \frac{1}{h}\left(D_{C,L1}^{\alpha-1} Z_{j+1} - D_{C,L1}^{\alpha-1} Z_j\right) \\
&= -\frac{1}{h^\alpha \Gamma(3-\alpha)} \left[\sum_{k=0}^{j} (Z_{k+1} - Z_k) d_{j+1-k} - \sum_{k=0}^{j-1} (Z_{k+1} - Z_k) d_{j-k}\right] \\
&= -\frac{1}{h^\alpha \Gamma(3-\alpha)} \left[(Z_1 - Z_0) d_{j+1} + \sum_{k=0}^{j-1} (Z_{k+2} - 2Z_{k+1} + Z_k) d_{j-k}\right] \\
&= -\frac{1}{h^\alpha \Gamma(3-\alpha)} \left[(Z_1 - Z_0) d_{j+1}\right] - D_{C,L2}^{\alpha} Z_j,
\end{aligned}$$

where $D_{C,L2}^{\alpha}$ is the L2 discretization [19, (4.1)] of the Caputo fractional derivative $D_C^\alpha u(x_j)$. Evidently this formula is a discretisation of (1.2).

It is easy to see that the terms d_j in (3.2) satisfy

$$(2-\alpha)(j-1)^{1-\alpha} \le d_j \le (2-\alpha) j^{1-\alpha} \quad \text{and} \quad d_{j-1} > d_j \text{ for } j \ge 2, \tag{3.3}$$

and the proof of [19, Lemma 4.2] shows that for $j = 1,2,\ldots,N-1$ one has $-d_{j-k} + 2d_{j-k+1} - d_{j-k+2} < 0$ for $k = 2,3,\ldots,j-1$ and $k = j+1$.

Analogously to the continuous problem, the finite difference operator (3.1) satisfies a discrete comparison principle. This principle guarantees the existence and uniqueness of the solution of (3.1).

Lemma 3.1 (Discrete Comparison Principle for L_N) *Assume* (2.5) *and that the mesh width h satisfies*

$$h \le \left[\frac{2(d_1 - 2d_2 + d_3)}{\|b\|_\infty \Gamma(3-\alpha)}\right]^{1/(\alpha-1)}. \tag{3.4}$$

Let $\{Z_j\}_{j=0}^N$ *be a mesh function that satisfies* $-D^+Z_0 \ge 0,\ Z_N + \beta_1 D^+ Z_{N-1} \ge 0$ *and* $L_N Z_j \ge 0$ *for* $j = 1,2,\dots,N-1$. *Then* $Z_j \ge 0$ *for* $j = 0,1,\dots,N$.

Proof Let the $(N+1)\times(N+1)$ matrix $A = (a_{jk})_{j,k=0}^N$ be associated with the discretisation (3.1). The entries of the 0^{th} and N^{th} rows of A are, from the boundary conditions (3.1b),

$$a_{00} = 1/h,\ a_{01} = -1/h,\ a_{0k} = 0 \text{ if } 1 < k \le N$$

and

$$a_{Nj} = 0 \ \text{ for } \ 0 \le j < N-1,\ a_{N,N-1} = -\beta_1/h,\ a_{NN} = 1 + \beta_1/h.$$

For $0 < j < N$, the entries of the j^{th} row of A correspond to the difference formula $L_N Z_j$ of (3.1a), viz.,

$$a_{j0} = \frac{d_{j+1} - d_j}{h^\alpha \Gamma(3-\alpha)} - \delta_{j,1}\frac{b_1}{2h}, \tag{3.5a}$$

$$a_{jk} = \frac{-d_{j-k} + 2d_{j-k+1} - d_{j-k+2}}{h^\alpha \Gamma(3-\alpha)} + \frac{b_j}{2h}(\delta_{j,k-1} - \delta_{j,k+1}) + \delta_{j,k}c_j \quad \text{for } k = 1,2,\dots,j+1, \tag{3.5b}$$

$$a_{jk} = 0 \text{ for } k = j+2, j+3, \dots, N, \tag{3.5c}$$

where

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

For the main diagonal entries one has

$$a_{jj} = \frac{2d_1 - d_2}{h^\alpha \Gamma(3-\alpha)} + c_j > 0 \ \text{ for } 0 < j < N.$$

Recalling that $-d_{j-k} + 2d_{j-k+1} - d_{j-k+2} < 0$ for $k \in \{1,2,3,\dots,j-1\}$ and $k = j+1$, we obtain

$$a_{jk} \le 0 \quad \text{if } |j-k| > 1 \text{ and } j = 1,2,\dots,N-1.$$

Using $d_{j+1} < d_j$, we have

$$a_{j0} < 0 \quad \text{ for } j > 1.$$

It remains to discuss the signs of the entries $a_{j,j-1}$ and $a_{j,j+1}$ for $j=1,2,\ldots,N-1$; here we distinguish two cases depending on the sign of b_j. If $b_j \geq 0$, then from (3.5) one has $a_{j,j-1}<0$, and the entries

$$a_{j,j+1} = \frac{-1}{h^\alpha \Gamma(3-\alpha)} + \frac{b_j}{2h} < 0 \quad \text{for } j=1,2,\ldots,N-1,$$

because the assumption (3.4) implies (see [9, Remark 1]) that

$$h < \left[\frac{2}{\|b\|_\infty \Gamma(3-\alpha)}\right]^{1/(\alpha-1)}.$$

If $b_j \leq 0$, then $a_{j,j+1}<0$ for $j=1,2,\ldots,N-1$ from (3.5), and the entries

$$a_{j,j-1} = \frac{-d_1+2d_2-d_3}{h^\alpha \Gamma(3-\alpha)} - \frac{b_j}{2h} \leq 0, \qquad \text{for } j=2,\ldots,N-1,$$

from the hypothesis (3.4). Finally, $a_{10}<0$ because

$$h < \left[\frac{2(d_1-d_2)}{\|b\|_\infty \Gamma(3-\alpha)}\right]^{1/(\alpha-1)},$$

which follows from (3.4) since $d_3<d_2$.

In summary, the matrix A has positive diagonal entries and non-positive off-diagonal entries.

From (3.1) and (3.2), we have

$$\sum_{k=0}^{N} a_{jk} = c_j \geq 0 \text{ for } j=1,2,\ldots,N-1, \ \sum_{k=0}^{N} a_{0k} = 0 \text{ and } \sum_{k=0}^{N} a_{Nk} = 1,$$

and hence the matrix A is diagonally dominant. In addition, if $\beta_1 \neq 0$ the matrix A is irreducible (see for example [21, p.18]). Therefore, the matrix A is irreducibly diagonally dominant [21, p.23] and invoking [21, Corollary 3.20, p.91] one has $A^{-1}>0$. But by hypothesis $A\vec{Z} \geq 0$ where $\vec{Z}=(Z_0,Z_1,\ldots,Z_N)^T$, and the result of the lemma follows. If $\beta_1=0$, one can apply the same argument to the submatrix $\tilde{A}=\{a_{ij}\}_{i,j=0}^{N-1}$ formed by eliminating the last row and last column of A. This submatrix is irreducible and satisfies

$$\sum_{k=0}^{N-1} a_{jk} = c_j \geq 0 \text{ for } j=1,2,\ldots,N-2, \ \sum_{k=0}^{N-1} a_{0k} = 0 \text{ and}$$
$$\sum_{k=0}^{N-1} a_{N-1,k} \geq c_{N-1} - a_{N-1,N} > 0 \qquad \text{as } a_{N-1,N}<0.$$

Thus, $\tilde{A}$ is irreducibly diagonally dominant and therefore $\tilde{A}^{-1}>0$ by [21, Corollary 3.20, p.91]. By hypothesis $Z_N \geq 0$ and we have now that $\tilde{A}(Z_0,Z_1,\ldots,Z_{N-1})^T \geq (0,0,\ldots,0,-a_{N-1,N}Z_N)^T$ with $-a_{N-1,N}Z_N \geq 0$, which completes the proof.

Remark 3.1 The mesh restriction (3.4) can be removed if, instead of the central difference approximation D^0U_j in (3.1a), one approximates the term bu' using upwinding, viz.,

$$b(x_j)u'(x_j) \approx \begin{cases} b_jD^+U_j & \text{if } b(x_j) < 0, \\ b_jD^+U_{j-1} & \text{if } b(x_j) \geq 0. \end{cases}$$

We have used central differencing because, in general, it can be more accurate than upwinding.

We shall also use the following result in our error analysis of the scheme (3.1).

Lemma 3.2 (Discrete Comparison Principle for $D^{\alpha-1}_{C,L1}$) *Let $\{Z_j\}_{j=0}^N$ be a mesh function that satisfies $Z_0 \geq 0$ and $D^{\alpha-1}_{C,L1}Z_j \geq 0$ for $j = 1,2,\dots,N$. Then $Z_j \geq 0$ for $j = 0,1,\dots,N$.*

Proof The discrete operator (3.2) can be written as

$$D^{\alpha-1}_{C,L1}Z_j = \frac{1}{h^{\alpha-1}\Gamma(3-\alpha)}\left(Z_j - d_jZ_0 + \sum_{k=1}^{j-1} Z_k(d_{j+1-k} - d_{j-k})\right) \text{ for } j \geq 1.$$

Hence, the hypothesis $D^{\alpha-1}_{C,L1}Z_j \geq 0$ implies that

$$Z_j \geq d_jZ_0 + \sum_{k=1}^{j-1} Z_k(d_{j-k} - d_{j+1-k}) \text{ for } j = 1,2,\dots,N.$$

Here $d_j > 0$ and $d_{j-k} - d_{j+1-k} > 0$ from (3.3). The result follows using a simple inductive argument.

4 Error analysis

We now prove some error estimates for the scheme (3.1) by a truncation error estimate combined with a stability argument.

4.1 Truncation error

The truncation errors of our discretisation (3.1) of (2.3) are given by

$$\begin{aligned} L_N(u-U)(x_j) &= -D^+D^{\alpha-1}_{C,L1}(u-U)(x_j) + b_jD^0(u-U)(x_j) + c_j(u-U)(x_j) \\ &= -(D^+D^{\alpha-1}_{C,L1} - D^{\alpha}_{RLC})u(x_j) + b_j\left(D^0 - \frac{d}{dx}\right)u(x_j) \text{ for } 0 < x_j < L, \end{aligned}$$

$$-D^+(u-U)(0) = \frac{u(0)-u(h)}{h},$$

$$(u-U)(x_N)+\beta_1 D^+(u-U)(x_{N-1}) = \beta_1\left(\frac{u(x_N)-u(x_{N-1})}{h} - u'(x_N)\right).$$

Our analysis uses two standard interpolation estimates. If $\bar{u}$ is the piecewise linear interpolant of u on $\bar{\omega}^N$ and $x_{j-1} < x < x_j$, then

$$|(u-\bar{u})'(x)| = \frac{1}{h}\left|\int_{s=x_{j-1}}^{x_j}\left(\int_{t=s}^{x} u''(t)\,dt\right)ds\right| \le C\min\{x_j^{\alpha-1}, hx_{j-1}^{\alpha-2}\} \tag{4.1a}$$

and

$$|(u-\bar{u})(x)| = \frac{1}{h}\left|\int_{r=x_{j-1}}^{x}\left(\int_{s=x_{j-1}}^{x_j}\int_{t=s}^{r} u''(t)\,dt\,ds\right)dr\right| \le Chx_j^{\alpha-1}, \tag{4.1b}$$

where we have used $|u''(t)| \le Ct^{\alpha-2}$ from Corollary 2.1. For brevity, we denote the interpolation error by $v := u - \bar{u}$.

Lemma 4.1 *(Truncation error bound) Assume* (2.5) *and that $b, c, f \in C^{q,\mu}(0,L]$ with $q \ge 2$ and $\mu \le 2-\alpha$. Then the truncation errors satisfy*

$$|D^+(u-U)(0)| \le Ch^{\alpha-1}, \quad |(u-U)(x_N) + \beta_1 D^+(u-U)(x_{N-1})| \le C\beta_1 h, \tag{4.2a}$$

$$|L_N(u-U)(x_j)| \le Chx_j^{-1} \text{ for } j = 1,2,\ldots,N. \tag{4.2b}$$

Proof The hypothesis (2.5) ensures (by Corollary 2.2) that (2.3) has a unique solution. Consequently we can invoke the bounds of Corollary 2.1.

Recall that $u'(0) = 0$ by Lemma 2.1. Then (3.1b) and the estimates of Corollary 2.1 yield

$$|D^+(u-U)(0)| = h^{-1}\left|\int_{t=0}^{h}\left(\int_{s=0}^{t} u''(s)\,ds\right)dt\right| \le Ch^{-1}\int_{t=0}^{h}\left(\int_{s=0}^{t} s^{\alpha-2}\,ds\right)dt \le Ch^{\alpha-1}.$$

Consider $x_N = L$. If $\beta_1 = 0$, then $(u-U)(x_N) = 0$. If $\beta_1 > 0$, then we use again the estimates from Corollary 2.1 to deduce that

$$\begin{aligned}|(u-U)(x_N) + \beta_1 D^+(u-U)(x_{N-1})| &= \beta_1\left|\frac{u(x_N)-u(x_{N-1})}{h} - u'(x_N)\right| \\ &\le \frac{\beta_1}{h}\int_{r=x_{N-1}}^{x_N}\left(\int_{s=r}^{x_N}|u''(s)|\,ds\right)dr \\ &\le C\beta_1 hx_{N-1}^{\alpha-2} \\ &\le C\beta_1 h.\end{aligned}$$

Hence, the truncation error bounds (4.2a) have been established.

For $0 < x_j < L$, the truncation error is decomposed into three terms, each of which we estimate separately:

$$\begin{aligned}L_N(u-U)(x_j) &= \left(D^+D_{C,L_1}^{\alpha-1} - \frac{d}{dx}D_C^{\alpha-1}\right)u(x_j) + b_j\left(D^0 - \frac{d}{dx}\right)u(x_j) \\ &= \left(D^+ - \frac{d}{dx}\right)D_C^{\alpha-1}u(x_j) + D^+\left(D_{C,L1}^{\alpha-1} - D_C^{\alpha-1}\right)u(x_j) \\ &\quad + b_j\left(D^0 - \frac{d}{dx}\right)u(x_j).\end{aligned} \tag{4.3}$$

Consider the first term in (4.3). Define $G(x) := D_C^{\alpha-1}u(x)$. Then by Theorem 2.1 one has $G' \in C^{q,2-\alpha}(0,L]$. Thus, $|G''(x)| \le Cx^{\alpha-2}$ and

$$\begin{aligned}\left|\left(D^+ - \frac{d}{dx}\right)G(x_j)\right| &= \left|\frac{1}{h}\int_{t=x_j}^{x_{i+1}}\left(\int_{s=x_j}^{t} G''(s)\,ds\right)dt\right| \\ &\le \frac{C}{h}\int_{t=x_j}^{x_{j+1}}\left(\int_{s=x_j}^{t} s^{\alpha-2}\,ds\right)dt \\ &\le Chx_j^{\alpha-2}. \end{aligned} \tag{4.4}$$

For the second term in (4.3), equations (1.1) and (3.1c) give

$$\begin{aligned}T(x_j) &:= D^+\left(D_{C,L1}^{\alpha-1} - D_C^{\alpha-1}\right)u(x_j) \\ &= \frac{1}{h\Gamma(2-\alpha)}\left(\int_{s=0}^{x_{j+1}}(x_{j+1}-s)^{1-\alpha}v'(s)\,ds - \int_{s=0}^{x_j}(x_j-s)^{1-\alpha}v'(s)\,ds\right)\end{aligned}$$

for $j \ge 1$. At the first interior mesh point, one has

$$\begin{aligned}|T(x_1)| &= \frac{1}{h\Gamma(2-\alpha)}\left|\int_{s=0}^{2h}(2h-s)^{1-\alpha}v'(s)\,ds - \int_{s=0}^{h}(h-s)^{1-\alpha}v'(s)\,ds\right| \\ &= \frac{1}{h\Gamma(2-\alpha)}\left|\int_0^h(2h-s)^{1-\alpha}v'(s)\,ds + \int_{s=0}^{h}(h-s)^{1-\alpha}\big(v'(s+h)-v'(s)\big)\,ds\right| \\ &\le Ch^{-\alpha}\int_{s=0}^{h}|v'(s)|ds + Ch^{-1}\int_{s=0}^{h}(h-s)^{1-\alpha}\left(\int_{t=s}^{s+h}|v''(t)|dt\right)ds \\ &\le C + Ch^{-1}\int_{s=0}^{h}(h-s)^{1-\alpha}\left(\int_{t=s}^{s+h}|u''(t)|dt\right)ds \\ &\le C + Ch^{-1}\int_{s=0}^{h}(h-s)^{1-\alpha}\left(\int_{t=s}^{s+h}t^{\alpha-2}dt\right)ds \\ &\le C + C\int_{s=0}^{h}(h-s)^{1-\alpha}s^{\alpha-2}\,ds,\end{aligned}$$

where we used (4.1a) and Corollary 2.1. The standard bound on Euler's Beta function (see, for example, [3, Theorem D.6]) now gives

$$|T(x_1)| \le C. \tag{4.5}$$

For $j = 2,3,\ldots,N-1$ we split $T(x_j)$ into two parts:

$$\begin{aligned}T(x_j) &= T_L(x_j) + T_R(x_j) \\ &= \frac{1}{h\Gamma(2-\alpha)}\left(\int_{s=0}^{x_{\lceil j/2\rceil+1}}(x_{j+1}-s)^{1-\alpha}v'(s)\,ds - \int_{s=0}^{x_{\lceil j/2\rceil}}(x_j-s)^{1-\alpha}v'(s)\,ds\right) \\ &\quad + \frac{1}{h\Gamma(2-\alpha)}\left(\int_{s=x_{\lceil j/2\rceil+1}}^{x_{j+1}}(x_{j+1}-s)^{1-\alpha}v'(s)\,ds - \int_{s=x_{\lceil j/2\rceil}}^{x_j}(x_j-s)^{1-\alpha}v'(s)\,ds\right).\end{aligned}$$

We use the property $v(x_j)=0$ for all j when integrating by parts below:

$$\begin{aligned}
h\Gamma(2-\alpha)T_L(x_j) &= \int_{s=0}^{x_{\lceil j/2\rceil+1}} (x_{j+1}-s)^{1-\alpha} v'(s)\,ds - \int_{s=0}^{x_{\lceil j/2\rceil}} (x_j-s)^{1-\alpha} v'(s)\,ds \\
&= \int_{s=x_{\lceil j/2\rceil}}^{x_{\lceil j/2\rceil+1}} (x_{j+1}-s)^{1-\alpha} v'(s)\,ds + \int_{s=0}^{x_{\lceil j/2\rceil}} \Big((x_{j+1}-s)^{1-\alpha} - (x_j-s)^{1-\alpha}\Big) v'(s)\,ds \\
&= \int_{s=x_{\lceil j/2\rceil}}^{x_{\lceil j/2\rceil+1}} (x_{j+1}-s)^{1-\alpha} v'(s)\,ds + (1-\alpha)\int_{s=0}^{x_{\lceil j/2\rceil}} \Big((x_{j+1}-s)^{-\alpha} - (x_j-s)^{-\alpha}\Big) v(s)\,ds \\
&= \int_{s=x_{\lceil j/2\rceil}}^{x_{\lceil j/2\rceil+1}} (x_{j+1}-s)^{1-\alpha} v'(s)\,ds + (\alpha-1)\alpha\int_{s=0}^{x_{\lceil j/2\rceil}} \Big(\int_{t=x_j-s}^{x_{j+1}-s} t^{-1-\alpha}\,dt\Big) v(s)\,ds.
\end{aligned}$$

By the interpolation bound (4.1), one gets

$$\begin{aligned}
h|T_L(x_j)| &\le C x_{\lceil j/2\rceil}^{1-\alpha} \int_{s=x_{\lceil j/2\rceil}}^{x_{\lceil j/2\rceil+1}} |v'(s)|\,ds + Ch\int_{s=0}^{x_{\lceil j/2\rceil}} (x_j-s)^{-1-\alpha}|v(s)|\,ds \\
&\le Ch^2 x_{\lceil j/2\rceil}^{1-\alpha} x_{\lceil j/2\rceil}^{\alpha-2} + Ch^2 x_{\lceil j/2\rceil}^{\alpha-1}\int_{s=0}^{x_{\lceil j/2\rceil}} (x_j-s)^{-1-\alpha}\,ds \\
&\le Ch^2 x_{\lceil j/2\rceil}^{-1} + Ch^2 x_{\lceil j/2\rceil}^{-1} \\
&\le Ch^2 x_j^{-1}.
\end{aligned}$$

Thus,

$$|T_L(x_j)| \le Chx_j^{-1} \quad \text{for } j\ge 2. \tag{4.6}$$

Next, for $s\in[x_{k-1},x_k]$ with $k>\lceil j/2\rceil$, we have

$$\begin{aligned}
v'(s+h)-v'(s) &= u'(s+h)-u'(s) - \frac{1}{h}\left(\int_{t=x_k}^{x_{k+1}} u'(t)\,dt - \int_{t=x_{k-1}}^{x_k} u'(t)\,dt\right) \\
&= \frac{1}{h}\int_{t=x_{k-1}}^{x_k} \big[u'(s+h)-u'(s)-(u'(t+h)-u'(t))\big]\,dt \\
&= \frac{1}{h}\int_{t=x_{k-1}}^{x_k}\int_{r=t}^{s} \big[u''(r+h)-u''(r)\big]\,dr\,dt \\
&= \frac{1}{h}\int_{t=x_{k-1}}^{x_k}\int_{r=t}^{s}\int_{w=r}^{r+h} u'''(w)\,dw\,dr\,dt;
\end{aligned}$$

consequently

$$|v'(s+h)-v'(s)| \le Ch^2 \max_{x_{k-1}\le x\le x_{k+1}} |u'''(x)| \le Ch^2 x_{k-1}^{\alpha-3} \quad \text{for } s\in[x_{k-1},x_k].$$

Substituting this bound into

$$T_R(x_j) = Ch^{-1}\int_{s=x_{\lceil j/2\rceil}}^{x_j} (x_j-s)^{1-\alpha}\Big(v'(s+h)-v'(s)\Big)\,ds$$

gives

$$|T_R(x_j)| \le Chx_j^{2-\alpha}x_j^{\alpha-3} = Chx_j^{-1}. \tag{4.7}$$

Finally, consider the third term in (4.3). If $j = 1$, then from Corollary 2.1 one has

$$\begin{aligned} |D^0 u(h) - u'(h)| &= \frac{1}{2h} \left| \int_{s=0}^{2h} \left(\int_{t=h}^{s} u''(t)\, dt \right) ds \right| \\ &\le Ch^{-1} \int_{s=0}^{2h} \left(\int_{t=0}^{2h} t^{\alpha-2}\, dt \right) ds \\ &\le Ch^{\alpha-1}. \end{aligned} \tag{4.8}$$

If $j \ge 2$, then using again Corollary 2.1 and $x_j \le 2x_{j-1}$, we obtain

$$\begin{aligned} |D^0 u(x_j) - u'(x_j)| &= \frac{1}{2h} \left| \int_{s=x_{j-1}}^{x_{j+1}} \left(\int_{t=x_j}^{s} u''(t)\, dt \right) ds \right| \\ &\le Ch^{-1} \int_{s=x_{j-1}}^{x_{j+1}} \left(\int_{t=x_{j-1}}^{x_{j+1}} t^{\alpha-2}\, dt \right) ds \\ &\le Chx_{j-1}^{\alpha-2} \\ &\le Chx_j^{\alpha-2}. \end{aligned} \tag{4.9}$$

The bound (4.2b) now follows from (4.3)–(4.9).

4.2 Discrete barrier functions

We use the discrete comparison principle of Lemma 3.1 to deduce appropriate error estimates for the scheme (3.1). More specifically, we shall define a grid function $\{\Psi_j\}_{j=0}^N$ (called a *discrete barrier function*) such that

$$\begin{aligned} |-D^+(U-u)(x_0)| &\le -D^+\Psi_0, \\ |L_N(U-u)(x_j)| &\le L_N\Psi_j \ \text{ for } j = 1,2,\ldots,N-1, \end{aligned}$$

and

$$|(u-U)(x_N) + \beta_1 D^+(u-U)(x_{N-1})| \le \Psi_N + \beta_1 D^+\Psi_{N-1}.$$

Then $|(U-u)(x_j)| \le \Psi_j$ for $j = 0,1,\ldots,N$ by Lemma 3.1.

The following technical result is very useful for constructing barrier functions.

Lemma 4.2 *If a grid function $\{B_j\}_{j=0}^N$ satisfies $B_0 = 0$ and $B_j \le B_k$ for $j \le k$, then*

$$D_{C,L1}^{\alpha-1} B_j \ge \frac{B_j}{x_j^{\alpha-1}\Gamma(2-\alpha)} \ \textit{ for } j = 1,2,\ldots,N-1.$$

Proof Using (3.2), (3.3) and the hypotheses on $\{B_j\}$, one gets

$$\begin{aligned} D^{\alpha-1}_{C,L1}B_j &= \frac{1}{h^{\alpha-1}\Gamma(3-\alpha)}\sum_{k=0}^{j-1}(B_{k+1}-B_k)d_{j-k} \\ &\geq \frac{d_j}{h^{\alpha-1}\Gamma(3-\alpha)}\sum_{k=0}^{j-1}(B_{k+1}-B_k) \\ &= \frac{d_j}{h^{\alpha-1}\Gamma(3-\alpha)}(B_j-B_0) \\ &\geq \frac{1}{x_j^{\alpha-1}\Gamma(2-\alpha)}B_j. \end{aligned}$$

Remark 4.1 An alternative proof of Lemma 4.2 follows from [8, Lemma 5] by replacing the piecewise power basis functions (which generate the fitted scheme of that paper) by the standard piecewise-linear hat functions (which generate the L1 scheme).

We now define a grid function $\{M_j\}_{j=0}^N$ that will be central in the construction of our discrete barrier functions. Some properties for $\{M_j\}_{j=0}^N$ are also given that we shall use later.

This discrete function is defined by

$$D^{\alpha-1}_{C,L1}M_j = \frac{1}{\Gamma(2-\alpha)}x_j^{|\ln h|^{-1}}, \quad j\geq 1, \quad M_0=0. \tag{4.10}$$

From Lemma 3.2, this function satisfies $M_j \geq 0$ for all j. We explicitly determine M_1 as it is required later. From (4.10) with $j=1$, one has

$$D^{\alpha-1}_{C,L1}M_1 = \frac{M_1-M_0}{h^{\alpha-1}\Gamma(3-\alpha)} = \frac{1}{\Gamma(2-\alpha)}h^{|\ln h|^{-1}} = \frac{e^{-1}}{\Gamma(2-\alpha)}.$$

Hence,

$$M_1 = (2-\alpha)e^{-1}h^{\alpha-1}. \tag{4.11}$$

We prove now that M_j is a non-decreasing function. Noting that

$$\begin{aligned} 0 &\leq \frac{x_{j+1}^{|\ln h|^{-1}} - x_j^{|\ln h|^{-1}}}{\Gamma(2-\alpha)} \\ &= \frac{1}{h^{\alpha-1}\Gamma(3-\alpha)}\left(\sum_{k=0}^{j}(M_{k+1}-M_k)d_{j+1-k} - \sum_{k=0}^{j-1}(M_{k+1}-M_k)d_{j-k}\right), \end{aligned}$$

we obtain

$$\sum_{k=0}^{j-1}(M_{k+1}-M_k)(d_{j-k}-d_{j+1-k}) \leq (M_{j+1}-M_j),$$

with $M_1-M_0=(2-\alpha)e^{-1}h^{\alpha-1}\geq 0$. Using (3.3), a simple inductive argument yields

$$M_{j+1}-M_j \geq 0, \quad \text{for } 0\leq j<N.$$

We also give an upper bound for M_j. Define

$$B_j = x_j^{|\ln h|^{-1}+\alpha-1}, \quad 0 \le j \le N.$$

It is an increasing function with $B_0 = 0$. From Lemma 4.2, one has

$$D_{C,L1}^{\alpha-1} B_j \ge \frac{1}{\Gamma(2-\alpha)} \frac{B_j}{x_j^{\alpha-1}} = \frac{1}{\Gamma(2-\alpha)} x_j^{|\ln h|^{-1}}. \tag{4.12}$$

Comparing (4.10) and (4.12), we deduce that B_j is a barrier function for M_j, i.e.,

$$0 \le M_j \le B_j = x_j^{|\ln h|^{-1}+\alpha-1}, \quad 0 \le j \le N. \tag{4.13}$$

4.3 Convergence of the scheme

In this section we establish an error estimate for our scheme. In the proof, we distinguish between the two cases of a Dirichlet boundary condition when $\beta_1 = 0$ and the case where $\beta_1 > 0$ in the right boundary condition $u(L) + \beta_1 u'(L) = \gamma_1$ of problem (2.3). In each case an appropriate barrier function will be defined in terms of (4.10). Difficulties in the construction of a suitable barrier arise if $b > 0$, which emanate primarily from the non-decreasing character of the grid function (4.10). For this reason, in order to establish an error bound we shall assume that $b(x) \le 0$ for $x \in [0, L]$. The general case (without any sign restriction on b) requires further investigation and it will be investigated in a future paper.

Theorem 4.1 *Assume that the hypotheses of Lemmas 3.1 and 4.1 are satisfied. Assume also that $b(x) \le 0$ for $x \in [0, L]$. Then there exists a constant C such that*

$$|u(x_j) - U_j| \le Ch|\ln h|, \quad 0 \le j \le N.$$

Proof The proof involves two cases: $\beta_1 = 0$ and $\beta_1 > 0$. In the first case, define the discrete function

$$\Psi_j = C_1 h|\ln h|(L^{|\ln h|^{-1}+\alpha-1} - M_j), \quad 0 \le j \le N, \tag{4.14}$$

where M_j is defined in (4.10). We want to prove that $|u(x_j) - U_j| \le \Psi_j$. Observe that $\Psi_j \ge 0$ for all j by (4.13). In particular, $|u(x_N) - U_N| = 0 \le \Psi_N$. At the endpoint $x = 0$, from (4.11),

$$-D^+\Psi_0 = -C_1 h|\ln h| \frac{(M_1 - M_0)}{h} = -C_1(2-\alpha)e^{-1}h^{\alpha-1}|\ln h|.$$

If $0 < x_j < L$, using $c \geq 0$ and $b \leq 0$ on $[0,L]$, $\Psi_j \geq 0$ and M_j an increasing function so $D^0 M_j \geq 0$, we have

$$\begin{aligned}
L_N \Psi_j &= -D^+ D^{\alpha-1}_{C,L1} \Psi_j + b_j D^0 \Psi_j + c_j \Psi_j \\
&\geq C_1 h|\ln h| D^+ D^{\alpha-1}_{C,L1} M_j - C_1 h|\ln h| b_j D^0 M_j \\
&\geq \frac{C_1 h|\ln h|}{\Gamma(2-\alpha)} D^+ x_j^{|\ln h|^{-1}} \quad \text{by (4.10)} \\
&\geq \frac{C_1 h}{\Gamma(2-\alpha)} x_{j+1}^{|\ln h|^{-1}-1} \quad \text{by the mean value theorem} \\
&\geq \frac{C_1 h e^{-1}}{\Gamma(2-\alpha)} x_{j+1}^{-1} \quad \text{as } x_{j+1} \geq h \text{ and } h^{|\ln h|^{-1}} = e^{-1}, \\
&\geq \frac{C_1 h e^{-1}}{2\Gamma(2-\alpha)} x_j^{-1} \quad \text{as } x_{j+1} \leq 2x_j.
\end{aligned}$$

Thus, Ψ_j is a barrier function for the error $|u(x_j) - U_j|$ and the result follows from Lemma 3.1. This completes the case $\beta_1 = 0$.

When $\beta_1 > 0$, note that

$$\begin{aligned}
\Psi_N + \beta_1 D^+ \Psi_{N-1} &= C_1 h|\ln h| \left(L^{|\ln h|^{-1}+\alpha-1} - M_N\right) + C_1 \beta_1 |\ln h| (M_{N-1} - M_N) \\
&\geq C_1 \beta_1 |\ln h| (M_{N-1} - M_N),
\end{aligned}$$

and $M_{N-1} - M_N \leq 0$. From [7, Theorem 4], we have

$$M_{N-1} - M_N = (L-h)^{|\ln h|^{-1}+\alpha-1} - L^{|\ln h|^{-1}+\alpha-1} \pm Ch \geq -C_2 h.$$

Therefore,

$$\Psi_N + \beta_1 D^+ \Psi_{N-1} \geq -C_1 C_2 \beta_1 h |\ln h|. \tag{4.15}$$

Hence, to deal with the case $\beta_1 > 0$ we require a modification to the barrier function.

Consider the discrete function

$$\widetilde{\Psi}_j = \Psi_j + \Phi_j$$

where Ψ_j is defined in (4.14) and

$$\Phi_j = C_3 h|\ln h| \times \begin{cases} \frac{h}{\beta_1} + 2, & \text{if } 0 \leq j \leq N-1, \\ 2, & \text{if } j = N. \end{cases}$$

Note that at $x = 0$

$$-D^+ \widetilde{\Psi}_0 = -D^+ \Psi_0 - D^+ \Phi_0 = -D^+ \Psi_0 = -C_1 (2-\alpha) e^{-1} h^{\alpha-1} |\ln h|.$$

In addition, the discrete function Φ_j also satisfies

$$D^{\alpha-1}_{C,L1} \Phi_j = 0, \quad \text{for } 1 \leq j \leq N-1, \quad D^+ (D^{\alpha-1}_{C,L1} \Phi_j) = 0, \quad \text{for } 1 \leq j \leq N-2.$$

Thus,

$$L^N\widetilde{\Psi}_j = L^N\Psi_j + L^N\Phi_j = L^N\Psi_j + c_j\Phi_j \geq L^N\Psi_j \geq \frac{C_1 he^{-1}}{2\Gamma(2-\alpha)}x_j^{-1}, \quad \text{for } 1 \leq j \leq N-2.$$

We now analyse $L^N\Phi_{N-1}$. Note that

$$\begin{aligned} D_{C,L1}^{\alpha-1}\Phi_N &= \frac{1}{h^{\alpha-1}\Gamma(3-\alpha)}\sum_{k=0}^{N-1}(\Phi_{k+1}-\Phi_k)d_{N-k} \\ &= \frac{\Phi_N - \Phi_{N-1}}{h^{\alpha-1}\Gamma(3-\alpha)} \\ &= -\frac{C_3 h^{3-\alpha}|\ln h|}{\beta_1\Gamma(3-\alpha)} \\ &\leq 0. \end{aligned}$$

Thus, $-D^+D_{C,L1}^{\alpha-1}\Phi_{N-1} \geq 0$. Using $b \leq 0$, we then have

$$\begin{aligned} L^N\widetilde{\Psi}_{N-1} &= L^N\Psi_{N-1} + L^N\Phi_{N-1} \\ &\geq L^N\Psi_{N-1} + b_{N-1}\frac{\Phi_N - \Phi_{N-2}}{2h} \\ &= L^N\Psi_{N-1} - \frac{C_3 b_{N-1} h|\ln h|}{2\beta_1} \\ &\geq L^N\Psi_{N-1} \\ &\geq \frac{C_1 he^{-1}}{2\Gamma(2-\alpha)}x_{N-1}^{-1}. \end{aligned}$$

Finally, from (4.15), at $x = L$ one has

$$\begin{aligned} \widetilde{\Psi}_N + \beta_1 D^+\widetilde{\Psi}_{N-1} &= \big(\Psi_N + \beta_1 D^+\Psi_{N-1}\big) + \big(\Phi_N + \beta_1 D^+\Phi_{N-1}\big) \\ &\geq (C_3 - C_1C_2\beta_1)h|\ln h|. \end{aligned}$$

Choosing C_3 sufficiently large so that $C_3 - C_1C_2\beta_1 > C$, then $\widetilde{\Psi}_N + \beta_1 D^+\widetilde{\Psi}_{N-1} \geq Ch|\ln h|$. Therefore, $\widetilde{\Psi}_j$ is a barrier function and the result follows for the case $\beta_1 > 0$.

5 Numerical experiments

In this section numerical results for two examples are given. The coefficients of the first example are constant and the exact solution can be obtained using Laplace transforms. The solution of the second example is unknown and the orders of convergence are estimated using the two-mesh principle [6]. The computed orders of convergence in both examples corroborate the convergence of our scheme for all the values of α considered.

Example 5.1 In this problem b and f are constants. Consider

$$-D_{RLC}^{\alpha}u - 0.5u' = 1 \text{ on } (0,1), \quad D^{\alpha-1}u(0) = 0, \; u(1) = 0.$$

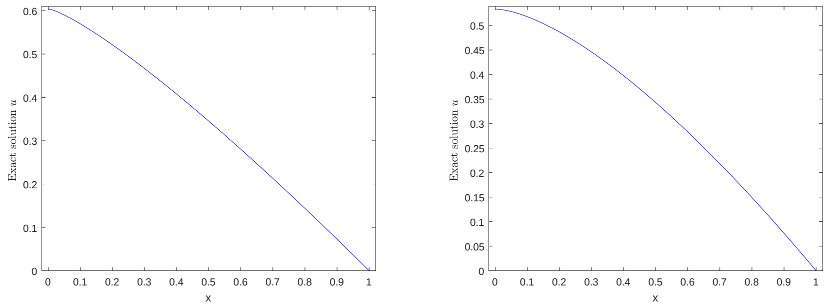
The exact solution can be obtained in closed form (see Appendix). The maximum error in the computed solution $\{U_j\}$ is denoted by

$$E_N := \max_{0 \le j \le N} |U_j - u(x_j)|.$$

The orders of convergence are computed from these values in a standard way:

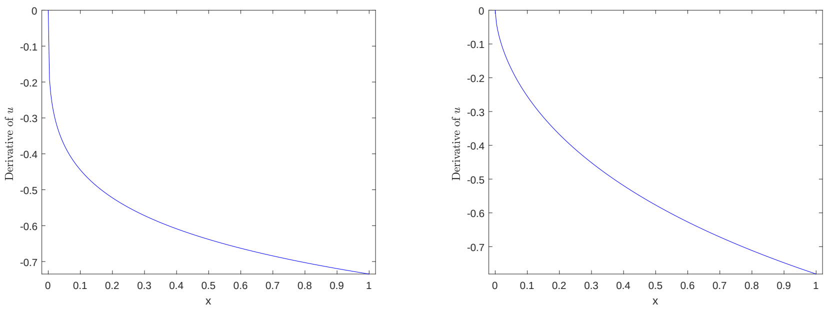
$$p_N := \log_2 \left(\frac{E_N}{E_{2N}} \right).$$

The exact solution u of Example 5.1 and its derivative u' are displayed for $N = 256$ and $\alpha = 1.3, 1.6$ in Figures 5.1 and 5.2, respectively. In Figure 5.2 we see that u'' blows up at $x = 0$.



(a) $\alpha = 1.3$ (b) $\alpha = 1.6$

Fig. 5.1 Example 5.1: Exact solution for $\alpha = 1.3, 1.6$



(a) $\alpha = 1.3$ (b) $\alpha = 1.6$

Fig. 5.2 Example 5.1: Derivative of u for $\alpha = 1.3, 1.6$

The numerical results in Table 5.1 indicate that the method is first-order convergent for all values of α, which is slightly better than the almost first-order convergence (due to the logarithmic factor) proved in Theorem 4.1.

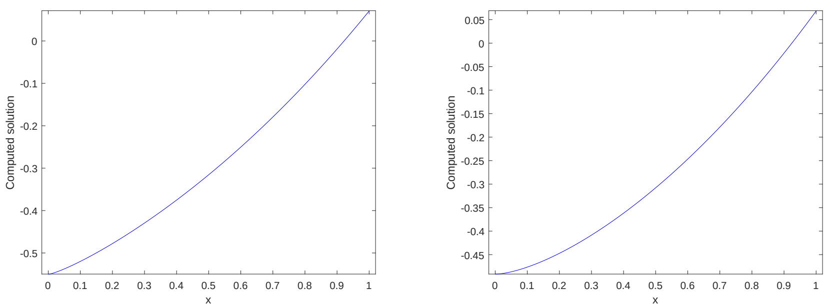
Table 5.1 Example 5.1: Maximum errors E_N and orders of convergence p_N

	N=64	N=128	N=256	N=512	N=1024	N=2048
$\alpha = 1.1$	8.946E-03 1.000	4.473E-03 1.000	2.237E-03 1.000	1.118E-03 1.000	5.592E-04 1.000	2.796E-04
$\alpha = 1.2$	9.207E-03 0.999	4.605E-03 1.000	2.303E-03 1.000	1.152E-03 1.000	5.759E-04 1.000	2.880E-04
$\alpha = 1.3$	9.457E-03 0.998	4.734E-03 0.999	2.368E-03 0.999	1.185E-03 1.000	5.925E-04 1.000	2.963E-04
$\alpha = 1.4$	9.681E-03 0.997	4.852E-03 0.998	2.430E-03 0.998	1.216E-03 0.999	6.085E-04 0.999	3.044E-04
$\alpha = 1.5$	9.848E-03 0.993	4.948E-03 0.995	2.482E-03 0.997	1.244E-03 0.998	6.231E-04 0.998	3.119E-04
$\alpha = 1.6$	9.902E-03 0.987	4.994E-03 0.991	2.513E-03 0.993	1.263E-03 0.995	6.338E-04 0.996	3.178E-04
$\alpha = 1.7$	9.748E-03 0.980	4.943E-03 0.984	2.500E-03 0.987	1.261E-03 0.989	6.353E-04 0.991	3.195E-04
$\alpha = 1.8$	9.236E-03 0.971	4.711E-03 0.975	2.396E-03 0.979	1.216E-03 0.982	6.156E-04 0.984	3.111E-04
$\alpha = 1.9$	8.142E-03 0.969	4.160E-03 0.971	2.122E-03 0.974	1.080E-03 0.976	5.493E-04 0.978	2.789E-04

Example 5.2 Consider the following variable-coefficient problem:

$$-D^{\alpha}_{RLC}u - (1+x^2)u' + xu = -e^x \text{ for } x \in (0,1),$$
$$D^{\alpha-1}u(0) = 0, \quad u(1) + u'(1) = 1.$$

The solution of Example 5.2 that is computed by our scheme for $N = 256$ and $\alpha = 1.3, 1.6$ is shown in Figure 5.3.



(a) $\alpha = 1.3$ (b) $\alpha = 1.6$

Fig. 5.3 Example 5.2: Computed solution for $N = 256$ and $\alpha = 1.3, 1.6$

The exact solution of Example 5.2 is unknown and the orders of convergence are estimated using the two-mesh principle [6]. That is, solutions $\{U_j\}_{j=0}^{N}$ and $\{\hat{U}_j\}_{j=0}^{2N}$ are computed by the scheme (3.1) on two uniform meshes $\{x_j\}_{j=0}^{N}$ and $\{\hat{x}_j\}_{j=0}^{2N}$ respectively. Observe that $x_j = \hat{x}_{2j}$ for $j = 0, 1, \ldots, N$. These computed solutions are used to calculate the two-mesh differences

$$D_N := \max_{0\le j\le N} |U_j - \hat{U}_{2j}|,$$

and the orders of convergence are estimated by

$$q_N := \log_2 \left(\frac{D_N}{D_{2N}} \right).$$

The numerical results for Example 5.2 are given in Table 5.2 and, similarly to Example 5.1, first-order convergence of the method is apparent.

Table 5.2 Example 5.2: Maximum two-mesh differences D_N and orders of convergence q_N

	N=64	N=128	N=256	N=512	N=1024	N=2048
$\alpha = 1.1$	5.718E-03 1.003	2.853E-03 1.001	1.425E-03 1.001	7.123E-04 1.000	3.560E-04 1.000	1.780E-04
$\alpha = 1.2$	5.859E-03 1.002	2.925E-03 1.001	1.462E-03 1.000	7.306E-04 1.000	3.653E-04 1.000	1.826E-04
$\alpha = 1.3$	6.003E-03 1.001	3.000E-03 1.000	1.500E-03 1.000	7.502E-04 1.000	3.752E-04 1.000	1.876E-04
$\alpha = 1.4$	6.146E-03 0.999	3.076E-03 0.998	1.540E-03 0.999	7.707E-04 0.999	3.856E-04 0.999	1.929E-04
$\alpha = 1.5$	6.277E-03 0.995	3.149E-03 0.996	1.579E-03 0.996	7.915E-04 0.997	3.965E-04 0.998	1.985E-04
$\alpha = 1.6$	6.381E-03 0.991	3.210E-03 0.992	1.614E-03 0.993	8.110E-04 0.994	4.071E-04 0.996	2.041E-04
$\alpha = 1.7$	6.429E-03 0.986	3.246E-03 0.987	1.638E-03 0.989	8.254E-04 0.990	4.155E-04 0.992	2.089E-04
$\alpha = 1.8$	6.366E-03 0.982	3.223E-03 0.982	1.632E-03 0.983	8.255E-04 0.985	4.170E-04 0.987	2.104E-04
$\alpha = 1.9$	6.090E-03 0.983	3.080E-03 0.982	1.560E-03 0.982	7.899E-04 0.982	3.998E-04 0.983	2.022E-04

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Appendix: Constant coefficient problem

We use Laplace transforms to derive the general solution of the differential equation

$$-D^{\alpha}_{RLC}w + bw' = f \quad \text{on } (0,L), \tag{5.1}$$

where b and f are nonzero constants. The Laplace transform of the Caputo fractional derivative is given by [18, (2.253)]

$$\mathscr{L}\{D^{\alpha-1}_{C}w\} = s^{\alpha-1}\mathscr{L}(w) - s^{\alpha-2}w(0), \quad 1 < \alpha \le 2.$$

Hence, using the well-known property $\mathscr{L}(f'(s)) = s\mathscr{L}(f(s)) - f(0^+)$, one obtains

$$\mathscr{L}\{D^{\alpha}_{RLC}w\} = s\left[s^{\alpha-1}\mathscr{L}(w) - s^{\alpha-2}w(0)\right] - D^{\alpha-1}_{C}w(0).$$

Thus, applying a Laplace transform to (5.1), we obtain

$$-s\left[s^{\alpha-1}\mathscr{L}(w) - s^{\alpha-2}w(0)\right] + D^{\alpha-1}_{C}w(0) + b\left(s\mathscr{L}(w) - w(0)\right) = \frac{f}{s}, \tag{5.2}$$

which gives

$$\mathscr{L}(w) = -\frac{f}{s^2(s^{\alpha-1}-b)} + \frac{D^{\alpha-1}_{C}w(0)}{s(s^{\alpha-1}-b)} + \frac{w(0)}{s}.$$

The two-parameter Mittag-Leffler function is defined by

$$E_{\delta,\gamma}(z) = \frac{1}{\Gamma(\gamma)} + \sum_{k=1}^{\infty}\frac{z^k}{\Gamma(\delta k+\gamma)} \qquad \text{for } \delta,\gamma,z \in \mathbb{R} \text{ with } \delta > 0,$$

From [18, (1.80),(1.82)], one has

$$\mathscr{L}\left\{x^{\gamma-1}E_{\delta,\gamma}(\pm bx^{\delta})\right\} = \frac{s^{\delta-\gamma}}{s^{\delta}\mp b}. \tag{5.3}$$

Therefore, from (5.2) and (5.3), we obtain

$$w(x) = -f x^{\alpha}E_{\alpha-1,\alpha+1}(bx^{\alpha-1}) + D^{\alpha-1}_{C}w(0)x^{\alpha-1}E_{\alpha-1,\alpha}(bx^{\alpha-1}) + w(0). \tag{5.4}$$

Thus, near $x = 0$ the solution of (5.1) behaves like x^{α} if $D^{\alpha-1}_{C}w(0) = 0$ and like $x^{\alpha-1}$ otherwise.

Remark 5.1 (Reaction-diffusion problem) The general solution of the differential equation

$$-D^{\alpha}_{RLC} v + cv = f,\ x \in (0,L), \tag{5.5}$$

with nonzero constants c and f can also be obtained using Laplace transforms. Here

$$-s\left[s^{\alpha-1}\mathscr{L}(v) - s^{\alpha-2}v(0)\right] + D^{\alpha-1}_{C} v(0) + c\mathscr{L}(v) = \frac{f}{s}\,,$$

so

$$\mathscr{L}(v) = -\frac{f}{s(s^{\alpha}-c)} + \frac{D^{\alpha-1}_{C} v(0)}{(s^{\alpha}-c)} + \frac{s^{\alpha-1}v(0)}{s^{\alpha}-c}\,.$$

Invoking (5.3), one gets

$$v(x) = -f\,x^{\alpha}E_{\alpha,1+\alpha}(cx^{\alpha}) + D^{\alpha-1}_{C} v(0)\,x^{\alpha-1}E_{\alpha,\alpha}(cx^{\alpha}) + v(0)E_{\alpha,1}(cx^{\alpha}).$$

Near $x = 0$ this solution behaves similarly to $w(x)$ in (5.4); it again depends on whether $D^{\alpha-1}_{C} v(0) = 0$.