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Equivalent definitions of Caputo derivatives and applications to subdiffusion equations

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Abstract. An equivalent definition of the fractional Caputo derivative $\mathbf{D}_t^\nu g$, for $\nu \in (0,1)$, is found, within suitable assumptions on g. Some applications to the fractional calculus and to the theory of fractional partial differential equations are then discussed. In particular, this alternative definition is used to prove the maximum principle for the classical solutions to the linear subdiffusion equation subject to nonhomogeneous boundary conditions. This approach also allows to construct numerical solutions to the initial-boundary value problem for the subdiffusion equation with memory.

Contents

1. Introduction

Fractional calculus is a widespread branch of modern Mathematics that has attracted the interest of several people from different areas, like Physics, Engineering,

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Life and Social Sciences (see e.g. [**4, 12, 13, 15, 24, 25, 26**] and references therein). Various types of fractional derivatives have been introduced and studied, the best known of which are named after Riemann-Liuoville, Caputo, Hadamard, Marchaud, Grünvald-Letnikov and Riesz. We refer to [**11, 15, 26**] for their definitions and related properties. The key feature of fractional derivatives is their effectiveness in the description of memory or delay phenomena, which are structurally present in real-life models. This leads in a natural way to the study of fractional differential equations (FDEs).

In this paper, we focus on the (left) Caputo fractional derivative of order $\nu \in (0,1)$, defined as (see (2.4.1) in [**15**])

$$\mathbf{D}_t^\nu g(t) = \frac{1}{\Gamma(1-\nu)} \frac{d}{dt} \int_0^t \frac{g(\tau) - g(0)}{(t-\tau)^\nu} d\tau, \tag{1.1}$$

Γ being the Euler Gamma-function. In the limit cases $\nu \downarrow 0$ and $\nu \uparrow 1$, the Caputo fractional derivatives of g boil down to $(g(t) - g(0))$ and $g'(t)$, respectively. Whenever g is differentiable, it is easily verified that $\mathbf{D}_t^\nu g(t)$ can be given by the equivalent definition (see [**26**, Sec.13])

$$\mathbf{D}_t^\nu g(t) = \frac{1}{\Gamma(1-\nu)} \frac{g(t) - g(0)}{t^\nu} + \frac{\nu}{\Gamma(1-\nu)} \int_0^t \frac{g(t) - g(\tau)}{(t-\tau)^{\nu+1}} d\tau. \tag{1.2}$$

Actually, as we will see later, (1.2) turns out to be more convenient for certain type of calculations. However, the function g involved, typically, does not possess enough regularity to pass from (1.1) to (1.2). In this respect, the first achievement of this work is showing the equivalence of the two formulations within the milder assumption that both the function g and its Caputo fractional derivative $\mathbf{D}_t^\nu g$, in the sense of (1.1), belong to the Hölder classes $\mathcal{C}^\beta([0,T])$, for some fixed $\beta \in (0,1)$. After that, we discuss the consequences of the obtained equivalence in the fractional calculus as well as in the qualitative analysis of FDEs (with particular reference to the maximum principle for classical solutions), and, last but not least, in the numerical study of initial-boundary value problems for FDEs.

In connection with the fractional calculus, taking into account (1.2), we are able to obtain some useful properties of the Caputo fractional derivative, such as the fractional differentiation of a product, and an integration by parts formula. It is worth noting that an integration by parts formula, but containing both the left and the right fractional derivatives, has been previously devised in [**3, 26, 15**] (see also the references therein). Here, under suitable (albeit reasonably mild) assumptions, we give a representation in terms of one-side derivatives only (either left or right). Coming to the Leibniz rule for fractional derivatives, this is an issue already analyzed for the Riemann-Liouville fractional derivative $\partial_t^\nu(g_1 g_2)$ of order $\nu \in (0,1)$ in [**1**], where the authors require that at least one between g_1 and g_2 belongs to $\mathcal{C}^\beta([0,T])$ with $\beta > \nu$. In our case, the restriction $\beta > \nu$ is removed.

Another important application of (1.2), as anticipated above, concerns with the proof of the maximum principle for the classical solutions of the initial-boundary value problems for the subdiffusion equations. More precisely, given a bounded domain $\Omega \subset \mathbb{R}^n$ with smooth boundary $\partial\Omega$, and given an arbitrarily fixed time $T > 0$, we denote

$$\Omega_T = \Omega \times (0,T) \qquad \text{and} \qquad \partial\Omega_T = \partial\Omega \times [0,T].$$

For a fixed $\nu \in (0,1)$, we consider the subdiffusion equation in the unknown $u = u(x,t) : \Omega_T \to \mathbb{R}$

$$\mathbf{D}_t^\nu u - \sum_{ij=1}^{n} a_{ij}(x,t)\frac{\partial^2 u}{\partial x_i \partial x_j} - \sum_{i=1}^{n} a_i(x,t)\frac{\partial u}{\partial x_i} + a_0(x,t)u = f(x,t), \tag{1.3}$$

supplemented with the initial condition

$$u(x,0) = u_0(x) \quad \text{in } \bar{\Omega}, \tag{1.4}$$

and subject to the Neumann boundary condition

$$\sum_{i=1}^{n} b_i(x,t)\frac{\partial u}{\partial x_i} + b_0(x,t)u = \psi(x,t) \quad \text{on } \partial\Omega_T, \tag{1.5}$$

where the functions a_{ij}, a_i, b_i ψ, u_0, f are prescribed. There are a lot of papers in the current literature devoted to study of the maximum principle for equations like (1.3) with Caputo or Riemann-Liouville derivatives (see e.g. [**1, 2, 5, 8, 17, 18, 20, 21, 22, 23**] and references therein). In particular, [**22, 23**] provide a detailed survey of the state of the art. The common assumption in the above-mentioned papers (with the exception of [**17, 18**]) is the existence, at least in a weak sense, of $\frac{\partial u}{\partial t}$. In more precise term, the assumption reads

$$u \in \mathcal{C}^1((0,T]) \qquad \text{and} \qquad \frac{\partial u}{\partial t} \in L^1(0,T).$$

Here, we establish the maximum principle for the classical solutions to (1.3)-(1.5) without such an assumption. Moreover, contrary to [**17, 18**], we are able to quantify the estimates in a precise way.

In the final Appendix, based on formula (1.2) and some recent results of the present authors [**16, 17, 18**], we construct numerical solutions to the initial-boundary value problems for the quasilinear subdiffusion equations with memory. The motivation for the study of equations of this kind arise from theoretical and experimental investigations of materials with memory [**4, 6, 7, 17**].

Outline of the paper. The paper is organized as follows: in Section 2, we introduce the notation and the functional setting. The main Theorem 3.1 on the equivalence between (1.1) and (1.2) and related consequences are stated in Section 3, whereas in Section 4 we state the results on the maximum principle for the classical solution to the subdiffusion equation (1.4). The proofs of the results are carried out in Sections 6 and 7. Some preliminary definitions and auxiliary results from fractional calculus, playing a key role in the course of the investigation, are anticipated in Section 5. In the Appendix, some numerical simulations are discussed.

2. Function Spaces and Notation

Throughout this work, the symbol C will denote a *generic* positive constant, depending only on the structural quantities of the model. We will carry out our analysis in the framework of the fractional Hölder spaces. To this end, in what follows, we take two arbitrary (but fixed) parameters

$$\alpha, \nu \in (0,1).$$

For any nonnegative integer l, for any $p > 1$ and any Banach space $(\mathbf{X}, \|\cdot\|_{\mathbf{X}})$, we consider the usual spaces

$$\mathcal{C}([0,T],\mathbf{X}), \qquad \mathcal{C}^{l+\alpha}(\bar{\Omega}), \qquad L^p(0,T).$$

Besides, denoting for $\beta \in (0,1)$

$$\langle v\rangle^{(\beta)}_{x,\Omega_T} = \sup_{\bar{\Omega}_T} \frac{|v(x,t)-v(\bar{x},t)|}{|x-\bar{x}|^\beta}, \quad x \neq \bar{x},$$
$$\langle v\rangle^{(\beta)}_{t,\Omega_T} = \sup_{\bar{\Omega}_T} \frac{|v(x,t)-v(x,\bar{t})|}{|t-\bar{t}|^\beta}, \quad t \neq \bar{t},$$
$$\langle w\rangle^{(\beta)}_{t,[0,T]} = \sup_{[0,T]} \frac{|w(t)-w(\bar{t})|}{|t-\bar{t}|^\beta}, \quad t \neq \bar{t},$$

we introduce the fractional Hölder spaces

$$\mathcal{C}^\beta_\nu([0,T]) \qquad \text{and} \qquad \mathcal{C}^{l+\alpha,\frac{l+\alpha}{2}\nu}(\bar{\Omega}_T), \quad l=0,1,2,$$

according to the following definition.

DEFINITION 2.1. The functions $v = v(x,t)$ and $w = w(x,t)$ belong to the classes $\mathcal{C}^{l+\alpha,\frac{l+\alpha}{2}\nu}(\bar{\Omega}_T)$ for $l = 0,1,2$, and $\mathcal{C}^\beta_\nu([0,T])$, respectively, if v and w together with the corresponding derivatives are continuous and the norms here below are finite:

$$\|v\|_{\mathcal{C}^{l+\alpha,\frac{l+\alpha}{2}\nu}(\bar{\Omega}_T)} = \|v\|_{\mathcal{C}([0,T],\mathcal{C}^{l+\alpha}(\bar{\Omega}))} + \sum_{j=0}^{l} \langle D^j_x v\rangle^{(\frac{l+\alpha-j}{2}\nu)}_{t,\Omega_T}, \quad l=0,1,$$

$$\|v\|_{\mathcal{C}^{2+\alpha,\frac{2+\alpha}{2}\nu}(\bar{\Omega}_T)} = \|v\|_{\mathcal{C}([0,T],\mathcal{C}^{2+\alpha}(\bar{\Omega}))} + \|\mathbf{D}^\nu_t v\|_{\mathcal{C}^{\alpha,\frac{\alpha}{2}\nu}(\bar{\Omega}_T)} + \sum_{j=1}^{2} \langle D^j_x v\rangle^{(\frac{2+\alpha-j}{2}\nu)}_{t,\Omega_T},$$

$$\|w\|_{\mathcal{C}^\beta_\nu([0,T])} = \|w\|_{\mathcal{C}([0,T])} + \|\mathbf{D}^\nu_t w\|_{\mathcal{C}([0,T])} + \langle \mathbf{D}^\nu_t w\rangle^{(\beta)}_{t,[0,T]}.$$

In a similar way, for $l = 0,1,2$, we define the space $\mathcal{C}^{l+\alpha,\frac{l+\alpha}{2}\nu}(\partial\Omega_T)$. We address the reader to [**18**] for a more detailed discussion on these spaces.

3. Equivalence of (1.1) and (1.2) and Applications

The main result of the section reads as follows.

THEOREM 3.1. *Assume that for some fixed $\beta \in (0,1)$ and $T > 0$ the functions $g(t)$ belongs to the class $\mathcal{C}^\beta_\nu([0,T])$. Then, for every $t \in [0,T]$, we have the equality*

$$\mathbf{D}^\nu_t g(t) = \frac{1}{\Gamma(1-\nu)} \frac{g(t)-g(0)}{t^\nu} + \frac{\nu}{\Gamma(1-\nu)} \int_0^t \frac{g(t)-g(\tau)}{(t-\tau)^{1+\nu}} d\tau. \tag{3.1}$$

The proof of the theorem, which is rather technical, will be postponed to the forthcoming Section 6.

REMARK 3.2. If the function g is also absolutely continuous on $[0,T]$, then the conclusion of Theorem 3.1 holds for the different notion of fractional derivative given by

$$D^\nu_t g(t) = \frac{1}{\Gamma(1-\nu)} \int_0^t (t-\tau)^{-\nu} \frac{dg}{d\tau}(\tau) d\tau.$$

We proceed with a straightforward corollary, which in particular establishes the Leibniz rule.

Corollary 3.1. Let the assumption of Theorem 3.1 hold.

(i) If in addition the function $g(t)$ attains its maximum at the point $t_0 \in [0,T]$, then the Caputo fractional derivative $\mathbf{D}_t^\nu g$ is nonnegative at t_0, i.e.

$$\mathbf{D}_t^\nu g(t_0) \geq 0.$$

(ii) If the functions $g_1,\ g_2 \in \mathcal{C}_\nu^\beta([0,T])$ and $\mathbf{D}_t^\nu(g_1 g_2) \in \mathcal{C}^\beta([0,T])$, then we have the equalities

$$\begin{aligned}\mathbf{D}_t^\nu(g_1g_2)(t) &= g_2(t)\mathbf{D}_t^\nu g_1(t) + g_1(0)\mathbf{D}_t^\nu g_2(t)\\ &\quad + \frac{\nu}{\Gamma(1-\nu)}\int_0^t \frac{[g_2(t)-g_2(\tau)][g_1(\tau)-g_1(0)]}{(t-\tau)^{1+\nu}}d\tau\\ &= g_1(t)\mathbf{D}_t^\nu g_2(t) + g_2(0)\mathbf{D}_t^\nu g_1(t)\\ &\quad + \frac{\nu}{\Gamma(1-\nu)}\int_0^t \frac{[g_1(t)-g_1(\tau)][g_2(\tau)-g_2(0)]}{(t-\tau)^{1+\nu}}d\tau.\end{aligned}$$

Making use of the Leibniz rule, we readily obtain the integration by parts formula.

Corollary 3.2. Let the functions g_1 and g_2 be as in point (ii) above. Then we have the following relations:

$$\begin{aligned}2\int_0^t \mathbf{D}_\tau^\nu(g_1g_2)(\tau)d\tau &= \int_0^t g_2(\tau)\mathbf{D}_\tau^\nu g_1(\tau)d\tau + \int_0^t g_1(\tau)\mathbf{D}_\tau^\nu g_2(\tau)d\tau\\ &\quad + g_1(0)\int_0^t \mathbf{D}_\tau^\nu g_2(\tau)d\tau + g_2(0)\int_0^t \mathbf{D}_\tau^\nu g_1(\tau)d\tau\\ &\quad + \frac{\nu}{\Gamma(1-\nu)}\int_0^t\int_0^\tau \frac{[g_2(\tau)-g_2(s)][g_1(s)-g_1(0)]}{(\tau-s)^{1+\nu}}dsd\tau\\ &\quad + \frac{\nu}{\Gamma(1-\nu)}\int_0^t\int_0^\tau \frac{[g_1(\tau)-g_1(s)][g_2(s)-g_2(0)]}{(\tau-s)^{1+\nu}}dsd\tau,\end{aligned}$$

and

$$\begin{aligned}2g_1(t)g_2(t) &= g_1(0)g_2(t) + g_2(0)g_1(t) + I_t^\nu(g_1\mathbf{D}_\tau^\nu g_2)(t) + I_t^\nu(g_2\mathbf{D}_\tau^\nu g_1)(t)\\ &\quad + \frac{\nu}{\Gamma(1-\nu)}I_t^\nu\left(\int_0^\tau \frac{[g_2(\tau)-g_2(s)][g_1(s)-g_1(0)]}{(\tau-s)^{1+\nu}}ds\right)(t)\\ &\quad + \frac{\nu}{\Gamma(1-\nu)}I_t^\nu\left(\int_0^\tau \frac{[g_1(\tau)-g_1(s)][g_2(s)-g_2(0)]}{(\tau-s)^{1+\nu}}ds\right)(t).\end{aligned}$$

In the last formula, the term I_t^ν is the Riemann-Liouville fractional integral (see Section 5 for more details).

Remark 3.3. It is worth mentioning that all the statements above, with slight modifications, hold in the case of the right Caputo fractional derivative, defined as

$$_t\mathbf{D}^\nu g(t) = \frac{1}{\Gamma(1-\nu)}\frac{\partial}{\partial t}\int_t^T \frac{g(T)-g(\tau)}{(\tau-t)^\nu}d\tau.$$

4. The Maximum Principle

We begin by stipulating the set of hypotheses on the structural quantities appearing in (1.3)-(1.5).

h1 (Ellipticity conditions): There are positive constants μ_1, μ_2, $\mu_1 < \mu_2$, such that for any $(x, t, \xi) \in \bar{\Omega}_T \times \mathbb{R}^n$

$$\mu_1|\xi|^2 \leq \sum_{ij=1}^{n} a_{ij}(x,t)\xi_i\xi_j \leq \mu_2|\xi|^2,$$

and there exists $\mu_3 > 0$ such that

$$\sum_{i=1}^{n} b_i(x,t)N_i(x) \geq \mu_3,$$

for any $(x,t) \in \partial\Omega_T$, where $N = \{N_1(x), ..., N_n(x)\}$ is the unit outward normal vector to Ω.

h2 (Smoothness of the coefficients): For $i, j = 1, ..., n$, we assume

$$a_{ij}(x,t), a_i(x,t), a_0(x,t) \in \mathcal{C}(\bar{\Omega}_T),$$

and

$$b_i(x,t), b_0(x,t) \in \mathcal{C}(\partial\Omega_T).$$

h3 (Smoothness of the given functions): We require

$$u_0(x) \in \mathcal{C}(\bar{\Omega}),$$
$$f(x,t) \in \mathcal{C}(\bar{\Omega}_T),$$
$$\psi(x,t) \in \mathcal{C}(\partial\Omega_T).$$

Our next results are concerned with the maximum principle for the classical solution to the subdiffusion equation (1.3), and to the initial-boundary value problem (1.3)-(1.5). In this respect, Theorem 3.1 plays a key role.

Theorem 4.1. *Let* **h1**-**h2** *hold. Assume that*

$$a_0(x,t) \geq 0 \quad in \quad \Omega_T. \tag{4.1}$$

Then, for any classical solution $u \in \mathcal{C}^{2+\alpha, \frac{2+\alpha}{2}\nu}(\bar{\Omega}_T)$ *to equation* (1.3)*, the following hold:*

(i) *If* $f(x,t) \leq 0$ *in* Ω_T*, then either* $u(x,t) \leq 0$ *in* $\bar{\Omega}_T$*, or the function* u *attains its positive maximum on the bottom of* Ω_T *or on the boundary* $\partial\Omega_T$*, i.e., for all* $(x,t) \in \bar{\Omega}_T$*,*

$$u(x,t) \leq \max\{0, \max_{\partial\Omega_T} u, \max_{\Omega\times\{0\}} u\}.$$

(ii) *If* $f(x,t) \geq 0$ *in* Ω_T*, then the specular result holds, i.e., for all* $(x,t) \in \bar{\Omega}_T$*,*

$$u(x,t) \geq \min\{0, \min_{\partial\Omega_T} u, \min_{\Omega\times\{0\}} u\}.$$

In fact, if we require also the continuity of f, as stated in **h3**, condition (4.1) can be relaxed.

THEOREM 4.2. *Let* **h1**-**h2** *hold, and let* $f(x,t) \in \mathcal{C}(\bar{\Omega}_T)$. *Assume that*

$$a_0(x,t) \geq -A_0 \quad in \quad \Omega_T, \tag{4.2}$$

for some positive constant A_0. *Then, any classical solution* $u \in \mathcal{C}^{2+\alpha,\frac{2+\alpha}{2}\nu}(\bar{\Omega}_T)$ *to equation* (1.3) *fulfills the estimates, for all* $(x,t) \in \bar{\Omega}_T$,

$$u(x,t) \leq E_\nu((1+A_0)T^\nu) \max\left\{0, \max_{\Omega_T} \frac{f}{E_\nu((1+A_0)t^\nu)}, \max_{\partial\Omega_T} \frac{u}{E_\nu((1+A_0)t^\nu)}, \max_{\Omega\times\{0\}} u\right\}$$

and

$$u(x,t) \geq \min\left\{0, \min_{\Omega_T} \frac{f}{E_\nu((1+A_0)t^\nu)}, \min_{\partial\Omega_T} \frac{u}{E_\nu((1+A_0)t^\nu)}, \min_{\Omega\times\{0\}} u\right\},$$

where

$$E_\nu(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(1+\nu n)}$$

denotes the Mittag-Leffler function of the order ν.

Next, we state the maximum principle for the classical solution to the initial-boundary value problem (1.3)-(1.5). To this end, we need to introduce a function $G = G(x) : \bar{\Omega} \to \mathbb{R}$ belonging to $\mathcal{C}^2(\bar{\Omega})$ and possessing the following properties:

$$G(x) = 1 \quad \text{on } \partial\Omega,$$

$$G(x) \geq 1 \quad \text{in } \bar{\Omega},$$

$$-\frac{\partial G}{\partial N} \geq \mu_4 \quad \text{on } \partial\Omega,$$

for some given constant $\mu_4 > 0$. Recall that here N denotes the outward normal to Ω. The procedure to construct a function of this kind is described in [**10**, Lemma 3.1].

Denoting

$$m_1 = \min_{\bar{\Omega}_T}\left\{a_0(x,t) - \frac{2\sum_{ij=1}^n a_{ij} G_{x_i} G_{x_j}}{G^2} + \frac{\sum_{ij=1}^n a_{ij} G_{x_i x_j}}{G} + \frac{\sum_{i=1}^n a_i G_{x_i}}{G}\right\},$$

and choosing a number λ such that $\lambda > 1 - m_1$, we have

THEOREM 4.3. *Let* **h1**-**h3** *and* (4.2) *hold. Let there exist* $B_0 > 0$ *such that*

$$b_0(x,t) \geq -B_0 \quad on\ \partial\Omega_T,$$

$$\mu_4 > \frac{(B_0+1)}{\mu_3}.$$

Then the classical solution $u(x,t) \in \mathcal{C}^{2+\alpha,\frac{2+\alpha}{2}\nu}(\bar{\Omega}_T)$ *to* (1.3)-(1.5) *satisfies, for each* $(x,t) \in \bar{\Omega}_T$,

$$u(x,t) \leq C_1 E_\nu(\lambda T^\nu) \max\left\{0, \max_{\Omega_T} \frac{f}{E_\nu(\lambda t^\nu)}, \max_{\partial\Omega_T} \frac{\psi}{E_\nu(\lambda t^\nu)}, \max_{\bar{\Omega}} u_0\right\}$$

and

$$u(x,t) \geq C_2 \min\left\{0, \min_{\Omega_T} \frac{f}{E_\nu(\lambda t^\nu)}, \min_{\partial\Omega_T} \frac{\psi}{E_\nu(\lambda t^\nu)}, \min_{\bar{\Omega}} u_0\right\}.$$

The positive constants C_1 and C_2 depend only on $\|G\|_{\mathcal{C}^2(\bar{\Omega})}$, besides the structural parameters of the model.

Remark 4.4. It is apparent that if the right-hand sides in (1.3)-(1.5) are nonnegative and $u|_{\partial\Omega} \geq 0$, then Theorems 4.2 and 4.3 provide the positivity of a solution to (1.3)-(1.4) with either the Neumann condition (1.5) or the Dirichlet boundary condition. Likewise, reversing the signs.

Remark 4.5. As it will clear from the proofs in Section 7, the assumption $u \in \mathcal{C}^{2+\alpha,\frac{2+\alpha}{2}\nu}(\bar{\Omega}_T)$ can be relaxed. Indeed, Theorems 4.1-4.3 continue to hold if for some fixed $\beta \in (0,1)$

$$\mathbf{D}_t^\nu u \in \mathcal{C}^\beta([0,T], \mathcal{C}(\Omega)), \qquad u \in \mathcal{C}((0,T), \mathcal{C}^2(\Omega)),$$

and $u \in \mathcal{C}(\bar{\Omega}_T)$ in the case of Theorems 4.1 and 4.2, while $u \in \mathcal{C}([0,T], \mathcal{C}^1(\bar{\Omega}))$ in the case of Theorem 4.3.

We finally observe that conditions **h2-h3** on the smoothness of the given functions do not provide in general the classical solvability of problems like (1.3)-(1.5) (see [**16**]). Nevertheless, these assumptions are sufficient in order to prove the maximum principle, as stated in our theorems.

5. Some Technical Results

Throughout the paper, for any $\theta > 0$ we denote

$$\omega_\theta(t) = \frac{t^{\theta-1}}{\Gamma(\theta)},$$

and we introduce the usual time-convolution product on $(0,t)$, namely,

$$(h_1 \star h_2)(t) = \int_0^t h_1(t-s) h_2(s) ds.$$

We define the fractional Riemann-Liouville integral of order ν of a function $g(\cdot,t)$ with respect to t as (see formula (2.1.1) in [**15**])

$$I_t^\nu g(\cdot,t) = (\omega_\nu \star g(\cdot,t)).$$

We now give some useful properties of fractional derivatives and integrals.

Proposition 5.1. The following hold:

(i) Let a function $g(t)$ and its Caputo fractional derivative $\mathbf{D}_t^\nu g(t)$ be continuous on $[0,T]$. Then for each $t \in [0,T]$ the function $g(t)$ we have the equalities

$$I_t^\nu \mathbf{D}_t^\nu g(t) = g(t) - g(0),$$

$$g(t) = g(0) + t^\nu \frac{\mathbf{D}_t^\nu g(0)}{\Gamma(1+\nu)} + \frac{1}{\Gamma(\nu)} \int_0^t (t-\tau)^{\nu-1} [\mathbf{D}_\tau^\nu g(\tau) - \mathbf{D}_\tau^\nu g(0)] d\tau.$$

(ii) If in addition $g \in \mathcal{C}_\nu^\beta([0,T])$ for some fixed $\beta \in (0,1)$, then

$$\|I_t^\nu [\mathbf{D}_t^\nu g - \mathbf{D}_t^\nu g(0)]\|_{\mathcal{C}^{\nu+\beta}([0,T])} \leq C \|g\|_{\mathcal{C}_\nu^\beta([0,T])}.$$

(iii) For every $t \in [0,T]$ the following inequality holds

$$J := \left| \int_0^t \frac{t^\nu - \tau^\nu}{(t-\tau)^{\nu+1}} d\tau \right| \leq \frac{\pi\nu}{\sin \pi\nu}.$$

PROOF. Point (i) is proved in [**19**, Lemma 2], while (ii) is a simple consequence of [**26**, Theorem 3.1]. Indeed, applying this theorem to the function $I_t^\nu[\mathbf{D}_t^\nu g - \mathbf{D}_t^\nu g(0)]$, one gets

$$\|I_t^\nu[\mathbf{D}_t^\nu g - \mathbf{D}_t^\nu g(0)]\|_{\mathcal{C}^{\nu+\beta}([0,T])} \leq C\|\mathbf{D}_t^\nu g - \mathbf{D}_t^\nu g(0)\|_{\mathcal{C}^\beta([0,T])} \leq C\|g\|_{\mathcal{C}_\nu^\beta([0,T])}.$$

We are left to show (iii). Introducing the new variable $z = 1 - \tau/t$, we have

$$\begin{aligned} J &= \left| \int_0^1 \frac{1-(1-z)^\nu}{z^{\nu+1}} dz \right| \\ &= \left| \int_0^1 \frac{dz}{z^{\nu+1}} \int_0^1 \frac{\partial}{\partial q}(1-qz)^\nu dq \right| \\ &= \nu \int_0^1 z^{-\nu} dz \int_0^1 (1-zq)^{\nu-1} dq \\ &\leq \nu \int_0^1 z^{-\nu}(1-z)^{\nu-1} dz \\ &= \frac{\pi\nu}{\sin \pi\nu}. \end{aligned}$$

The last integral is computed via formula (1.5.20) in [**15**]. □

We conclude this preliminary section recalling some properties of the Mittag-Leffler function (see e.g. [**11**, Section 4]).

PROPOSITION 5.2. For any positive λ, the function $\varphi(t) = E_\nu(\lambda t^\nu)$ belongs to the space $\mathcal{C}_\nu^\beta([0,T])$ and solves the Cauchy problem

$$\begin{cases} \mathbf{D}_t^\nu \varphi(t) = \lambda\varphi, & t \in (0,T], \\ \varphi(0) = 1. \end{cases}$$

Besides, φ is monotonically increasing and $\varphi(t) \geq 1$ for all $t \in [0,T]$.

6. Proof of Theorem 3.1

The strategy of the proof is the following: first, we show that, within our assumptions on the function g, the right-hand side in (3.1) is bounded. Then we prove that the Caputo derivative defined by (1.1) boils down to the right-hand side of (3.1).

In order to estimate the first term of (3.1), we apply point (i) of Proposition 5.1. This yields

$$\begin{aligned} \frac{|g(t)-g(0)|}{t^\nu} &\leq \frac{|\mathbf{D}_t^\nu g(0)|}{\Gamma(1+\nu)} + \frac{t^{-\nu}}{\Gamma(\nu)} \int_0^t (t-\tau)^{\nu-1} |\mathbf{D}_\tau^\nu g(\tau) - \mathbf{D}_\tau^\nu g(0)| d\tau \\ &\leq \frac{|\mathbf{D}_t^\nu g(0)|}{\Gamma(1+\nu)} + \frac{t^{-\nu} \langle \mathbf{D}_\tau^\nu g \rangle_{t,[0,T]}^{(\beta)}}{\Gamma(\nu)} \int_0^t (t-\tau)^{\nu-1} \tau^\beta d\tau \\ &\leq C(1+T^\beta)\|g\|_{\mathcal{C}_\nu^\beta([0,T])}, \end{aligned}$$

ensuring the sought bound of the first term of (3.1). Concerning the second term of (3.1), taking into account point (i) of Proposition 5.1, we first write the difference $g(t) - g(\tau)$ as

$$g(t) - g(\tau) = \frac{\mathbf{D}_t^\nu g(0)}{\Gamma(1+\nu)}[t^\nu - \tau^\nu] + I_t^\nu[\mathbf{D}_t^\nu g - \mathbf{D}_t^\nu g(0)](t) - I_\tau^\nu[\mathbf{D}_\tau^\nu g - \mathbf{D}_\tau^\nu g(0)](\tau).$$

Then, using points (ii)-(iii) of the same proposition, we obtain the inequality

$$\Big|\int_0^t \frac{g(t)-g(\tau)}{(t-\tau)^{\nu+1}}d\tau\Big| \leq C\left[\frac{\pi\nu}{\sin\pi\nu}\frac{|\mathbf{D}_t^\nu g(0)|}{\Gamma(1+\nu)} + \int_0^t \frac{(t-\tau)^{\nu+\beta}}{(t-\tau)^{\nu+1}}d\tau\|\mathbf{D}_t^\nu g\|_{\mathcal{C}^\beta([0,T])}\right]$$
$$\leq C\|g\|_{\mathcal{C}_\nu^\beta([0,T])}[1+T^\beta].$$

Collecting the obtained estimates, we end up the bound

$$\left|\frac{1}{\Gamma(1-\nu)}\frac{g(t)-g(0)}{t^\nu} + \frac{\nu}{\Gamma(1-\nu)}\int_0^t \frac{g(t)-g(\tau)}{(t-\tau)^{\nu+1}}d\tau\right| \leq C(1+T^\beta)\|g\|_{\mathcal{C}_\nu^\beta([0,T])}.$$

This completes the first step of our plan.

At this point, as $g\in\mathcal{C}_\nu^\beta([0,T])$, Proposition 5.1 tells that

$$g(t)-g(0) = I_t^\nu\Phi(t),$$

where

$$\Phi(t) = \mathbf{D}_t^\nu g.$$

Besides, in light of the smoothness of g, we have the embedding

$$\mathbf{D}_t^\nu g \in L^p(0,T), \quad \forall p\geq 1.$$

Then Theorem 13.1 from [**26**] is applied, providing the identity

$$\frac{1}{\Gamma(1-\nu)}\frac{g(t)-g(0)}{t^\nu} + \frac{\nu}{\Gamma(1-\nu)}\int_0^t \frac{g(t)-g(\tau)}{(t-\tau)^{\nu+1}}d\tau = \Phi(t) = \mathbf{D}_t^\nu g,$$

which finishes the proof of Theorem 3.1. □

Remark 6.1. It is worth noting that, in the case of $g\in\mathcal{C}([0,T])\cap B_{1,1}^\nu(0,T)$, where $B_{1,1}^\nu(0,T)$ is the usual Besov space, the standard approach for proving integral identities based on the approximation by smooth functions can be exploited to show the equivalence between (1.1) and (1.2) in the following sense:

$$\frac{\psi(T)}{\Gamma(1-\nu)}\int_0^T \frac{g(t)-g(0)}{(T-t)^\nu}dt + \int_0^T [g(t)-g(0)]\,{}_t\mathbf{D}^\nu\psi(t)dt$$
$$= \frac{1}{\Gamma(1-\nu)}\int_0^T \frac{g(t)-g(0)}{t^\nu}\psi(t)dt + \frac{\nu}{\Gamma(1-\nu)}\int_0^T \psi(t)\int_0^t \frac{g(t)-g(t-\tau)}{\tau^{1+\nu}}d\tau dt,$$

for any $\psi\in\mathcal{C}^1([0,T])$.

We conclude this section with an important inequality, which is a consequence of Theorem 3.1, and will play a key role in the proofs of the forthcoming Theorems 4.2 and 4.3.

Proposition 6.1. Let $g_1,g_2\in\mathcal{C}_\nu^\beta([0,T])$, for some fixed $\beta\in(0,1)$, and let there exist $M>0$ such that

$$|g_2(t)|>M, \quad \forall t\in[0,T].$$

Then the ratio $g=g_1/g_2$ belongs to $\mathcal{C}^\beta([0,T])$ and satisfies the inequality

$$\left|\frac{g(t)-g(0)}{\Gamma(1-\nu)t^\nu} + \frac{\nu}{\Gamma(1-\nu)}\int_0^t \frac{g(t)-g(\tau)}{(t-\tau)^{\nu+1}}d\tau\right|$$
$$\leq \frac{C\|g_1\|_{\mathcal{C}_\nu^\beta([0,T])}}{M}\left[1+\frac{\|g_2\|_{\mathcal{C}_\nu^\beta([0,T])}}{M}+\frac{\|g_2\|^2_{\mathcal{C}_\nu^\beta([0,T])}}{M^2}\right].$$

PROOF. The smoothness of g follows immediately from the properties of the functions g_1 and g_2. By straightforward calculations, together with Theorem 3.1, we establish the equality

$$\begin{aligned}&\frac{g(t)-g(0)}{\Gamma(1-\nu)t^{\nu}}+\frac{\nu}{\Gamma(1-\nu)}\int_0^t\frac{g(t)-g(\tau)}{(t-\tau)^{\nu+1}}d\tau\\&=\frac{\mathbf{D}_t^{\nu}g_1(t)}{g_2(t)}-\frac{g_1(0)\mathbf{D}_t^{\nu}g_2(t)}{g_2(0)g_2(t)}\\&\quad-\frac{\nu}{\Gamma(1-\nu)g_2(t)}\int_0^t\frac{[g_2(t)-g_2(\tau)][g_1(\tau)-g_1(0)]d\tau}{(t-\tau)^{1+\nu}g_2(\tau)}\\&\quad+\frac{\nu}{\Gamma(1-\nu)}\frac{g_1(0)}{g_2(0)g_2(t)}\int_0^t\frac{[g_2(t)-g_2(\tau)][g_2(\tau)-g_2(0)]d\tau}{(t-\tau)^{1+\nu}g_2(\tau)}.\end{aligned}$$

The desired inequality then follows by estimating each term in the right-had side by means of the very same arguments employed in the proof of Theorem 3.1. □

7. Proof of Theorems 4.1-4.3

7.1. Proof of Theorem 4.1. We will carry out the detailed arguments of the first inequality. The proof of the second one is identical, and left to the interested reader. By virtue of continuity of the function $u(x,t)$ on the bounded closed domain Ω_T, there is a point $(x_0,t_0)\in\bar{\Omega}_T$ such that

$$u(x,t)\leq u(x_0,t_0),\quad \forall(x,t)\in\bar{\Omega}_T. \tag{7.1}$$

Then we have two possibilities. The first one is

$$u(x_0,t_0)\leq 0,$$

which immediately completes the proof of Theorem 4.3. Otherwise,

$$u(x_0,t_0)>0.$$

In this case, if $(x_0,t_0)\in\partial\Omega_T$ or $t_0=0$, then inequality (7.1) provides the estimate

$$u(x,t)\leq\max\{\max_{\partial\Omega_T}u,\ \max_{\Omega\times\{0\}}u\},$$

which finishes the proof. Thus, we are left to analyze the case where (x_0,t_0) is an interior point of Ω_T. It is well known, that in the maximum point the following inequalities hold

$$\begin{aligned}\sum_{ij=1}^{n}a_{ij}(x_0,t_0)\frac{\partial^2u(x_0,t_0)}{\partial x_i\partial x_j}&\leq 0,\\\frac{\partial u(x_0,t_0)}{\partial x_i}&=0,\quad i=1,2,...,n,\\a_0(x_0,t_0)u(x_0,t_0)&\geq 0.\end{aligned}$$

Here we used assumptions **h1** and (4.1) on the coefficients. Moreover, since

$$u\in\mathcal{C}^{2+\alpha,\frac{2+\alpha}{2}\nu}(\bar{\Omega}_T),$$

we can employ Corollary 3.1 to conclude that

$$\mathbf{D}_t^{\nu}u(x_0,t_0)\geq 0. \tag{7.2}$$

On account of these inequalities together with the non-positivity of the function f, from equation (1.3) written at the point (x_0, t_0), we come to the estimates

$$\begin{aligned}
0 &\geq f(x_0, t_0) \\
&= \mathbf{D}_t^\nu u(x_0, t_0) - \sum_{ij=1}^n a_{ij}(x_0, t_0)\frac{\partial^2 u(x_0, t_0)}{\partial x_i \partial x_j} - \sum_{i=1}^n a_i(x_0, t_0)\frac{\partial u(x_0, t_0)}{\partial x_i} \\
&+ a_0(x_0, t_0)u(x_0, t_0) \geq 0.
\end{aligned}$$

Two situations may occur:

• either $f(x_0, t_0) = 0$,

• or the positive maximum $u(x, t)$ can not be attained in the interior point (x_0, t_0).

It is apparent that in the second case the proof of the theorem is finished. Let us analyze the first situation. The obtained estimate tells that every term in (1.3) vanishes, in particular,

$$\mathbf{D}_t^\nu u(x_0, t_0) = 0.$$

Due to Theorem 3.1, this is equivalent to

$$\frac{u(x_0, t_0) - u(x_0, 0)}{\Gamma(1-\nu)t_0^\nu} + \frac{\nu}{\Gamma(1-\nu)}\int_0^{t_0} \frac{u(x_0, t_0) - u(x_0, \tau)}{(t_0 - \tau)^{1+\nu}} d\tau = 0,$$

where, as it follows from the very definition of (x_0, t_0), both terms are above non-negative. Thus, the equality holds only if each term is zero. Consequently, we deduce that

$$u(x_0, t_0) = u(x_0, 0).$$

But this contradicts the assumption that the positive maximum of $u(x, t)$ is not attained in $\Omega \times \{0\}$. The proof of Theorem 4.1 is now completed. □

7.2. Proof of Theorem 4.2. In this proof, as we did for Theorem 4.1, it is enough to obtain the first estimate, being the second verified with the analogous arguments.

First, we define the function $v = v(x, t) : \bar{\Omega}_T \to \mathbb{R}$ by

$$v(x, t) = \frac{u(x, t)}{\varphi(t)},$$

where

$$\varphi(t) = E_\nu((A_0 + 1)t^\nu).$$

By Proposition 5.2,

$$v(x, 0) = u(x, 0).$$

Then, we rewrite equation (1.3) in terms of v as

$$\begin{aligned}
&\varphi(0)\left[\frac{v(x, t) - v(x, 0)}{\Gamma(1-\nu)t^\nu} + \frac{\nu}{\Gamma(1-\nu)}\int_0^t \frac{v(x, t) - v(x, \tau)}{(t-\tau)^{1+\nu}} d\tau\right] \\
&+ \frac{\nu}{\Gamma(1-\nu)}\int_0^t \frac{[v(x, t) - v(x, \tau)][\varphi(\tau) - \varphi(0)]}{(t-\tau)^{1+\nu}} d\tau \\
&- \sum_{ij=1}^n a_{ij}(x, t)\varphi(t)\frac{\partial^2 v}{\partial x_i \partial x_j} - \sum_{i=1}^n a_i(x, t)\varphi(t)\frac{\partial v}{\partial x_i} + [a_0\varphi + \mathbf{D}_t^\nu \varphi]v = f \quad \text{in} \quad \Omega_T.
\end{aligned}$$

Here, we applied Theorem 3.1 to calculate $\mathbf{D}_t^\nu u = \mathbf{D}_t^\nu(v\varphi)$. Moreover, on account of Propositions 5.2 and 6.1, all the terms of the equality above are bounded. From the smoothness of u and φ, along with the positivity of φ, we deduce that $v \in \mathcal{C}(\bar{\Omega}_T)$. As consequence, there is a point $(x_0, t_0) \in \bar{\Omega}_T$ such that

$$v(x,t) \leq v(x_0,t_0), \quad \forall (x,t) \in \bar{\Omega}_T.$$

Arguing exactly as in the proof of Theorem 4.1, we can restrict our analysis to the case where (x_0, t_0) is an interior point of Ω_T and $v(x_0, t_0) > 0$, for otherwise

$$v(x,t) \leq \max\{0, \max_{\partial\Omega_T} v, \max_{\Omega\times\{0\}} v\},$$

or, in terms of u,

$$u(x,t) \leq \varphi(t) \max\left\{0, \max_{\partial\Omega_T} \frac{u}{\varphi}, \max_{\Omega\times\{0\}} u\right\} \leq \varphi(T) \max\left\{0, \max_{\partial\Omega_T} \frac{u}{\varphi}, \max_{\Omega\times\{0\}} u\right\}.$$

Accordingly, let us dwell on the case when the positive maximum of v is attained at an interior point. Taking into account Proposition 5.2, we get the (equality and) inequalities in the maximum point

$$\sum_{ij=1}^{n} a_{ij}(x_0,t_0)\varphi(t_0)\frac{\partial^2 v(x_0,t_0)}{\partial x_i \partial x_j} \leq 0, \qquad \sum_{i=1}^{n} a_i(x_0,t_0)\varphi(t_0)\frac{\partial v(x_0,t_0)}{\partial x_i} = 0,$$

$$\frac{v(x_0,t_0)-v(x_0,0)}{\Gamma(1-\nu)t_0^{\nu}} + \frac{\nu}{\Gamma(1-\nu)}\int_0^{t_0} \frac{v(x_0,t_0)-v(x_0,\tau)}{(t_0-\tau)^{1+\nu}}d\tau$$
$$+ \frac{\nu}{\Gamma(1-\nu)}\int_0^{t_0} \frac{[v(x_0,t_0)-v(x_0,\tau)][\varphi(\tau)-\varphi(0)]}{(t_0-\tau)^{1+\nu}}d\tau > 0,$$

$$[a_0(x_0,t_0)\varphi(t_0) + \mathbf{D}_t^{\nu}\varphi(t_0)]v(x_0,t_0) = [a_0(x_0,t_0) + A_0 + 1]\varphi(t_0)v(x_0,t_0) > 0.$$

Hence, from the equation for v we deduce that

$$f(x_0,t_0) \geq [A_0 + 1 + a_0(x_0,t_0)]\varphi(t_0)v(x_0,t_0) > \varphi(t_0)v(x_0,t_0) > 0,$$

which in particular forces the strict inequality $f(x_0, t_0) > 0$. Therefore, for each $(x, t) \in \bar{\Omega}_T$,

$$v(x,t) \leq v(x_0,t_0) < \frac{f(x_0,t_0)}{\varphi(t_0)} \leq \max_{\bar{\Omega}_T} \frac{f(x,t)}{\varphi(t)},$$

or, in terms of u,

$$u(x,t) \leq \varphi(t)\max_{\bar{\Omega}_T} \frac{f(x,t)}{\varphi(t)} \leq \varphi(T)\max_{\bar{\Omega}_T} \frac{f(x,t)}{\varphi(t)}.$$

This finishes the proof of Theorem 4.2. □

7.3. Proof of Theorem 4.3. Here, similarly to Theorems 4.1 and 4.2, we verify only the first inequality. Introducing the new unknown function

$$w(x,t) = \frac{u(x,t)}{\varphi(t)}G(x) \qquad \text{with} \qquad \varphi(t) = E_{\nu}(\lambda t^{\nu}),$$

and denoting

$$\begin{aligned}
\bar{a}_{ij} &= \varphi a_{ij}, \\
\bar{a}_i &= \varphi\left[a_i - \frac{2}{G}\sum_{j=1}^{n}\frac{\partial G}{\partial x_j}a_{ij}\right], \\
\bar{a}_0 &= \varphi\left[\lambda + a_0 - \frac{2}{G^2}\sum_{ij=1}^{n}\frac{\partial G}{\partial x_i}\frac{\partial G}{\partial x_j}a_{ij} + \frac{1}{G}\sum_{ij=1}^{n}\frac{\partial^2 G}{\partial x_i \partial x_j}a_{ij} + \frac{1}{G}\sum_{i=1}^{n}\frac{\partial G}{\partial x_i}a_i\right], \\
\bar{b}_0 &= b_0 - \frac{1}{G}\sum_{i=1}^{n}\frac{\partial G}{\partial x_i}b_i,
\end{aligned}$$

we rewrite problem (1.3)-(1.5) in the form

$$\begin{cases}
\dfrac{w(x,t)-w(x,0)}{\Gamma(1-\nu)t^{\nu}} + \dfrac{\nu}{\Gamma(1-\nu)}\displaystyle\int_0^t \dfrac{w(x,t)-w(x,\tau)}{(t-\tau)^{1+\nu}}d\tau \\
\quad + \dfrac{\nu}{\Gamma(1-\nu)}\displaystyle\int_0^t \dfrac{[w(x,t)-w(x,\tau)][\varphi(\tau)-\varphi(0)]}{(t-\tau)^{1+\nu}}d\tau \\
\quad - \displaystyle\sum_{ij=1}^{n}\bar{a}_{ij}\dfrac{\partial^2 w}{\partial x_i \partial x_j} - \sum_{i=1}^{n}\bar{a}_i\dfrac{\partial w}{\partial x_i} + \bar{a}_0 w = fG \qquad \text{in } \Omega_T, \\
\displaystyle\sum_{i=1}^{n} b_i \dfrac{\partial w}{\partial x_i} + \bar{b}_0 w = \dfrac{\psi G}{\varphi} \qquad \text{on } \partial\Omega_T, \\
w(x,0) = G(x)u_0(x) \qquad \text{in } \bar{\Omega}.
\end{cases}$$

Here, in order to obtain the first equation we applied successively Theorem 3.1 and Proposition 6.1 together with Proposition 5.2. The properties of u, G and φ yield the continuity of w in $\bar{\Omega}_T$, which consequently attains its maximum at some $(x_0, t_0) \in \bar{\Omega}_T$. We can restrict our analysis to the case of a positive maximum of w attained on the boundary $\partial\Omega_T$, since all the remaining cases can be tackled by analogous arguments to those of the proof of Theorem 4.2, yielding the inequality

$$\begin{aligned}
u(x,t) &\le CE_\nu(\lambda t^\nu)\max\left\{0, \max_{\Omega_T}\frac{f}{E_\nu(\lambda t^\nu)}, \max_{\Omega\times\{0\}} u\right\} \\
&\le CE_\nu(\lambda T^\nu)\max\left\{0, \max_{\Omega_T}\frac{f}{E_\nu(\lambda t^\nu)}, \max_{\Omega\times\{0\}} u\right\}
\end{aligned}$$

for some $C > 0$ depending on the structural parameters of the model. Coming back to the more interesting case $(x_0, t_0) \in \partial\Omega_T$, and making use of the relation

$$b_i(x_0,t_0)\frac{\partial w}{\partial x_i}(x_0,t_0) \ge 0,$$

together with the boundary condition for w, we are led to

$$[\bar{b}(x_0,t_0) - 1]w(x_0,t_0) + w(x_0,t_0) \le \frac{G(x_0)\psi(x_0,t_0)}{\varphi(t_0)} = \frac{\psi(x_0,t_0)}{\varphi(t_0)},$$

and

$$\begin{aligned}[\bar{b}(x_0,t_0)-1] &= b_0(x_0,t_0) - G^{-1}(x_0,t_0)\sum_{i=1}^{n} b_i(x_0,t_0)\frac{\partial G}{\partial x_i}(x_0,t_0) - 1 \\ &\geq \mu_3\mu_4 - 1 - B_0 > 0.\end{aligned}$$

The last inequality follows from the assumption on μ_4. Collecting the two relations, we obtain the bound

$$0 < w(x_0,t_0) \leq \frac{\psi(x_0,t_0)}{\varphi(t_0)},$$

implying in particular that $\psi(x_0,t_0) > 0$. Therefore, for each $(x,t) \in \bar{\Omega}_T$, we end up with

$$w(x,t) \leq C \max_{\partial\Omega_T} \frac{\psi(x,t)}{\varphi(t)},$$

or, in terms of u,

$$u(x,t) \leq C\,\varphi(t) \max_{\partial\Omega_T} \frac{\psi(x,t)}{\varphi(t)} \leq C\,\varphi(T) \max_{\partial\Omega_T} \frac{\psi(x,t)}{\varphi(t)}.$$

This last estimate completes the proof of Theorem 4.3. □

Appendix: Numerical Simulations

In this Appendix, we show the effectiveness of the alternative definition (3.1) of Caputo fractional derivative $\mathbf{D}_t^\nu u$ in the construction of numerical solutions to the boundary value problem for the quasilinear subdiffusion equation with memory, introduced and studied in the previous works [**16, 17, 18**], where the global classical solvability has been proved in the fractional Hölder spaces (and to which we address the interested reader for the physical motivations of the model).

We consider initial-boundary value problem in the one-dimensional domain $\Omega = (0, L)$

$$\text{(A.1)} \qquad \begin{cases} \mathbf{D}_t^\nu u - a(x,t)u_{xx} + d(x,t)u_x - \displaystyle\int_0^t \mathsf{K}(t-s)b(x,s)u_{xx}(x,s)ds \\ \qquad = f(x,t,u) + f_0(x,t) \quad \text{in } \Omega_T, \\ u(x,0) = u_0(x) \quad \text{in } [0,L], \\ c_1 u_x(0,t) + c_2 u(0,t) = \varphi_1(t) \quad \text{in } [0,T], \\ c_3 u_x(L,t) + c_4 u(L,t) = \varphi_2(t) \quad \text{in } [0,T]. \end{cases}$$

All the coefficients above are sufficiently smooth. In particular, $a(x,t)$ is positive definite, while the nonlinearity $f(x,t,u)$ is Lipschitz in x,t and locally Lipschitz in u. Finally, the memory kernel K is a summable function such that

$$|\mathsf{K}(t)| \leq \frac{C}{t^\beta}, \quad 0 < \beta < 1.$$

For the precise assumptions on the coefficients we address the reader to [**17**]. Within these hypotheses, problem (A.1) admits a unique global classical solution (see [**17**, Theorem 3.4])

$$u \in \mathcal{C}^{2+\alpha, \frac{2+\alpha}{2}\nu}(\bar{\Omega}_T).$$

In particular, the regularity of u tells that u and $\mathbf{D}_t^\nu u$ fall into the conditions of Theorem 3.1, which entitle us to apply formula (3.1) when dealing with the Caputo fractional derivative of u in the numerical scheme.

Introducing the space-time mesh with nodes

$$x_k = kh, \quad \tau_j = j\tau, \quad k = 0, 1, \dots, \mathcal{N}, \quad j = 0, 1, \dots, \mathcal{M}, \quad h = L/\mathcal{N}, \quad \tau = T/\mathcal{M},$$

and approximating the differential equation in (A.1) at each level τ_{j+1}, we derive the following finite-difference scheme:

$$\begin{aligned}&\frac{\tau^{-\nu}}{\Gamma(2-\nu)} u_k^{j+1} - \sum_{m=0}^{j} \omega_m^{j+1} u_k^m - \frac{a_k^{j+1}}{h^2}(u_{k-1}^{j+1} - 2u_k^{j+1} + u_{k+1}^{j+1}) + \frac{d_k^{j+1}}{2h}(u_{k+1}^{j+1} - u_{k-1}^{j+1})\\ &= \sum_{m=0}^{j} \left(b_k^m \frac{u_{k-1}^m - 2u_k^m + u_{k+1}^m}{h^2} + b_k^{m+1} \frac{u_{k-1}^{m+1} - 2u_k^{m+1} + u_{k+1}^{m+1}}{h^2} \right) \frac{\mathsf{K}_{m,j}}{2}\\ &\quad + f(x_k, \tau_j, u_k^j) + f_0(x_k, \tau_{j+1}),\end{aligned}$$

for

$$k = 1, \dots, \mathcal{N} - 1 \quad \text{and} \quad j = 0, 1, \dots, \mathcal{M} - 1,$$

where we denoted the finite-difference approximation of the function u at the point (x_k, τ_j) by u_k^j, and we put

$$a_k^{j+1} = a(x_k, \tau_{j+1}),\ d_k^{j+1} = d(x_k, \tau_{j+1}),\ b_k^j = b(x_k, \tau_j),\ \mathsf{K}_{m,j} = \int_{\tau_m}^{\tau_{m+1}} \mathsf{K}(\tau_{j+1} - s) ds,$$

and

$$\omega_m^j = \frac{1}{\Gamma(1-\nu)} \begin{cases} \nu \displaystyle\int_0^{t_j} (t_j - s)^{-\nu-1} \phi_m(s) ds, & 0 < m \le j - 1, \\ \dfrac{1}{t_j^\nu} + \nu \displaystyle\int_0^{t_j} (t_j - s)^{-\nu-1} \phi_0(s) ds, & m = 0. \end{cases}$$

Here, $\phi_m(\cdot)$ are the standard piecewise-linear "hat" functions, that provide a piecewise linear approximation of the integrand in (3.1), thereby realizing the trapezoid-like approximation of the integral in (3.1) on each segment $[t_m, t_{m+1}]$. We also took advantage of the equality

$$\sum_{m=0}^{j-1} \omega_m^j = \frac{\tau^{-\nu}}{\Gamma(2-\nu)},$$

to collect the coefficients at the value u_k^{j+1} (see, e.g. [**5**]). The derivatives u_x and u_{xx} are approximated by the second-order finite-difference formulas, while the trapezoid-rule is employed to approximate the integrals in the sum

$$\sum_{m=0}^{j} \int_{\tau_m}^{\tau_{m+1}} \mathsf{K}(\tau_{j+1} - s) b(x, s) u_{xx}(x, s) ds.$$

Finally, we used two fictitious mesh points outside the spatial domain to approximate the Neumann boundary conditions with the second order of accuracy (see, e.g. [**14**]).

Four different numerical tests are considered. In all the analyzed examples we can exhibit the exact solution u, and the absolute error $\delta = \max |u - u_{\mathsf{N}}|$ between u and the numerical solution u_{N} (the maximum is taken over all the grid points in the space-time mesh) are listed in Tables 1-4.

EXAMPLE A.1. Consider problem (A.1) with $L = 1$, $T = 0.1$ and

$$a(x,t) = \cos \pi x/4 + t, \qquad d(x,t) = x + t, \qquad b(x,t) = t^{1/3} + \sin \pi x,$$
$$\mathsf{K}(t) = t^{-1/3}, \qquad u_0(x) = \cos \pi x, \qquad f(x,t,u) = xt \sin(u^2),$$
$$f_0(x,t) = 1 + \pi^2 \Big(\cos \frac{\pi x}{4} + t + \frac{3t^{2/3} \sin(\pi x)}{2} + \frac{t\pi}{3 \sin \pi/3} \Big) \cos \pi x$$
$$- (x+t)\pi \sin \pi x - xt \sin \Big(\cos \pi x + \frac{t^\nu}{\Gamma(1+\nu)} \Big)^2,$$
$$c_1 = c_3 = 1, \qquad c_2 = c_4 = 0, \qquad \varphi_1(t) = \varphi_2(t) = 0.$$

The function

$$u(x,t) = \cos \pi x + \frac{t^\nu}{\Gamma(1+\nu)}$$

solves the initial-boundary value problem (A.1) with the parameters specified above. In our numerical calculations we set $\mathcal{M} = \mathcal{N} = 10^3$.

TABLE 1. The absolute error δ in Example A.1

ν	δ
0.1	3.5620e-02
0.2	2.5033e-02
0.3	1.2993e-02
0.4	5.8764e-03
0.5	2.4260e-03
0.6	9.2511e-04
0.7	3.2262e-04
0.8	1.1020e-04
0.9	4.2003e-05

EXAMPLE A.2. Consider problem (A.1) with $L = 1$, $T = 1$ and

$$a(x,t) = 1, \qquad d(x,t) = 0, \qquad b(x,t) = 1,$$
$$\mathsf{K}(t) = \frac{t^{-\nu}}{\Gamma(1-\nu)}, \qquad u_0(x) = \cos \pi x, \qquad f(x,t,u) = 0,$$

$$f_0(x,t) = \Big[\Gamma(1+\nu) + \pi^2(1+t^\nu) + \pi^2 t(1+\Gamma(1+\nu)) + \frac{1+\pi^2}{\Gamma(2-\nu)} t^{1-\nu}$$
$$+ \frac{\pi^2}{\Gamma(3-\nu)} t^{2-\nu} \Big] \cos \pi x,$$

$$c_1 = c_3 = 1, \qquad c_2 = c_4 = 0, \qquad \varphi_1(t) = \varphi_2(t) = 0.$$

In this example, the exact solution has the form

$$u(x,t) = [1 + t + t^\nu] \cos \pi x.$$

In the numerical calculations we set $\mathcal{M} = \mathcal{N} = 10^3$.

TABLE 2. The absolute error δ in Example A.2

ν	δ
0.15	9.3646e-03
0.25	1.1117e-02
0.35	9.6659e-03
0.45	6.7121e-03
0.55	3.9127e-03
0.65	1.9790e-03
0.75	8.6936e-04
0.85	3.3379e-04
0.95	3.3733e-04

EXAMPLE A.3. Consider problem (A.1) with $L = 1$, $T = 1$ and

$$a(x,t) = (x+1)(t+1), \qquad d(x,t) = x\sin t, \qquad b(x,t) = 0,$$
$$\mathsf{K}(t) = 0, \qquad u_0(x) = 2x - x^2, \qquad f(x,t,u) = 0,$$
$$f_0(x,t) = E_\nu(t^\nu)[2x - x^2 + 2(x+1)(t+1) + x(2-2x)\sin t],$$
$$c_1 = c_3 = 1, \quad c_2 = -2, \quad c_4 = 0, \quad \varphi_1(t) = 2E_\nu(t^\nu), \quad \varphi_2(t) = 0.$$

Here the exact solution reads

$$u(x,t) = [2x - x^2]E_\nu(t^\nu).$$

In the numerical calculations we set $\mathcal{M} = \mathcal{N} = 500$.

TABLE 3. The absolute error δ in Example A.3

ν	δ
0.1	3.8610e-02
0.2	3.2700e-02
0.3	2.4142e-02
0.4	1.5880e-02
0.5	9.4498e-03
0.6	5.1052e-03
0.7	2.4788e-03
0.8	1.1052e-03
0.9	4.2044e-04

EXAMPLE A.4. Consider problem (A.1) with $L = 1$, $T = 1$ and

$$a(x,t) = 1, \qquad d(x,t) = 0, \qquad b(x,t) = 1,$$
$$\mathsf{K}(t) = \frac{t^{-\nu}}{\Gamma(1-\nu)}, \qquad u_0(x) = \cos \pi x, \qquad f(x,t,u) = 0,$$
$$f_0(x,t) = \left[(1+t^2)\pi^2 + \frac{2t^{2-\nu}}{\Gamma(3-\nu)} + \frac{\pi^2 t^{1-\nu}}{\Gamma(2-\nu)} + \frac{2\pi^2 t^{3-\nu}}{\Gamma(4-\nu)}\right]\cos \pi x,$$
$$c_1 = c_3 = 1, \qquad c_2 = c_4 = 0, \qquad \varphi_1(t) = \varphi_2(t) = 0.$$

The corresponding exact solution is

$$u(x,t) = (1+t^2)\cos \pi x.$$

In the numerical calculations we set $\mathcal{M} = \mathcal{N} = 10^3$.

TABLE 4. The absolute error δ in Example A.4

ν	δ
0.13	1.6976e-06
0.23	2.1854e-06
0.33	3.3378e-06
0.43	6.0408e-06
0.53	1.2325e-05
0.63	2.6798e-05
0.73	5.9804e-05
0.83	1.3432e-04
0.93	3.0081e-04

In Example A.4, decreasing the order ν leads to an increase of the computation accuracy. This matches the results in [**5**]. Namely, the fractional derivative is approximated with accuracy $O(\tau^{2-\nu})$ in the finite-difference scheme applied above, provided that $\partial^2 u/\partial t^2$ is bounded on $[0,L]\times[0,T]$. This requirement is not fulfilled in Examples A.1-A.3, due to the fact that integer-order derivatives with respect to t have singularities at $t=0$. Hence, the numerical results for the first three tests fit into the general pattern, predicting that the accuracy decreases with order ν in the case of weakly singular solutions, especially near the singularity point $t=0$ (see [**9**] for more details).

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