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Regularity of solutions to a time-fractional diffusion equation

by

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Abstract

The paper proves estimates for the partial derivatives of the solution to a time-fractional diffusion equation, posed over a bounded spatial domain. Such estimates are needed for the analysis of effective numerical methods, particularly since the solution is less regular than in the well-known case of classical diffusion.

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1 Introduction

In classical diffusion, the density u(x,t) of particles at position x and time t obeys the parabolic partial differential equation

$$u_t - \nabla \cdot (K\nabla u) = f, \tag{1}$$

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where $u_t = \partial u/\partial t$, f = f(x,t) is the density of sources, K > 0 is the diffusivity, and ∇u is the spatial gradient of u. In anomalous subdiffusion, u instead satisfies the partial integrodifferential equation

$$u_t - \nabla \cdot (\omega_\nu * K \nabla u)_t = f, \tag{2}$$

with $0 < \nu < 1$, where $\omega_{\nu}(t) = t^{\nu-1}/\Gamma(\nu)$ and * denotes the Laplace convolution. Our aim is to describe the smoothness, or lack thereof, of solutions to (2).

We can interpret the parameter ν at the microscopic level: the diffusing particles have a mean-square displacement $2Kt^{\nu}/\Gamma(1+\nu) \propto t^{\nu}$, in contrast to 2Kt in the classical setting of Brownian motion; see [4, 10].

For any $\mu > 0$, the convolution

$$(\omega_{\mu} * v)(t) = \int_{0}^{t} \frac{(t-s)^{\mu-1}}{\Gamma(\mu)} v(s) ds$$

defines the Riemann–Liouville fractional integral of v of order μ , and we may interpret $(\omega_{\nu} * v)_t$ as the fractional derivative $\partial_t^{1-\nu}u$. If $\nu \to 1$ then $(\omega_{\nu} * v)_t \to v$. In this way, the classical diffusion equation (1) is a limiting case of (2).

For a bounded domain $\Omega \subseteq \mathbb{R}^d$ with spatial dimension $d \geq 1$, we impose homogenous boundary conditions, either of Dirichlet type,

$$u(x,t) = 0 \quad \text{for } x \in \partial\Omega \text{ and } t > 0,$$
 (3)

or else of Neumann type,

$$\partial_n u(x,t) = 0 \quad \text{for } x \in \partial \Omega \text{ and } t > 0,$$
 (4)

where n denotes the outward unit normal to Ω . We also assume the initial condition

$$u(x,0) = u_0(x)$$
 for $x \in \Omega$.

It will be convenient to define the second-order, self-adjoint, elliptic partial differential operator $Au = -\nabla \cdot (K\nabla u)$, and to rewrite (2) as

$$u_t + (\omega_\nu * Au)_t = f(t). \tag{5}$$

An understanding of the regularity of u is crucial for the design of effective numerical methods for (5), especially since u is less regular than in the classical case. For a simple example, let $f \equiv 0$ and $u_0 = \phi$, where ϕ is an eigenfunction of A, say $A\phi = \lambda \phi$. It follows from (12) and (14) below that

$$u(x,t) = \phi(x) \left(1 - \frac{\lambda t^{\nu}}{\Gamma(1+\nu)} + O(t^{2\nu}) \right) \text{ as } t \to 0,$$

so, since $0 < \nu < 1$, the derivatives of u with respect to t are unbounded as $t \to 0$. The motivation for this paper came from an analysis of discontinuous Galerkin methods in [7, 11], which assumed regularity estimates of the form

$$t^{\nu} \|Au'(t)\| + t^{1+\nu} \|Au''(t)\| + t^{2+\nu} \|Au'''(t)\| \le Ct^{\sigma-1}$$
 (6)

and

$$||u'(t)|| + t||u''(t)|| \le Ct^{\sigma - 1},$$
 (7)

for $0 < t \le T$, with $\sigma > 0$.

In Section 2, we solve the initial boundary value problem for (2) using separation of variables and Laplace transformation. This construction is standard so we merely outline the main steps, introducing our notation in the process. Section 3 summarizes some key facts concerning the function space $\dot{H}^r \subseteq H^r(\Omega)$ that we use to measure the spatial regularity of u.

Having dealt with these preliminaries, in Section 4 we suppose $f \equiv 0$ and prove bounds of the form

$$t^{q} \| u^{(q)}(t) \|_{\dot{H}^{r+\mu}} \le C t^{-\mu\nu/2} \| v \|_{\dot{H}^{r}}, \tag{8}$$

for $q \in \{1, 2, 3, ...\}$ and $0 \le r < \infty$. Here, the additional smoothing in space is limited to $0 \le \mu \le 2$, in contrast to the classical case $\nu = 1$ where μ may be arbitrarily large. The method of proof was used previously in [6, 8] to deal with a fractional wave equation, corresponding to the case $1 < \nu < 2$. We also obtain an expansion for u in powers of t^{ν} as $t \to 0$.

A different approach, based on a contour integral representation of u and a resolvent estimate for A, was used in [9, Theorem 2.1] to prove bounds like (8) in the maximum norm; for instance, $t^q ||Au^{(q)}(t)||_{L_{\infty}(\Omega)} \leq Ct^{-\nu}||v||_{L_{\infty}(\Omega)}$, corresponding to the case $\mu = 2$. Cuesta, Lubich and Palencia [1] used an essentially similar approach, in the guise of an operational calculus. Note that $\nu = 1 - \alpha$ in the notation of [1], whereas $\nu = 1 + \alpha$ in the notation of [9].

In Section 5, we suppose $u_0 = 0$ and allow a nonzero f. Again, techniques used in [6] carry over to the present case, allowing us to show that

$$t^{q} \|u^{(q)}(t)\|_{\dot{H}^{r+\mu}} \le C t^{-\mu\nu/2} \sum_{j=0}^{q+1} \int_{0}^{t} s^{j} \|f^{(j)}(s)\|_{\dot{H}^{r}} ds,$$

for $0 \le \mu \le 2$. The previously cited work [9] proved only a basic estimate for the inhomogenous problem,

$$\int_0^t ||Au'(s)||_{L_{\infty}(\Omega)} ds \le Ct^{1-\nu} \bigg(||f(0)||_{L_{\infty}(\Omega)} + \int_0^t ||f'(s)||_{L_{\infty}(\Omega)} ds \bigg).$$

Finally, in Section 6, we investigate the behaviour of the solution when the initial datum u_0 does not satisfy the boundary condition, in the simple case when $f \equiv 0$ and the spatial dimension d = 1. It follows that $u_0 \in \dot{H}^r$ only when $r < \frac{1}{2}$ for a Dirichlet boundary condition, and only when $r < \frac{3}{2}$ for a Neumann boundary condition, limiting the applicability of our regularity estimates (8).

2 Separation of variables

For much of our analysis, we treat A in (5) as an abstract, unbounded, self-adjoint linear operator in a real Hilbert space \mathbb{H} . We make the following assumptions:

- 1. the eigenfunctions ϕ_0 , ϕ_1 , ϕ_2 , ... of A form a complete orthonormal system in \mathbb{H} ;
- 2. the associated eigenvalues $\lambda_0, \lambda_1, \lambda_2, \dots$ are all non-negative.

We will write $\phi_m = \phi_m^D$ and $\lambda_m = \lambda_m^D$, or $\phi_m = \phi_m^N$ and $\lambda_m = \lambda_m^N$, whenever it is necessary to be specific about the boundary condition, that is,

$$\phi_m^{\rm D} = 0$$
 and $\frac{\partial \phi_m^{\rm N}}{\partial n} = 0$ on $\partial \Omega$.

Without loss of generality, we may also assume for convenience that

$$0 = \lambda_0 \le \lambda_1 \le \lambda_2 \le \cdots$$
.

These assumptions are satisfied in the case $Au = -\nabla \cdot (K\nabla u)$ and $\mathbb{H} = L_2(\Omega)$. Note that $\lambda_0^{\mathrm{D}} > 0$ in the case of the Dirichlet boundary condition (3), but $\lambda_0^{\mathrm{N}} = 0$ for the Neumann boundary condition (4).

Denote the inner product and norm in \mathbb{H} by $\langle u, v \rangle$ and ||u||, respectively. It is convenient to treat u as a function of t taking values in \mathbb{H} . Assumption 1 above implies that

$$u(t) = \sum_{m=0}^{\infty} u_m(t)\phi_m$$
, where $u_m(t) = \langle u(t), \phi_m \rangle$,

and we likewise put $f_m(t) = \langle f(t), \phi_m \rangle$ and $u_{0m} = \langle u_0, \phi_m \rangle$.

Taking the inner product of ϕ_m with (5) gives a scalar initial-value problem

$$\frac{du_m}{dt} + \lambda_m(\omega_\nu * u_m)_t = f_m(t) \quad \text{for } t > 0, \text{ with } u_m(0) = u_{m0}, \tag{9}$$

for each $m \geq 0$. We will construct the solution u_m using the Laplace transform,

$$\hat{v}(z) = \mathcal{L}\{v(t)\} = \int_0^\infty e^{-zt} v(t) dt.$$

Since $\hat{\omega}_{\nu}(z) = z^{-\nu}$, the problem (9) becomes

$$z\hat{u}_m(z) - u_{0m} + \lambda_m z^{1-\nu}\hat{u}_m(z) = \hat{f}_m(z)$$

and so

$$\hat{u}_m(z) = \frac{u_{0m} + \hat{f}_m(z)}{z + \lambda_m z^{1-\nu}}. (10)$$

A geometric series expansion shows that

$$\mathcal{L}^{-1}\left\{\frac{1}{z+\lambda z^{1-\nu}}\right\} = E_{\nu}(-\lambda t^{\nu}),\tag{11}$$

where the Mittag-Leffler function [2, p 206–212] is defined by

$$E_{\nu}(t) = \sum_{p=0}^{\infty} \frac{t^p}{\Gamma(1+\nu p)}.$$
(12)

Therefore, the representation (10) implies that

$$u_m(t) = u_{0m} E_{\nu}(-\lambda_m t^{\nu}) + \int_0^t E_{\nu} \left(-\lambda_m (t-s)^{\nu}\right) f_m(s) \, ds, \tag{13}$$

leading us to define the linear operator

$$\mathcal{E}(t)v = \sum_{m=0}^{\infty} E_{\nu}(-\lambda_m t^{\nu}) \langle v, \phi_m \rangle \phi_m. \tag{14}$$

The solution of the fractional diffusion equation (5) is then given by the Duhamel formula,

$$u(t) = \mathcal{E}(t)u_0 + \int_0^t \mathcal{E}(t-s)f(s) ds.$$
 (15)

By deforming the integration contour in the Laplace inversion formula, it follows from (11) that

$$E_{\nu}(-t^{\nu}) = \frac{1}{\pi} \int_0^{\infty} \frac{e^{-xt} x^{\nu-1} \sin \pi \nu \, dx}{(x^{\nu} + \cos \pi \nu)^2 + \sin^2 \pi \nu};\tag{16}$$

see [3, equation (23)]. Hence, $E_{\nu}(-t^{\nu})$ is positive and decreasing for $0 < t < \infty$, and since $E_{\nu}(0) = 1$ it follows that $0 \le E_{\nu}(-t) \le 1$ for all $t \ge 0$. Thus,

$$\|\mathcal{E}(t)v\|^2 = \sum_{m=0}^{\infty} \left(E_{\nu}(-\lambda_m t^{\nu}) \langle v, \phi_m \rangle \right)^2 \le \sum_{m=0}^{\infty} \langle v, \phi_m \rangle^2 = \|v\|^2,$$

and the formal construction above, leading to (15), does in fact define a function $u:[0,\infty)\to\mathbb{H}$, satisfying

$$||u(t)|| \le ||u_0|| + \int_0^t ||f(s)|| ds$$
 for $t \ge 0$.

3 Sobolev spaces

To measure the spatial regularity of $v \in \mathbb{H}$ we introduce the norm $||v||_r$ defined by

$$||v||_r^2 = ||(I+A)^{r/2}v||^2 = \sum_{m=0}^{\infty} (1+\lambda_m)^r \langle v, \phi_m \rangle^2 \text{ for } 0 \le r < \infty,$$

and define the associated Hilbert space $\dot{H}^r = \{ v \in \mathbb{H} : ||v||_r < \infty \}.$

For the concrete partial differential operator $Au = -\nabla \cdot (K\nabla u)$ and the space $\mathbb{H} = L_2(\Omega)$, we write $\dot{H}^r = \dot{H}^r_D$ if we want to emphasize that $\phi_m = \phi_m^D$, and $\dot{H}^r = \dot{H}^r_N$ if $\phi_m = \phi_m^N$. If Ω is C^{∞} , then

$$\dot{H}_{\rm D}^r = H^r(\Omega) \text{ for } 0 < r < \frac{1}{2} \quad \text{and} \quad \dot{H}_{\rm N}^r = H^r(\Omega) \text{ for } 0 < r < \frac{3}{2}, \quad (17)$$

and for $j = 1, 2, 3, \ldots$,

$$\dot{H}_{\rm D}^r = \{ v \in H^r(\Omega) : u = Au = \dots = A^{j-1}u = 0 \text{ on } \partial\Omega \}$$
for $2j - \frac{3}{2} < r < 2j + \frac{1}{2}$, (18)

and

$$\dot{H}_{N}^{r} = \left\{ v \in H^{r}(\Omega) : \partial_{n} u = \partial_{n} A u = \dots = \partial_{n} A^{j-1} u = 0 \text{ on } \partial\Omega \right\}$$
for $2j - \frac{1}{2} < r < 2j + \frac{3}{2}$. (19)

For the exeptional Dirichlet index $r=2j-\frac{3}{2}$, the condition $A^{j-1}u=0$ on $\partial\Omega$ is replaced by $A^{j-1}u\in \tilde{H}^{1/2}(\Omega)$, and similarly for the exceptional Neumann index $r=2j-\frac{1}{2}$ the condition $\partial_n A^{j-1}u=0$ on $\partial\Omega$ is replaced by $\partial_n A^{j-1}u\in \tilde{H}^{1/2}(\Omega)$. These results are proved using elliptic regularity theory and interpolation [12, page 34], [13, Theorem 4.3.3]. If Ω is not C^{∞} then we must restrict r accordingly; for instance, if Ω is Lipschitz then the above relations are valid for $r\leq 1$, and if Ω is convex or $C^{1,1}$, then we can allow $r\leq 2$.

4 Homogenous problem

In this section, we consider (5) when $f(t) \equiv 0$, so that the solution (15) reduces to $u(t) = \mathcal{E}(t)u_0$. Our results assume that $u_0 \in \dot{H}^r$ for some $r \geq 0$. In practice, for generic, reasonably smooth data, this assumption holds only for $r < \frac{1}{2}$ in the case of a Dirichlet boundary condition, and only for $r < \frac{3}{2}$ in the case of a Neumann boundary condition; see (17). If u_0 happens to satisfy the boundary condition, then by (18) and (19) these restrictions are relaxed to $r < \frac{5}{2}$ and $r < \frac{7}{2}$, respectively.

Let $\lambda_+ = \min\{\lambda_m : \lambda_m > 0\}$ denote the smallest, strictly positive eigenvalue of A. Since $E_{\nu}(0) = 1$, we make the splitting

$$\mathcal{E}(t) = \mathcal{E}_0 + \mathcal{E}_+(t),$$

where

$$\mathcal{E}_0 v = \sum_{\lambda_m = 0} \langle v, \phi_m \rangle \phi_m$$
 and $\mathcal{E}_+(t) v = \sum_{\lambda_m \ge \lambda_+} E_{\nu}(-\lambda_m t^{\nu}) \langle v, \phi_m \rangle \phi_m$;

of course, if $\lambda_0 > 0$, so that $\lambda_+ = \lambda_0$, then $\mathcal{E}_0 = 0$ and $\mathcal{E}_+(t) = \mathcal{E}(t)$. In studying the regularity of $\mathcal{E}(t)v$, it suffices to consider the part $\mathcal{E}_+(t)v$, because

$$\|\mathcal{E}_0 v\|_r = \|\mathcal{E}_0 v\| \le \|v\|$$
 for $0 \le r < \infty$.

The Mittag-Leffler function admits the asymptotic expansion [2, p 207]

$$E_{\nu}(-t) = \sum_{p=1}^{N} \frac{(-1)^{p+1} t^{-p}}{\Gamma(1-\nu p)} + O(t^{-N-1}) \quad \text{as } t \to \infty,$$
 (20)

so in the sum (14) the *m*th Fourier mode is damped by a factor $E_{\nu}(-\lambda_m t^{\nu}) \sim \lambda_m^{-1} t^{-\nu} / \Gamma(1-\nu)$, with the result that for t>0 the solution is smoother than the initial datum, as we see in the next theorem.

Theorem 4.1. Let $0 \le \mu \le 2$ and $0 \le r < \infty$. If $v \in \dot{H}^r$, then

$$\|\mathcal{E}(t)v\|_{r+\mu} \le C_T t^{-\mu\nu/2} \|v\|_r \quad \text{for } 0 < t \le T,$$

and

$$\|\mathcal{E}_{+}(t)v\|_{r+\mu} \le C(1+\lambda_{+}^{-1})^{\mu/2}t^{-\mu\nu/2}\|v\|_{r} \quad \text{for } 0 < t < \infty.$$

Proof. Put $g(t) = E_{\nu}(-t^{\nu})$ so that

$$\|\mathcal{E}(t)v\|_{r+\mu}^{2} = \sum_{m=0}^{\infty} (1+\lambda_{m})^{r+\mu} g(\lambda_{m}^{1/\nu}t)^{2} \langle v, \phi_{m} \rangle^{2}.$$

From the series definition (12) and the asymptotic expansion (20), we see that

$$g(t) \le C \min(1, t^{-\nu}) \le C(1 + t^{\nu})^{-\mu/2}$$
 for $0 < t < \infty$.

Thus, if $0 < t \le 1$ then

$$g(\lambda_m^{1/\nu}t)^2 \le C(1+\lambda_m t^{\nu})^{-\mu} = Ct^{-\mu\nu}(t^{-\nu}+\lambda_m)^{-\mu} \le Ct^{-\mu\nu}(1+\lambda_m)^{-\mu}$$

and so

$$\|\mathcal{E}(t)v\|_{r+\mu}^2 \le Ct^{-\mu\nu} \sum_{m=0}^{\infty} (1+\lambda_m)^r \langle v, \phi_m \rangle^2 = Ct^{-\mu\nu} \|v\|_r^2.$$

In addition, $g(t) \leq Ct^{-\mu\nu/2}$ for $0 < t < \infty$, implying that

$$g(\lambda_m^{1/\nu}t)^2 \le C\lambda_m^{-\mu}t^{-\mu\nu} = Ct^{-\mu\nu}\left(\frac{1+\lambda_m}{\lambda_m}\right)^{\mu}(1+\lambda_m)^{-\mu}$$

$$\le Ct^{-\mu\nu}(1+\lambda_+^{-1})^{\mu}(1+\lambda_m)^{-\mu} \quad \text{when } \lambda_m > 0,$$

from which the estimate for $\|\mathcal{E}_{+}(t)v\|_{r+\mu}$ follows at once.

In the case of classical diffusion, the *m*th Fourier mode of the initial datum is damped by a factor $E_1(-\lambda_m t) = e^{-\lambda_m t}$, with the result that $||u(t)||_{r+\mu} \le Ct^{-\mu/2}||v||_r$ for every $\mu > 0$. The weaker damping of the high frequency modes in the case of fractional diffusion accounts for the restriction $\mu \le 2$ in part 1 of Theorem 4.1.

The same method of proof works for the time derivatives of $\mathcal{E}(t)$.

Theorem 4.2. Let $-2 \le \mu \le 2$, $0 \le r < \infty$ and $q \in \{1, 2, 3, ...\}$. If $v \in \dot{H}^r$, then

$$t^q \| \mathcal{E}^{(q)}(t) v \|_{r+\mu} \le C_{q,T} t^{-\mu\nu/2} \| v \|_r \quad \text{for } 0 < t \le T,$$

and

$$t^q \|\mathcal{E}^{(q)}(t)v\|_{r+\mu} \le C_q (1+\lambda_{\perp}^{-1})^{\mu/2} t^{-\mu\nu/2} \|v\|_r \quad \text{for } 0 < t \le \infty.$$

Proof. Once again, we define $g(t) = E_{\nu}(-t^{\nu})$ so that $g(\lambda^{1/\nu}t) = E_{\nu}(-\lambda t^{\nu})$. For $0 < t < \infty$, the asymptotic expansion (20) implies that

$$|t^q|g^{(q)}(t)| \le C_q \min(t^{\nu}, t^{-\nu}) \le C_q t^{-\mu\nu/2}$$

so by the chain rule,

$$t^{q} \left| \left(\frac{d}{dt} \right)^{q} g(\lambda_{m}^{1/\nu} t) \right| = (\lambda_{m}^{1/\nu} t)^{q} \left| g^{(q)} (\lambda_{m}^{1/\nu} t) \right| \le C_{q} (\lambda_{m}^{1/\nu} t)^{-\mu\nu/2} = C_{q} t^{-\mu\nu/2} \lambda_{m}^{-\mu/2}$$

$$\le C_{q} t^{-\mu\nu/2} (1 + \lambda_{+}^{-1})^{\mu/2} (1 + \lambda_{m})^{-\mu/2} \quad \text{for } \lambda_{m} \ge \lambda_{+},$$

and the second estimate follows at once, noting that $\mathcal{E}^{(q)}(t) = \mathcal{E}^{(q)}_+(t)$. To prove the first estimate, we use

$$t^{q}|g^{(q)}(t)| \le \begin{cases} C_{q}t^{-\nu\mu/2}, & -2 \le \mu \le 0, \\ C_{q}(1+t^{\nu})^{-\mu/2}, & 0 \le \mu \le 2, \end{cases}$$

to obtain

$$t^{q} \left| \left(\frac{d}{dt} \right)^{q} g(\lambda_{m}^{1/\nu} t) \right| \leq \begin{cases} C_{q} \lambda_{m}^{-\mu/2} t^{-\mu\nu/2}, & -2 \leq \mu \leq 0, \\ C_{q} (1 + \lambda_{m} t^{\nu})^{-\mu/2}, & 0 \leq \mu \leq 2. \end{cases}$$
$$\leq C_{q} t^{-\mu\nu/2} (1 + \lambda_{m})^{-\mu/2} \quad \text{for } 0 < t \leq 1.$$

The following expansion describes in finer detail the behaviour of $\mathcal{E}(t)v$ as $t \to 0$.

Theorem 4.3. Let $0 \le \mu \le 2$ and $0 \le r < \infty$. If $v \in \dot{H}^{r+2M}$, then

$$\mathcal{E}(t)v = v + \sum_{p=1}^{M-1} \frac{(-1)^p t^{\nu p}}{\Gamma(1+\nu p)} A^p v + R_M(t) A^M v,$$

where the operator $R_M(t)$ satisfies

$$||R_M(t)v||_{r+\mu} \le C_{M,T} t^{M\nu-\mu\nu/2} ||v||_r \quad \text{for } 0 < t \le T.$$

Proof. From (12) and (20), we see that the function

$$g_M(t) = t^{-M\nu} \left(E_{\nu}(-t^{\nu}) - \sum_{\nu=0}^{M-1} \frac{(-1)^{\nu} t^{\nu p}}{\Gamma(1+\nu p)} \right),$$

satisfies $|g_M(t)| \leq C_M \min(1, t^{-\nu})$. Since

$$E_{\nu}(-\lambda t^{\nu}) = 1 + \sum_{p=1}^{M-1} \frac{(-1)^p t^{\nu p}}{\Gamma(1+\nu p)} \lambda^p + t^{M\nu} g_M(\lambda^{1/\nu} t) \lambda^M,$$

we may estimate $||R_M(t)v||_{r+\mu}$ by the same method as in the proof of Theorem 4.1.

Notice that the case M=1 with r=0 and $\mu=2-\alpha$ gives the estimate

$$||v - \mathcal{E}(t)v||_{2-\alpha} \le Ct^{\nu - (2-\alpha)\nu/2} = Ct^{\alpha\nu/2}||Av|| \text{ for } 0 \le \alpha \le 2,$$

and since $\mathcal{E}(t)$ commutes with $(I+A)^{(\alpha-2)/2}$,

$$||v - \mathcal{E}(t)v|| \le Ct^{\alpha\nu/2}||v||_{\alpha}$$
 for $0 \le \alpha \le 2$,

showing that $\mathcal{E}(t)v \to v$ in \mathbb{H} if $v \in \dot{H}^r$ for any r > 0.

To conclude this section, we show that bounds of the form (6) and (7) hold.

Theorem 4.4. If $\sigma = r\nu/2$ and $q \in \{1, 2, 3, ...\}$, then for $0 < t \le T$ the solution of the homogeneous problem, $u = \mathcal{E}(t)u_0$, satisfies

$$t^{q-1+\nu} ||Au^{(q)}(t)|| \le C_{q,T} t^{\sigma-1} ||u_0||_r \quad \text{for } 0 \le r \le 4,$$

and

$$t^{q-1} \|u^{(q)}(t)\| \le C_{q,T} t^{\sigma-1} \|u_0\|_r \quad \text{for } 0 \le r \le 2.$$

Proof. The first estimate follow by taking $\mu = 2 - r$ in Theorem 4.2, and the second by taking $\mu = -r$.

5 Inhomogenous problem

We now consider (5) with $u_0 = 0$ and nonzero f, so that (15) reduces to

$$u(t) = \int_0^t \mathcal{E}(t-s)f(s) \, ds. \tag{21}$$

For our regularity estimates, we will make use of several lemmas involving the differential operator D defined by

$$Dv(t) = tv(t).$$

The first shows that the bounds of Theorem 4.2 hold with $t^q \mathcal{E}^{(q)}(t)$ replaced by $D^q \mathcal{E}(t)$.

Lemma 5.1. For $q \in \{1, 2, 3, ...\}$ there exists constants a_{qj} and b_{qj} such that

$$D^q v(t) = \sum_{j=1}^q a_{qj} t^j v^{(j)}(t)$$
 and $t^q v^{(q)}(t) = \sum_{j=1}^q b_{qj} D^j v(t)$.

Proof. Use induction on q.

The next lemma shows how D acts on a convolution.

Lemma 5.2. We have the identities

1.
$$D(v*w) = v*w + (Dv)*w + v*(Dw),$$

2.
$$D\omega_{\mu} = (\mu - 1)\omega_{\mu}$$

3.
$$D(\omega_{\mu} * v) = \omega_{\mu} * (D + \mu)v$$
.

Proof. We observe that

$$\frac{\partial}{\partial t} \int_0^t v(t-s)w(s) \, ds = v(0)w(t) + \int_0^t v'(t-s)w(s) \, ds$$

SO

$$D(v * w)(t) = v(0)tw(t) + \int_0^t (Dv)(t-s)w(s) \, ds + \int_0^t sv'(t-s)w(s) \, ds.$$

Integration by parts gives

$$\int_0^t sv'(t-s)w(s)\,ds = -v(0)tw(t) + (v*w)(t) + (v*Dw)(t),$$

implying the identity in part 1. For part 2 we have $D\omega_{\mu}(t) = t\omega'_{\mu}(t) = t(\mu - 1)t^{\mu - 2}/\Gamma(\mu) = (\mu - 1)\omega_{\mu}(t)$, and together these first two results give

$$D(\omega_{\mu} * v) = \omega_{\mu} * v + (\mu - 1)\omega_{\mu} * v + \omega_{\mu} * (Dv) = \omega_{\mu} * (\mu v + Dv),$$

proving part 3.

Applying D^q to a convolution yields a sum of the following form.

Lemma 5.3. There exist constants a_{qjk} such that

$$D^{q}(v * w) = \sum_{j+k \le q} a_{qjk}(D^{j}v) * (D^{k}w).$$

Proof. We again use induction on q. Part 1 of Lemma 5.2 shows that the case q = 1 holds with $a_{100} = a_{110} = a_{101} = 1$, and that

$$D\big[(D^jv)*(D^kw)\big] = (D^jv)*(D^kw) + (D^{j+1}v)*(D^kw) + (D^jv)*(D^{k+1}w),$$

from which the inductive step follows at once.

We can now prove the analogue of Theorems 4.1 and 4.2 with $\mu = 0$.

Theorem 5.4. Let $0 \le r < \infty$ and $q \in \{0, 1, 2, ...\}$. Then,

$$t^q \| (\mathcal{E} * f)^{(q)}(t) \|_r \le C_q \sum_{j=0}^q \int_0^t s^j \| f^{(j)}(s) \|_r ds \quad \text{for } 0 < t < \infty.$$

Proof. Taking $\mu = 0$ in Theorems 4.1 and 4.2, we have $||D^q \mathcal{E}(t)v||_r \leq C_q ||v||_r$, so by Lemma 5.3,

$$||D^{q}(\mathcal{E} * f)||_{r} \leq C_{q} \sum_{j+k \leq q} \int_{0}^{t} ||(D^{j}E)(t-s)(D^{k}f)(s)||_{r} ds$$

$$\leq C_{q} \sum_{j=0}^{q} \int_{0}^{t} ||D^{j}f(s)||_{r} ds,$$

and the result follows by Lemma 5.1.

The preceding proof easily generalizes to show that

$$t^{q} \| (\mathcal{E} * f)^{(q)}(t) \|_{r+\mu} \le C_{q} \sum_{j=0}^{q} \int_{0}^{t} (t-s)^{-\mu\nu/2} s^{j} \| f^{(j)}(s) \|_{r} ds$$

for $0 \le \mu \le 2$ if q = 0, and for $-2 \le \mu \le 2$ if $q \ge 1$. However, we will derive an alternative bound in which the factor $(t-s)^{-\mu\nu/2}$ in the integrand is replaced by $t^{-\mu\nu/2}$ (for $0 \le \mu \le 2$), at the cost of adding a term with j = q+1.

We integrate (5) with respect to t, remembering that $u_0 = 0$, to see that $u = \mathcal{E} * f$ satisfies

$$u + \omega_{\nu} * Au = F$$
 where $F(t) = \int_0^t f(s) ds$.

Since $\omega_{1-\nu} * \omega_{\nu} = \omega_1$, it follows that

$$\omega_1 * Au = \omega_{1-\nu} * \omega_{\nu} * Au = \omega_{1-\nu} * (F-u),$$

or in other words,

$$\int_0^t Au(s) \, ds = \int_0^t \frac{(t-s)^{-\nu}}{\Gamma(1-\nu)} \left[F(s) - u(s) \right] ds.$$

Using part 3 of Lemma 5.2, we have

$$D(\omega_1 * Au) = D(\omega_{1-\nu} * (F-u)) = \omega_{1-\nu} * (D+1-\nu)(F-u),$$

implying that

$$tAu(t) = \int_0^t \frac{(t-s)^{-\nu}}{\Gamma(1-\nu)} (D+1-\nu) [F(s) - u(s)] ds.$$
 (22)

The desired estimate will follow using this representation and the following identities.

Lemma 5.5. There exist constants c_{qj} such that

$$t^q v^{(q)}(t) = t^{-1} \sum_{j=0}^q c_{qj} D^j(tv)$$
 and $D^q(tv) = t \sum_{j=0}^q \binom{q}{j} D^j v$.

Proof. Use induction on q.

We now arrive at the main result for this section.

Theorem 5.6. Let $0 \le \mu \le 2$, $0 \le r < \infty$ and $q \in \{0, 1, 2, ...\}$ Then,

$$t^{q} \| (\mathcal{E} * f)^{(q)}(t) \|_{r+\mu} \le C_{q,\nu} (1 + t^{-\mu\nu/2}) \sum_{j=0}^{q+1} \int_{0}^{t} s^{j} \| f^{(j)}(s) \|_{r} ds.$$

Proof. Put $u = \mathcal{E} * f$. The first identity in Lemma 5.5 shows that to bound $t^q ||u^{(q)}(t)||_{r+2}$ it suffices to consider

$$t^{-1}\|D^q(tu)\|_{r+2} = t^{-1}\|(I+A)D^q(tu)\|_r \le t^{-1}\|D^q(tu)\|_r + t^{-1}\|D^q(tAu)\|_r.$$

The second identity in Lemma 5.5 and the fact that, by (22),

$$D^{q}(tAu) = D^{q}(\omega_{1-\nu} * (D+1-\nu)(F-u)) = \omega_{1-\nu} * (D+1-\nu)^{q+1}(F-u)$$

then give

$$t^{-1} \|D^{q}(tu)\|_{r+2} \le C_{q} \left(\sum_{j=0}^{q} \|D^{j}u\|_{r} + t^{-1} \sum_{j=0}^{q+1} \omega_{1-\nu} * \|D^{j}(F-u)\|_{r} \right),$$

in which the first sum may be estimated using Theorem 5.4.

Part 2 of Lemma 5.2 and Lemma 5.3 give

$$D^{j}(F - u) = D^{j}(\omega_{1} * f - \mathcal{E} * f) = \omega_{1} * (D + 1)^{j} f - \sum_{k+l \le j} a_{jkl}(D^{k}\mathcal{E}) * (D^{l}f)$$

so by Theorem 4.1,

$$||D^{j}(F-u)||_{r} \leq C_{j} \sum_{k=0}^{j} \int_{0}^{t} ||D^{k}f(s)||_{r} ds = C_{j} \sum_{k=0}^{j} \omega_{1} * ||D^{k}f||_{r}$$

and hence

$$t^{-1}\omega_{1-\nu} * ||D^{j}(F-u)||_{r} \le C_{j} \sum_{k=0}^{j} t^{-1}\omega_{2-\nu} * ||D^{k}f||_{r}.$$

Since $\omega_{2-\nu} * ||D^k f||_r \le Ct^{1-\nu} \int_0^t ||D^k f(s)||_r ds$, we conclude that

$$|t^{-1}||D^q(tu)||_{r+2} \le C_q(1+t^{-\nu})\sum_{j=0}^{q+1}\int_0^t ||D^jf(s)||_r ds$$

and thus

$$t^{q} \|u^{(q)}(t)\|_{r+2} \le C_{q} \sum_{j=0}^{q} t^{-1} \|D^{j}(tu)\|_{r+2} \le C_{q} (1+t^{-\nu}) \sum_{j=0}^{q+1} \int_{0}^{t} \|D^{j}f(s)\| \, ds,$$

proving the result in the case $\mu = 2$. The general case follows by Theorem 5.4 using the interpolation inequality

$$||v||_{r+\mu} \le (||v||_r)^{1-\mu/2} (||v||_{r+2})^{\mu/2}.$$

We can further investigate the behaviour of $\mathcal{E} * f$ as $t \to 0$ using the expansion of $\mathcal{E}(t)v$ given in Theorem 4.3. For instance, if

$$f(t) = \frac{t^{\alpha - 1}}{\Gamma(\alpha)} v = \omega_{\alpha}(t)v$$
 for $\alpha > 0$ and $v \in \dot{H}^{r+2M}$,

then

$$\mathcal{E} * f = \left(\sum_{p=0}^{M-1} (-1)^p \omega_{1+\nu p} A^p + R_M A^M\right) * \omega_{\alpha} v$$
$$= \sum_{p=0}^{M-1} (-1)^p \omega_{1+\nu p+\alpha} A^p v + R_M * \omega_{\alpha} A^M v,$$

that is, since $||R_M * \omega_\alpha A^M v||_r \le C\omega_{1+\nu M} * \omega_\alpha ||A^M v||_r \le C\omega_{1+\nu M+\alpha} ||v||_{r+2M}$,

$$(\mathcal{E} * f)(t) = \frac{t^{\alpha}}{\Gamma(1+\alpha)} v + \sum_{p=1}^{M-1} \frac{(-1)^p t^{\nu p + \alpha}}{\Gamma(1+\nu p + \alpha)} A^p v + O(t^{\nu M + \alpha}) \quad \text{as } t \to 0.$$

As for the homogeneous problem, we have bounds of the form (6) and (7).

Theorem 5.7. If $\sigma = r\nu/2$, $0 \le r \le 2$ and $q \in \{1, 2, 3, ...\}$, then the solution $u = \mathcal{E} * f$ of the inhomogeneous problem with $u_0 = 0$ satisfies

$$t^{q-1+\nu} ||Au^{(q)}(t)|| \le C_{q,T} t^{\sigma-1} \sum_{j=0}^{q+1} \int_0^t s^j ||f^{(j)}(s)||_r ds.$$

and

$$|t^{q-1}||u^{(q)}(t)|| \le C_{q,T}t^{\sigma-1}\sum_{j=0}^q \int_0^t s^{j-\sigma}||f^{(j)}(s)|| ds$$

for $0 < t \le T$.

Proof. Take $\mu = 2 - r$ in Theorem 5.6 for the first estimate, and use Theorem 5.4 with r = 0 for the second, noting that

$$\int_0^t s^j \|f^{(j)}(s)\| \, ds \le t^{\sigma} \int_0^t s^{j-\sigma} \|f^{(j)}(s)\| \, ds.$$

The preceding analysis assumes that f(t) is sufficiently smooth as a function of t for t > 0. For an example of what happens if this assumption is not satisfied, suppose that f is piecewise smooth with just a single jump discontinuity at t = a for some a > 0. Writing $[f]_a = f(a^+) - f(a^-)$ we have

$$Df(t) = a[f]_a \delta(t - a) + v(t),$$

where v is piecewise smooth, and so, by Lemma 5.2,

$$D(\mathcal{E} * f)(t) = a\mathcal{E}(t - a)[f]_a + (\mathcal{E} * f + (D\mathcal{E}) * f + \mathcal{E} * v)(t) \quad \text{for } t > a.$$

6 Incompatible initial data

We will describe the behaviour of the solution when the initial datum u_0 is not compatible with the given boundary condition, in the simple case when the spatial domain is the positive half-axis $\Omega = (0, \infty)$, and $f(t) \equiv 0$.

Consider first the case $\Omega = (-\infty, \infty)$, that is,

$$u_t - K(\omega_{\nu} * u_{xx})_t = 0$$
 and $u(x, 0) = u_0(x)$,

for $-\infty < x < \infty$ and t > 0, with u(x,t) bounded as $x \to \pm \infty$. Denoting the Fourier transform of u by

$$\tilde{u}(\xi,t) = \mathcal{F}\{u(x,t)\} = \int_{-\infty}^{\infty} e^{-i\xi x} u(x,t) \, dx,$$

we see that

$$\tilde{u}_t + K\xi^2(\omega_\nu * \tilde{u})_t = 0$$
 with $\tilde{u}(\xi, 0) = \tilde{u}_0(\xi)$.

Thus, \tilde{u} satisfies an equation having the same form as (9), except that $K\xi^2$ takes the place of λ_m , and no source term is present. Hence, by (13),

$$\tilde{u}(\xi, t) = E_{\nu}(-K\xi^2 t^{\nu})\tilde{u}_0(\xi),$$

and therefore

$$u(x,t) = \int_{-\infty}^{\infty} G(x - y, t) u_0(y) \, dy$$
 (23)

where the Green function, or fundamental solution, is given by

$$G(x,t) = \mathcal{F}^{-1}\{E_{\nu}(-K\xi^{2}t^{\nu})\} = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\xi x} E_{\nu}(-K\xi^{2}t^{\nu}) d\xi.$$
 (24)

The inverse Fourier transform (24) may be expressed in terms of the M-Wright function [5],

$$M_{\alpha}(x) = \sum_{n=0}^{\infty} \frac{(-1)^n x^n}{n! \Gamma(1 - \alpha(n+1))} = \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n-1} x^{n-1}}{(n-1)!} \Gamma(\alpha n) \sin(\pi \alpha n),$$

where the identity $\Gamma(z)\Gamma(1-z) = \pi/\sin \pi z$ shows that the two series are equal. In fact [5, Section 4.5],

$$\mathcal{F}\{M_{\alpha}(|x|)\} = 2E_{2\alpha}(-\xi^2) \text{ for } 0 < \alpha < 1,$$

SO

$$G(x,t) = \frac{1}{2\sqrt{Kt^{\nu}}} M_{\nu/2} \left(\frac{|x|}{\sqrt{Kt^{\nu}}}\right).$$

Notice that for each t > 0, the function $x \mapsto G(x,t)$ is not differentiable at x = 0. However, in the limiting case when $\nu \to 1$, we have $M_{1/2}(x) = \pi^{-1/2} \exp(-x^2/4)$ and G(x,t) is just the classical heat kernel, which is C^{∞} for t > 0.

The behaviour of G(x,t) for large x may be seen from the asymptotic formula [5, equation (4.5)]

$$M_{\alpha}(x/\alpha) \sim \frac{x^{(\alpha-1/2)/(1-\alpha)}}{\sqrt{2\pi(1-\alpha)}} \exp(-(1-\alpha)r^{1/(1-\alpha)}/\alpha)$$
 as $x \to \infty$,

where $0 < \alpha < 1$. It follows that the integral (23) converges for t > 0 if u_0 is locally integrable and bounded on $(-\infty, \infty)$.

Now consider the problem on the half-line $\Omega = (0, \infty)$ with a Dirichlet boundary condition,

$$u_t - K(\omega_{\nu} * u_{xx})_t = 0, \qquad u(x,0) = u_0(x), \qquad u(0,t) = 0,$$
 (25)

for $0 < x < \infty$ and t > 0. By taking the odd extension of the initial datum to $(-\infty, \infty)$, so that $u_0(-x) = -u_0(x)$, we obtain the solution to (25):

$$u(x,t) = \int_{-\infty}^{\infty} G(x-y,t)u_0(y) \, dy = \int_{0}^{\infty} \left[G(x-y,t) - G(x+y,t) \right] u_0(y) \, dy.$$

Suppose now that $u_0(0) \neq 0$. This means that u_0 fails to satisfy the boundary condition, and so u(x,t) is discontinuous at (x,t) = (0,0). To see the nature of the discontinuity we rewrite the solution as

$$u(x,t) = \int_{-\infty}^{x} G(y,t)u_0(x-y) \, dy - \int_{x}^{\infty} G(y,t)u_0(y-x) \, dy.$$

Let $\psi(x,t)$ denote the solution in the special case when $u_0(x) = 1$ for all x > 0, that is

$$\psi(x,t) = \int_{-\infty}^{x} G(y,t) \, dy - \int_{x}^{\infty} G(y,t) \, dy, \tag{26}$$

then in the general case,

$$u(x,t) = u_0(0)\psi(x,t) + v(x,t),$$

where v is the solution with initial datum $u_0(x) - u_0(0)$, and is therefore continuous at (0,0). Since

$$\int_{-\infty}^{\infty} G(y,t) \, dy = \tilde{G}(0,t) = E_{\nu}(0) = 1,$$

we can simplify (26)

$$\psi(x,t) = 1 - 2 \int_{x}^{\infty} G(y,t) \, dy = 1 - \frac{1}{\sqrt{Kt^{\nu}}} \int_{x}^{\infty} M_{\nu/2} \left(\frac{|y|}{\sqrt{Kt^{\nu}}}\right) dy,$$

and obtain ψ in the form of a similarity solution,

$$\psi(x,t) = \Psi\left(\frac{x}{\sqrt{Kt^{\nu}}}\right)$$
 where $\Psi(x) = 1 - \int_{x}^{\infty} M_{\nu/2}(y) \, dy$.

If we fix t > 0 and let $x \to 0$, then $\psi(x,t) \to \Psi(0) = 0$, whereas if we fix x > 0 and let $t \to 0$, then $\psi(x,t) \to \Psi(\infty) = 1$.

To handle a Neumann boundary condition, $u_x(0,t) = 0$, we proceed in the same way except that we use the *even* extension of u_0 , so that $u_0(-x) = u_0(x)$ and

$$u(x,t) = \int_0^\infty \left[G(x-y,t) + G(x+y,t) \right] u_0(y) \, dy$$

= $\int_{-\infty}^x G(y,t) u_0(x-y) \, dy + \int_x^\infty G(y,t) u_0(y-x) \, dy.$

Although $u(x,t) \to u(0,0) = u_0$ as $(x,t) \to (0,0)$, the derivative

$$u_x(x,t) = \int_{-\infty}^{x} G(y,t)u_0'(x-y) \, dy - \int_{x}^{\infty} G(y,t)u_0'(y-x) \, dy$$

is discontinuous at (0,0). In the special case $u_0(x) = x$ for x > 0, we have $u_x(x,t) = \psi(x,t)$, and in general

$$u_x(x,t) = u'_0(0)\psi(x,t) + v(x,t),$$

with v continuous at (0,0).

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References

- [1] Eduardo Cuesta, Christian Lubich and Cesar Palencia. Convolution quadrature time discretization of fractional diffusion-wave equations, *Math. Comp.*, 75:673–696, 2006. http://dx.doi.org/10.1090/S0025-5718-06-01788-1
- [2] A. Erdelyi, *Higher Transendental Functions*, Volume 3, McGraw-Hill, 1955.
- [3] Rudolf Gorenflo, Joulia Loutchko and Yuri Luchko, Computation of the Mittag-Leffler function $E_{\alpha,\beta}(z)$ and its derivative, Fract. Calc. Appl. Anal., 5:491–518, 2002, and Correction, 6:111-112, 2003.
- [4] B. I. Henry and S. L. Wearne, Fractional reaction-diffusion, *Physica A*, 276:448-455, 2000.
- [5] Francesco Mainardi, Antonio Mura and Gianni Pagnini, The M-Wright function in time-fractional diffusion processes: a tutorial survey, International Journal of Differential Equations, Article ID 104505, 29 p, 2010. http://dx.doi.org/10.1155/2010/104505.
- [6] William McLean and Kassem Mustapha, A second-order accurate numerical method for a fractional wave equation, *Numer. Math.*, 105:481–510, 2007. http://dx.doi.org/10.1007/s00211-006-0045-y.

- [7] William McLean and Kassem Mustapha, Convergence analysis of a discontinuous Galerkin method for a fractional diffusion equation, *Numer. Algor.* 52:69–88, 2009. http://dx.doi.org/~10.1007/s11075-008-9258-8.
- [8] W. McLean and V. Thomée, Numerical solution of an evolution equation with a positive-type memory term, J. Austral. Math. Soc. Ser. B, 35:23– 70, 1993.
- [9] William McLean and Vidar Thomée, Maximum-norm error analysis of a numerical solution via Laplace transformation and quadrature of a fractional-order evolution equation, *IMA J. Numer. Anal.*, 30:208–230, 2010. http://dx.doi.org/10.1093/imanum/drp004.
- [10] Ralf Metzler and Joseph Klafter, The random walk's guide to anomalous diffusion: a fractional dynamics approach, *Physics Reports* 339:1–77, 2000. http://dx.doi.org/10.1016/S0370-1573(00)00070-3
- [11] Kassem Mustapha and William McLean, Piecewise-linear, discontinuous Galerkin method for a fractional diffusion equation, *Numer. Algor.*, to appear. http://dx.doi.org/10.1007/s11075-010-9379-8.
- [12] Vidar Thomée, Galerkin Finite Element Methods for Parabolic Problems, Springer Lecture Notes in Mathematics 1054, 1084.
- [13] Hans Triebel, Interpolation Theory, Function Spaces, Differential Operators, Johann Ambrosius Barth Verlag, 1995.