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SURVEY PAPER

FRACTIONAL DIFFUSION ON BOUNDED DOMAINS

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Abstract

The mathematically correct specification of a fractional differential equation on a bounded domain requires specification of appropriate boundary conditions, or their fractional analogue. This paper discusses the application of nonlocal diffusion theory to specify well-posed fractional diffusion equations on bounded domains.

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Key Words and Phrases: fractional diffusion, boundary value problem, nonlocal diffusion, well-posed equation

1. Introduction

The goal of this paper is to address an important open problem in the area of fractional diffusion. Over the past ten years, a wide variety of effective numerical methods have been developed to solve fractional partial differential equations, see for example [12, 13, 19, 24, 26, 28, 29, 43, 30, 37, 39, 45, 46]. However, for the most part, the underlying mathematical theory is lacking. Stability and consistency of the methods are proven, but generally it is not known whether the problems are well-posed, with unique solutions in some suitable class of functions. Since fractional derivatives are nonlocal operators, it is not even clear in general how one should specify boundary conditions. In this paper, we carefully describe this open problem, and outline one possible solution approach using the newly developed theory of nonlocal diffusion [1, 9, 14, 17, 42].

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2. **Fractional diffusion on bounded domains**

The positive and negative Riemann-Liouville fractional derivatives are defined by

$$\mathbb{D}^{\alpha}_{x,L} f(x) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_L^x \frac{f(\xi)}{(x-\xi)^{\alpha+1-n}} d\xi \,,$$

$$\mathbb{D}^{\alpha}_{-x,R} f(x) = \frac{(-1)^n}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_x^R \frac{f(\xi)}{(\xi-x)^{\alpha+1-n}} d\xi \,,$$

where $n-1 < \alpha \leq n$. The special case $L = -\infty$ or $R = +\infty$ is also called the Liouville derivative. If $f(x) = 0$ for all $x < L$, then we also have $\mathbb{D}^{\alpha}_{x,L} f(x) = \mathbb{D}^{\alpha}_{x,-\infty} f(x) := \mathbb{D}^{\alpha}_{x} f(x)$. If $f(x) = 0$ for all $x > R$, then $\mathbb{D}^{\alpha}_{-x,R} f(x) = \mathbb{D}^{\alpha}_{-x,\infty} f(x) := \mathbb{D}^{\alpha}_{-x} f(x)$.

In numerical solutions of space-fractional diffusion equations, one typically specifies the problem using the Riemann-Liouville fractional derivatives $\mathbb{D}^{\alpha}_{\pm x} f(x)$, but then in order to obtain numerical solutions, one has to replace these infinitely nonlocal operators by their finitely nonlocal counterparts $\mathbb{D}^{\alpha}_{x,L} f(x)$ and $\mathbb{D}^{\alpha}_{-x,R} f(x)$, since we cannot solve a numerical problem with an infinite number of grid points.

In a numerical scheme, we approximate the Riemann-Liouville fractional derivatives using a Grünwald-Letnikov finite difference scheme. For any $\alpha > 0$ we can define the Grünwald-Letnikov fractional derivative

$$\mathbf{D}^{\alpha}_{\pm x} f(x) = \lim_{h \to 0} h^{-\alpha} \Delta^{\alpha}_{\pm h} f(x),$$

where

$$\Delta^{\alpha}_{\pm h} f(x) = \sum_{j=0}^{\infty} \binom{\alpha}{j} (-1)^j f(x \mp jh), \quad \binom{\alpha}{j} = \frac{\Gamma(\alpha+1)}{j!\Gamma(\alpha-j+1)} \,. \qquad (2.1)$$

The equivalence between the Riemann-Liouville and Grünwald-Letnikov fractional derivatives is established in [33, Theorem 2.1]: If f is bounded, and $f^{(k)} \in L^1(\mathbb{R})$ for $k \leq n$, for some $n > 1 + \alpha$, then $\mathbf{D}^{\alpha}_{\pm x} f(x)$ exists, and its Fourier transform

$$\int_{-\infty}^{\infty} e^{-ikx} \mathbf{D}^{\alpha}_{\pm x} f(x) \, dx = (\pm ik)^{\alpha} \hat{f}(k).$$

Since the Riemann-Liouville fractional derivative has the same Fourier transform [41, Eq. (7.4)], it follows from the uniqueness of the Fourier transform that the two operators are the same for such functions.

Fourier transforms are fundamental to the theory of numerical analysis for fractional diffusion equations. For example, in order to construct a stable numerical scheme, one typically needs to employ a shifted version of the Grünwald-Letnikov fractional derivative, replacing $f(x \mp jh)$ in (2.1)

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by $f(x \mp (j+s)h)$, where s is an integer (if $1 < \alpha < 2$, we take $s = 1$). The proof of $O(h)$ convergence for the shifted finite difference, [28, Theorem 2.4], also uses Fourier transform methods.

Remark 2.1. It is also possible to use Fourier transform methods on a bounded domain. One simply needs to redefine $f(x) = 0$ outside the domain, and use Fourier transforms on the modified function, as in Chen and Deng [8]. In this way, one can establish rates of convergence and develop higher-order (e.g., 4th order) schemes. For example, if $1 < \alpha < 2$ and $f, \mathbb{D}_x^\alpha f(x)$ are in $L^1(\mathbb{R})$ with Fourier transforms in $L^1(\mathbb{R})$, then [8, Lemma 2.3] shows that

$$\mathbb{D}_{x,L}^\alpha f(x) = h^{-\alpha}\Delta_{h,L}^\alpha f(x) + O(h),$$

where

$$\Delta_{h,L}^\alpha f(x) = \sum_{j=0}^{[(x-L)/h]} \binom{\alpha}{j} (-1)^j f(x - jh) \tag{2.2}$$

using the fractional binomial coefficients defined in (2.1). The book of Podlubny [39, pp. 49–55 and 62–63] proves that $h^{-\alpha}\Delta_{h,L}^\alpha f(x) \to \mathbb{D}_{x,L}^\alpha f(x)$ as $h \to 0$ using combinatorial arguments, assuming that $f(x)$ and its derivatives of order up to $m+1$ exist and are continuous in the interval $[L, x]$, where $m < \alpha < m+1$. Podlubny [39, p. 224] then cites Lubich [25] to show that the numerical methods developed in [39, Chapter 8] are $O(h)$. This proof, which does not rely on Fourier transforms, is considerably longer.

3. Illustration

Consider the space-fractional diffusion equation with drift

$$\partial_t p(x,t) = -v(x,t)\partial_x p(x,t) + a(x,t)\mathbb{D}_x^\alpha p(x,t) + b(x,t)\mathbb{D}_{-x}^\alpha p(x,t) + g(x,t)$$

on a finite domain $L < x < R$, $0 \le t \le T$. If v, a, b are constants and $g = 0$, then the Green's function solutions to this equation on the real line are stable densities [33, Section 1.2], and there are widely available tools to compute these special functions (e.g., see [33, Chapter 5]). These solutions are useful for example in hydrology, where they model solute transport in underground aquifers [4, 5, 6] and rivers [12, 22, 23]. For the general, variable coefficient space-fractional diffusion equation, a number of effective numerical methods have been developed to compute solutions to this problem, see for example [12, 13, 19, 24, 26, 28, 29, 43, 30, 37, 39, 45, 46]. The most popular in practical applications are finite difference methods, based on the Grünwald-Letnikov approximation of the Riemann-Liouville fractional derivatives. These codes are *mass-preserving*, since

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$$\sum_{j=0}^{\infty} \binom{\alpha}{j} (-1)^j = 0.$$

For example, in an application to ground water hydrology, the general space-fractional diffusion equation with drift is used when the mean plume velocity v and the fractional diffusivities a, b vary with space and time. An initial function $p_0(x) = p(x, 0)$ describes the concentration of solute at location x, and the solution $p(x, t)$ predicts the concentration at a later time $t > 0$. In the absence of a source term ($g = 0$), the total mass $C_0 = \int p(x, t)\, dx$ will be a constant that does not vary over time. Since the finite difference codes are mass-preserving, the approximate numerical solution will have the same property, i.e., its total mass will not vary over time. This mass-preserving property is very useful in applications.

The following simple example from [43] is typical for the existing literature on finite difference solutions of fractional partial differential equations. As we shall see later in this paper, insights from the newly developed theory of nonlocal diffusion strongly suggest that this formulation *is not* well-posed. The space-fractional diffusion equation

$$\partial_t p(x, t) = a(x) \mathbb{D}_x^{1.8} p(x, t) + g(x, t) \tag{3.1}$$

on the bounded domain $0 < x < 1$ with

$$\begin{aligned} p(x, 0) &= x^3 \\ p(0, t) &= 0 \\ p(1, t) &= e^{-t} \\ a(x) &= \frac{\Gamma(2.2)}{6} x^{2.8} \\ g(x, t) &= -(1 + x) e^{-t} x^3 \end{aligned} \tag{3.2}$$

has exact solution $p(x, t) = e^{-t} x^3$ for all $t > 0$. Now a Crank-Nicolson scheme [43] with $\Delta t = 1/10$ and $\Delta x = h = 1/10$ gives the solution at time $t = 1.0$, see Figure 1. Evidently, even with this relatively large step size, we obtain a good match to the exact solution.

Because the Grünwald-Letnikov approximation of the Riemann-Liouville fractional derivative is $O(h)$ accurate, the Crank-Nicolson method is only first-order accurate. A standard application of Richardson extrapolation (e.g., see [20]) yields a second order method, as evidenced by the error analysis in Table 1.

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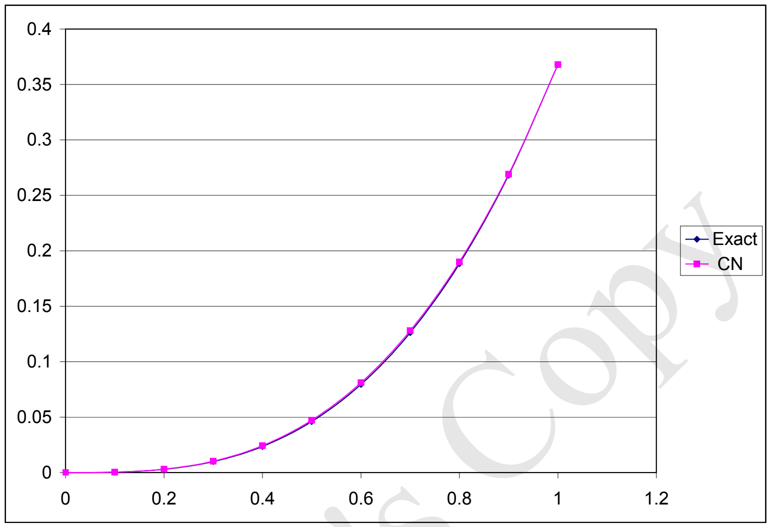

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FIGURE 1. Comparison of the exact and numerical solution to the example problem (3.1), from [43].

Δt	Δx	CN Error	Rate	RE Error	Rate
1/10	1/10	1.82×10^{-3}	–	1.77×10^{-4}	–
1/15	1/15	1.17×10^{-3}	$\approx 15/10$	7.85×10^{-5}	$\approx (15/10)^2$
1/20	1/20	8.64×10^{-4}	$\approx 20/15$	4.41×10^{-5}	$\approx (20/15)^2$
1/25	1/25	6.85×10^{-4}	$\approx 25/20$	2.83×10^{-5}	$\approx (25/20)^2$

TABLE 1. Error analysis for the numerical solution to the example problem (3.1), from [43].

Next we explain how the exact solution to the sample problem (3.1) has been computed. It is not hard to check that

$$
\begin{aligned}
\mathbb{D}^{\alpha}_{x,L}(x-L)^q &= \frac{\Gamma(q+1)}{\Gamma(q+1-\alpha)}(x-L)^{q-\alpha} \\
D^{\alpha}_{-x,R}(R-x)^q &= \frac{\Gamma(q+1)}{\Gamma(q+1-\alpha)}(R-x)^{q-\alpha}
\end{aligned}
\tag{3.3}
$$

see for example [33, Example 2.7]. Assume that $p(x,t) = 0$ for $x \le 0$, so that $\mathbb{D}_x^{1.8} p(x,t) = \mathbb{D}_{x,0}^{1.8} p(x,t)$. Now set $p(x,t) = e^{-t}x^3$ and compute

$$\partial_t p(x,t) = -e^{-t}x^3 \quad \text{and} \quad \mathbb{D}_x^{1.8} p(x,t) = \frac{\Gamma(4)}{\Gamma(2.2)}\, e^{-t}x^{1.2}.$$

Plug this into equation (3.1), and solve to obtain $g(x,t)$. By this calculation, we have shown that there exists *at least one* solution $p(x,t) = e^{-t}x^3$ to the fractional partial differential equation (3.1) on the bounded interval $0 < x < 1$, that satisfies the conditions (3.2).

What is often overlooked in this analysis is that we have *assumed* $p(x,t) = 0$ for $x \le 0$, to make $\mathbb{D}_x^{1.8} p(x,t) = \mathbb{D}_{x,0}^{1.8} p(x,t)$. Suppose instead that $p(x,t) = 1$ for $-1 < x < 0$, and $p(x,t) = 0$ for $x \le -1$. Then

$$\begin{aligned} \mathbb{D}_x^{1.8} p(x,t) &= \frac{\Gamma(4)}{\Gamma(2.2)}\, e^{-t}x^{1.2} + \frac{1}{\Gamma(0.2)} \frac{d^2}{dx^2} \int_{-1}^{0} \frac{1}{(x-\xi)^{0.8}} d\xi \\ &= \frac{6}{\Gamma(2.2)}\, e^{-t}x^{1.2} + \frac{0.8}{\Gamma(0.2)} \left[x^{-1.8} - (x+1)^{-1.8} \right], \end{aligned} \tag{3.4}$$

and hence the forcing function $g(x,t)$ must change in order to retain the same exact solution.

We *do not know* whether the exact solution $p(x,t) = e^{-t}x^3$ to the fractional diffusion equation (3.1) with initial and boundary conditions (3.2) is unique. What is clear is that values of $p(x,t)$ at every exterior point $x < 0$ affect the solution. If the problem also involves a negative fractional derivative, then values of $p(x,t)$ at exterior points $x > 1$ will also affect the solution. Hence it seems likely that a well-posed space-fractional diffusion problem on a bounded domain must also specify the value of the solution at points exterior to the domain, not just at the boundary.

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REMARK 3.1. In some applications [32, 47], it has proven useful to consider a *tempered* fractional diffusion equation like

$$\partial_t p(x,t) = a(x)\mathbb{D}_x^{\alpha,\lambda} p(x,t) + g(x,t). \tag{3.5}$$

The tempered fractional derivative $\mathbb{D}_x^{\alpha,\lambda} f(x)$ can be defined for any $\alpha > 0$ and $\lambda > 0$ as the function with Fourier transform $(\lambda + ik)^{-\alpha} F(k)$, for suitable functions $f(x)$ with Fourier transform $F(k) = \int e^{-ikx} f(x)dx$ [34, Theorem 2.9]. When $0 < \alpha < 1$, we can also define

$$\mathbb{D}_x^{\alpha,\lambda} f(x) = \lambda^\alpha f(x) + \frac{\alpha}{\Gamma(1-\alpha)} \int_{-\infty}^{x} \frac{f(x) - f(u)}{(x-u)^{\alpha+1}}\, e^{-\lambda(t-u)} du, \tag{3.6}$$

which reduces to the Marchaud fractional derivative [41, Section 5.4] when the tempering parameter $\lambda = 0$. For $0 < \alpha < 1$, we have from Sabzikar et al. [40, Theorem 5.1] that $\lim_{h\to 0} h^{-\alpha}\Delta_h^{\alpha,\lambda} f(x) = \mathbb{D}_x^{\alpha,\lambda} f(x)$, where

$$\Delta_h^{\alpha,\lambda} f(x) = \sum_{j=0}^{\infty} \binom{\alpha}{j} (-1)^j e^{-\lambda j h} f(x - jh) - (1 - e^{-\lambda h})^{\alpha} f(x).$$

A shifted version of this Grünwald-Letnikov approximation can be used to construct effective finite difference codes [2, 40]. These codes are mass-preserving since, by the fractional binomial formula, we have

$$\sum_{j=0}^{\infty} \binom{\alpha}{j} (-1)^j e^{-\lambda j h} = (1 - e^{-\lambda h})^{\alpha}$$

A Crank-Nicolson solution to the tempered fractional diffusion equation (3.5) on the bounded domain $0 < x < 1$ with $\alpha = 1,6$, $\lambda = 2$, $\beta = 2.8$, $p(0,t) = 0$, and

$$\begin{aligned} p(1,t) &= \frac{e^{-\lambda - t}}{\Gamma(\beta+1)} \\ p(x,0) &= \frac{x^{\beta} e^{-\lambda x}}{\Gamma(\beta+1)} \\ a(x) &= \frac{x^{\alpha}\Gamma(1+\beta-\alpha)}{\Gamma(\beta+1)} \\ g(x,t) &= c_1(x,t) e^{-\lambda x - t} \frac{\Gamma(1+\beta-\alpha)}{\Gamma(\beta+1)} \\ c_1(x,t) &= \frac{(1-\alpha)\lambda^{\alpha} x^{\alpha+\beta}}{\Gamma(\beta+1)} + \frac{\alpha\beta\lambda^{\alpha-1} x^{\alpha+\beta-1}}{\Gamma(\beta)} - \frac{2x^{\beta}}{\Gamma(1+\beta-\alpha)} \end{aligned} \tag{3.7}$$

was presented in [40, Example 5.3], and compared to the exact solution $p(x,t) = x^{\beta} e^{-\lambda x - t}/\Gamma(1+\beta)$. The exact solution to the tempered fractional diffusion equation (3.5) with boundary conditions (3.7) can be computed in the same manner as the exact solution to the fractional diffusion equation (3.1) with initial and boundary conditions (3.2), using (3.3) together with the fact [33, p. 209] that

$$\mathbb{D}_x^{\alpha,\lambda} f(x) = e^{-\lambda x}\, \mathbb{D}_x^{\alpha}[e^{\lambda x} f(x)]. \tag{3.8}$$

Here again, the exact solution assumes that $p(x,t) = 0$ for $x < 0$ and $t \geq 0$, and without this condition, the solution is not valid.

4. Nonlocal diffusion

In the previous section, we have presented a simple example to illustrate the basic issues in the specification of fractional boundary value problems. In this section, we discuss one possible path to resolving these issues.

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The theory of nonlocal diffusion is related to the study of *peridynamics*, which extends the physical models of continuum mechanics using integral equations in place of partial differential equations. Since Riemann-Liouville fractional derivatives are defined in terms of integrals, space-fractional differential equations can also be viewed as a special case of Volterra integral equations. Then the theory of nonlocal diffusion can be applied to illuminate the proper specification of fractional boundary value problems. In this theory, boundary values are replaced by *volume constraints* that specify values of a solution on a set of positive volume, exterior to the bounded domain of interest [9, 14, 17, **?**, 42]. The need for volume constraints from the point of view of probability is explained in [7].

In the remainder of this section, we describe the connection between nonlocal diffusion and fractional diffusion, summarize what can be immediately inferred about fractional diffusion problems on a bounded domain via the theory of nonlocal diffusion, and sketch some of the open problems for future research in this direction.

In order to explain the close connection between fractional calculus and nonlocal diffusion, we now recall another definition of the fractional derivative. The positive and negative Marchaud fractional derivatives [41, Section 5.4] (also called the generator form [33]) are defined as

$$\mathcal{D}_x^\alpha f(x) = \frac{\alpha}{\Gamma(1-\alpha)} \int_{-\infty}^{x} \frac{f(x)-f(u)}{(x-u)^{\alpha+1}} du$$

$$\mathcal{D}_{-x}^\alpha f(x) = \frac{\alpha}{\Gamma(1-\alpha)} \int_{x}^{+\infty} \frac{f(x)-f(u)}{(u-x)^{\alpha+1}} du$$

for $0 < \alpha < 1$. A slightly more complicated form pertains for $1 < \alpha < 2$, see [33, Chapter 3]. If f, f', f'' are continuous and integrable functions that vanish at infinity, then the Fourier transform of $\mathcal{D}_{\pm x}^\alpha f(x)$ is $(\pm ik)^\alpha \hat{f}(k)$ [33, Theorem 3.17 and Example 3.24], and hence this definition coincides with the Riemann-Liouville derivative for such functions. Hence the constant coefficient fractional diffusion equation

$$\partial_t p(x,t) = a\mathbb{D}_x^\alpha p(x,t) + b\mathbb{D}_{-x}^\alpha p(x,t)$$

for $0 < \alpha < 1$ can be rewritten in the form

$$\partial_t p(x,t) = \int_{\mathbb{R}} [p(x-u,t) - p(x,t)]\, \phi(u)\, du \tag{4.1}$$

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where the *Lévy jump intensity*

$$\phi(u) = \begin{cases} a\dfrac{\alpha}{\Gamma(1-\alpha)}|u|^{-\alpha-1} & u < 0, \\ b\dfrac{\alpha}{\Gamma(1-\alpha)}u^{-\alpha-1} & u > 0. \end{cases} \tag{4.2}$$

A change of variable $y = x - u$ in (4.1) yields

$$\partial_t p(x,t) = \int_{\mathbb{R}} [p(y,t) - p(x,t)]\,\gamma(y,x)\,dy, \tag{4.3}$$

where the *interaction kernel* $\gamma(y,x) = \phi(x-y)$. Equation (4.3) defines a Cauchy problem $\partial_t p = Lp; p(x,0) = p_0(x)$ on $L^2(\mathbb{R})$, where the nonlocal operator

$$Lf(x) = \int_{y\neq 0} [f(y) - f(x)]\,\gamma(y,x)\,dy \tag{4.4}$$

as in Du et al. [14]. If $a = b$, then L is proportional to the fractional Laplacian in one dimension. The same idea extends to $\mathbb{R}^d$, and if the interaction kernel $\gamma(y,x)$ is proportional to $|y-x|^{-\alpha-d}$ then L is proportional to the fractional Laplacian in d dimensions.

One way to define the nonlocal operator on a bounded domain D is to simply restrict the domain of integration in (4.4) to $y \in D$. Using that definition of the fractional Laplacian, Du et al. [14] prove that the constrained minimization problem

$$\min_{u\in H^{\alpha/2}(D)} Lu - \int_{x\in D} b(x)u(x)\,dx$$

is well-posed given the volume constraint $u = 0$ on the interaction domain

$$D_I := \{y \in \mathbb{R}\setminus D : \gamma(x,y) \neq 0 \;\exists\; x \in D\}.$$

Here $H^s(D)$ is the usual fractional Sobolev space [36], the natural domain of the fractional derivatives of order $\alpha = 2s$. Du et al. [14] also note that the same problem is ill-posed using Dirichlet boundary conditions $u = 0$ on ∂D. The volume constraint $u = 0$ for $x \in D_I$ is a kind of *nonlocal Dirichlet* condition, the proper nonlocal analogue of a Dirichlet boundary condition.

Du et al. [18] prove well-posedness for the Cauchy problem $\partial_t p = Lp; p(x,0) = p_0(x)$ on $L^2(\mathbb{R})$, where the integral in (4.4) is taken over the entire space, the interaction kernel $\gamma(x,y) = \gamma(y-x)$ is translation invariant, and vanishes off a ball of finite radius $|y-x| < \lambda$. They also assume a zero volume constraint on the interaction domain. This result could easily be generalized to include the non-homogeneous case $\partial_t p = Lp + g; p(x,0) = p_0(x)$.

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REMARK 4.1. The tempered fractional diffusion in Remark 3.1 is also a nonlocal diffusion whose interaction kernel

$$\gamma(y,x) = C(y-x)^{-\alpha-1}e^{-\lambda(y-x)}I_{y>x}$$

has an infinite interaction length. It would also be interesting to develop a suitable theory of well-posed tempered fractional diffusion on a bounded domain.

To demonstrate the practical utility of nonlocal diffusion theory for applications to fractional diffusion on a bounded domain, we offer the following result, which is a simple consequence of established nonlocal diffusion theory. Consider the fractional initial value problem

$$\begin{aligned} \partial_t p(x,t) &= \frac{1}{2}\left[\mathbb{D}_x^\alpha p(x,t) + \mathbb{D}_{-x}^\alpha p(x,t)\right] \\ p(x,0) &= p_0(x) \quad \text{for all } L < x < R \\ p(x,t) &= 0 \quad \text{for all } x \notin (L,R) \text{ and all } t \in [0,T] \end{aligned} \tag{4.5}$$

on the bounded domain $D = (L,R)$ for some $0 < \alpha < 1$ and some $T > 0$. Here the interaction length $\lambda = \infty$, and the interaction domain $D_I = \mathbb{R} \setminus D$. Define the nonlocal energy semi-norm

$$|||v||| := \frac{1}{2}\int_{\mathbb{R}\times\mathbb{R}} |v(x) - v(y)|^2 \phi(|y-x|)\, dy\, dx$$

where $\phi(u)$ is the Lévy jump intensity (4.2) with $a = b = 1/2$. Define the nonlocal energy space

$$V := \{v \in L^2(\mathbb{R}) : |||v||| < \infty\}$$

and the nonlocal volume-constrained energy space

$$V_c := \{v \in V : v(x) = 0 \ \forall\ x \notin (L,R)\}.$$

THEOREM 4.1. *For any $p_0 \in V_c$, the fractional diffusion problem* (4.5) *has a unique solution in* $L^\infty([0,T], V_c) \cap H^1([0,T], L^2(\mathbb{R}))$.

P r o o f. First, note that V_c is a Hilbert space, and a closed subspace of $L^2(\mathbb{R})$. For details and extensions, see [14, 35]. By the analysis of well-posedness of the steady state variational problem obtained by setting $\partial_t p(x,t) = 0$ in (4.5), it is easy to see that the bilinear form

$$a(u,v) = \int_{\mathbb{R}\times\mathbb{R}} \big(u(x) - u(y)\big)\big(v(x) - v(y)\big)\phi(|x-y|)\, dy\, dx$$

is coercive and continuous on $V_c \times V_c$. In particular, we have that $a(u,u) = |||u|||^2$. Moreover, it follows from a nonlocal version of Green's second identity [17], see also (5.7) in the next section, that $a(u,v) = (L(u),v)$, where L is defined by (4.4) with $\gamma(y,x) = \phi(x-y)$. Thus, the operator L generates a continuous semigroup, and hence the existence and uniqueness of a solution $p(x,t)$ in the space $L^\infty([0,T],V_c) \cap H^1([0,T],L^2(\mathbb{R}))$ follows from the standard theory [38]. □

Remark 4.2. The proof of Theorem 4.1 also extends to fractional diffusion problems on $\mathbb{R}^d$. If the interaction kernel $\gamma(\mathbf{x},\mathbf{y})$ is proportional to $|\mathbf{y}-\mathbf{x}|^{-\alpha-d}$, then the operator (4.4) is proportional to the fractional Laplacian in d dimensions. With a finite interaction length $\lambda > 0$, the interaction kernel is given by $\gamma(\mathbf{x},\mathbf{y}) = c|\mathbf{y}-\mathbf{x}|^{-\alpha-d}\mathbf{1}_{|\mathbf{y}-\mathbf{x}|\le\lambda}$, the interaction domain is given by $D_I := \{\mathbf{y} \in \mathbb{R}^d \setminus D : |\mathbf{x}-\mathbf{y}| < \lambda\}$, and the nonlocal diffusion problem

$$\begin{aligned} \partial_t p(\mathbf{x},t) &= Lp(\mathbf{x},t) + g(\mathbf{x},t) \quad \forall\, \mathbf{x} \in D,\ t \in (0,T] \\ p(\mathbf{x},0) &= p_0(\mathbf{x}) \quad \forall\, \mathbf{x} \in D \\ p(\mathbf{x},t) &= 0 \quad \forall\, \mathbf{x} \in D_I,\ t \in (0,T] \end{aligned} \tag{4.6}$$

with a zero volume constraint has a unique solution. If the interaction length $\lambda = \infty$, then $D_I = \mathbb{R}^d \setminus D$, and the problem (4.6) is equivalent to the nonlocal Dirichlet problem for the fractional Laplacian on the bounded domain D, with a zero exterior condition.

Remark 4.3. It is typical in the theory of nonlocal diffusion to assume a finite interaction length $\lambda < \infty$. This is not consistent with fractional diffusion problems, where the interaction length in the Riemann-Liouville derivative (or the fractional Laplacian) is infinite. To address this problem, D'Elia and Gunzburger[10] consider the steady state problem $0 = Lp + g$ on D with $p = 0$ on D_I, where L is the fractional Laplacian. They prove that solutions to this steady state problem can be obtained as the limit of solutions of the same nonlocal problem with a finite interaction length, by letting the interaction length tend to infinity [10, Theorem 3.1]. That is, they apply the interaction kernel $\gamma(y,x) = c|y-x|^{-\alpha-d}\mathbf{1}_{|y-x|\le\lambda}$ and let $\lambda \to \infty$. Specifically, the difference between the two solutions, measured in the $H^{\alpha/2}(D \cup D_I)$ norm, is proportional to $\lambda^{-\alpha}$ as $\lambda \to \infty$. It would be interesting to extend these results to the Cauchy problem $\partial_t p = Lp; p(x,0) = p_0(x)$, as well as other non-symmetric fractional derivative operators. For example, one can consider the anisotropic fractional derivative operator $L = \nabla_M^\alpha$ such that $Lf(x)$ has the Fourier transform

$$\int_{|\theta|=1} (ik\cdot\theta)^\alpha M(d\theta)\hat{f}(k),$$

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see [33, Section 6.5].

Remark 4.4. In numerical analysis, practical considerations necessitate a finite domain, with a finite interaction length. Hence in this setting, the finite interaction length typically assumed in the nonlocal theory is quite natural. For example, if one considers the space-fractional diffusion equation with drift

$$\partial_t p(x,t) = -v(x,t)\partial_x p(x,t) + a(x,t)\mathbb{D}^{\alpha}_{x,L} p(x,t) + b(x,t)\mathbb{D}^{\alpha}_{-x,L} p(x,t) + g(x,t)$$

on a finite domain $L < x < R$, $0 \le t \le T$, then nonlocal diffusion theory with a finite interaction length is directly applicable. Although the Riemann-Liouville fractional derivative $\mathbb{D}_{\pm x}$ is more natural in applications (e.g., to ground water hydrology), the imposition of a finite interaction length is inevitable in numerical work.

Another interesting open problem is the appropriate specification of reflecting (and other) boundary conditions. A first step in this direction was taken by Baeumer et al. [3]. Consider a Brownian motion reflected at the origin, so that particles remain in the positive half-line. The transition densities $p(x, y, t)$ of $Z_{t+s} = y$ given $Z_s = x$ solve the diffusion equation $\partial_t p(x, y, t) = \partial_y^2 p(x, y, t)$ together with the reflecting boundary condition

$$\partial_y p(x,y,t)\Big|_{y=0+} := \lim_{h\to 0+} \frac{p(x,y+h,t) - p(x,y,t)}{h}\Big|_{y=0} = 0 \quad \text{for all } t > 0,$$

see for example Itô and McKean [21, Eq. 8]. Replacing the Brownian motion by a negatively skewed stable Lévy motion with index $1 < \alpha < 2$, the corresponding transition densites solve the fractional diffusion equation $\partial_t p(x, y, t) = \mathbb{D}^{\alpha}_{-y} p(x, y, t)$ with the fractional reflecting boundary condition

$$\mathbb{D}^{\alpha-1}_{-y} p(x,y,t)\Big|_{y=0+} = 0 \quad \text{for all } t > 0. \tag{4.7}$$

Just like the classical case of a reflecting Brownian motion, the fractional reflecting boundary condition (4.7) enforces a no-flux condition at the point $y = 0$ in the state space. The boundary condition (4.7) can therefore be considered as the appropriate fractional analogue of a reflecting boundary condition in the traditional diffusion equation. It would be very interesting to extend this result to more general fractional diffusion equations in one and several dimensions.

In the nonlocal diffusion setting, the appropriate specification of such Neumann type volume constraints was discussed in [14, 17]; in short, Neumann constraints in the nonlocal diffusion theory simply require equation

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(5.6) in the following section to hold, not only for $\mathbf{x} \in D$, but also for $\mathbf{x} \in D_I$. It would be very interesting to connect (4.7) to the treatment of nonlocal Neumann volume constraints specified in [14, 17].

5. Nonlocal vector calculus

In this section, we describe the recently developed theory of nonlocal vector calculus, including nonlocal analogues of the divergence and gradient. Given vector-valued mappings $\boldsymbol{\nu}(\mathbf{x},\mathbf{y}), \boldsymbol{\beta}(\mathbf{x},\mathbf{y})\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ with $\boldsymbol{\beta}$ antisymmetric, i.e., $\boldsymbol{\beta}(\mathbf{y},\mathbf{x}) = -\boldsymbol{\beta}(\mathbf{x},\mathbf{y})$, the action of the *nonlocal divergence operator* $\mathcal{D}\colon \mathbb{R}^d \to \mathbb{R}$ on $\boldsymbol{\nu}$ is defined as

$$\mathcal{D}\big(\boldsymbol{\nu}\big)(\mathbf{x}) := \int_{\mathbb{R}^d} \big(\boldsymbol{\nu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\nu}(\mathbf{y},\mathbf{x})\big) \cdot \boldsymbol{\beta}(\mathbf{x},\mathbf{y})\, d\mathbf{y} \quad \forall\, \mathbf{x} \in \mathbb{R}^d. \tag{5.1a}$$

This definition follows from reasonable assumptions about how a divergence operator should act, followed by an application of the Schwarz kernel theorem; see [17].

Given a scalar-valued mapping $u(\mathbf{x})\colon \mathbb{R}^d \to \mathbb{R}$, the action of the adjoint operator $\mathcal{D}^*\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ on u is given by [14]

$$\mathcal{D}^*\big(u\big)(\mathbf{x},\mathbf{y}) = -\big(u(\mathbf{y}) - u(\mathbf{x})\big)\boldsymbol{\beta}(\mathbf{x},\mathbf{y}) \quad \forall\, \mathbf{x},\mathbf{y} \in \mathbb{R}^d; \tag{5.1b}$$

and we note that $-\mathcal{D}^*$ defines a *nonlocal gradient operator*.

Given a scalar-valued mapping $u(\mathbf{x})\colon \mathbb{R}^d \to \mathbb{R}$, the action of the operator $\mathcal{L}\colon \mathbb{R}^d \to \mathbb{R}$ on u is defined as

$$\mathcal{L}u := -\mathcal{D}(\boldsymbol{\Theta}\mathcal{D}^* u) + \mathcal{D}(\boldsymbol{\mu} u) \quad \forall\, \mathbf{x} \in \mathbb{R}^d, \tag{5.2}$$

where, without loss of generality [11], one can assume that $\boldsymbol{\Theta}(\mathbf{x},\mathbf{y}) = \boldsymbol{\Theta}^T(\mathbf{x},\mathbf{y}) = \boldsymbol{\Theta}(\mathbf{y},\mathbf{x})$ and $\boldsymbol{\mu}(\mathbf{x},\mathbf{y}) = \boldsymbol{\mu}(\mathbf{y},\mathbf{x})$. Using (5.1), $\mathcal{L}u$ has the explicit form

$$\mathcal{L}u(\mathbf{x}) = \int_{\mathbb{R}^d} \big(u(\mathbf{y})\gamma(\mathbf{y},\mathbf{x}) - u(\mathbf{x})\gamma(\mathbf{x},\mathbf{y})\big)\, d\mathbf{y} \quad \text{for } \mathbf{x} \in \mathbb{R}^d, \tag{5.3}$$

where

$$\gamma(\mathbf{x},\mathbf{y}) = \boldsymbol{\beta}(\mathbf{x},\mathbf{y}) \cdot \big(\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\boldsymbol{\beta}(\mathbf{x},\mathbf{y})\big) - \boldsymbol{\mu}(\mathbf{x},\mathbf{y}) \cdot \boldsymbol{\beta}(\mathbf{x},\mathbf{y}). \tag{5.4}$$

Given an open subset $D \subset \mathbb{R}^d$, recall that the interaction domain corresponding to D is defined by

$$D_I := \{\mathbf{y} \in \mathbb{R}^d \setminus D \quad \text{such that} \quad \boldsymbol{\beta}(\mathbf{x},\mathbf{y}) \neq \mathbf{0} \quad \forall\, \mathbf{x} \in D\} \tag{5.5}$$

so that D_I consists of those points outside of D that interact with points in D. In this case, we have that

$$\mathcal{L}u(\mathbf{x}) = \int_{D \cup D_I} \big(u(\mathbf{y})\gamma(\mathbf{y},\mathbf{x}) - u(\mathbf{x})\gamma(\mathbf{x},\mathbf{y})\big)\, d\mathbf{y} \quad \forall\, \mathbf{x} \in D. \tag{5.6}$$

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Note that the cases $D_I = \mathbb{R}^d \setminus D$ or $D = \mathbb{R}^d$ are not excluded.

In [17], a nonlocal vector calculus is developed for the operators $\mathcal{D}$ and $\mathcal{D}^*$ including nonlocal gradient and curl operators, mimicking the classical vector calculus for differential operators. Included in the nonlocal calculus are analogues of well-known vector identities and theorems such as the divergence theorem and the Green identities. Of special relevance to this study is the nonlocal Green's second identity: given $u(\mathbf{x})$ and $v(\mathbf{x})$ defined for $\mathbf{x} \in D \cup D_I$, then

$$\begin{aligned} \int_{D\cup D_I} v(\mathbf{x})\mathcal{D}(\boldsymbol{\Theta}\mathcal{D}^* u)(\mathbf{x})\, d\mathbf{x} \\ = \int_{D\cup D_I}\int_{D\cup D_I} \mathcal{D}^*(u)(\mathbf{x},\mathbf{y}) \cdot (\boldsymbol{\Theta}\mathcal{D}^* v)(\mathbf{x},\mathbf{y})\, d\mathbf{y}d\mathbf{x}. \end{aligned} \tag{5.7}$$

Remark 5.1. A fractional vector calculus has also been developed by Meerschaert et al. [31] and Tarasov [44]. The theory defines a fractional gradient, divergence, curl, and a fractional divergence theorem and Stokes theorem. It would be interesting to reconcile the vector fractional calculus in those papers with the nonlocal vector calculus described above. For example, the vector fractional calculus defines the β-fractional divergence [31, Eq. (12)] of a vector field $\boldsymbol{V} : \mathbb{R}^d \to \mathbb{R}^d$ as

$$\operatorname{div}_M^\beta \boldsymbol{V}(\mathbf{x}) := \int_{|\boldsymbol{\theta}|=1}\int_0^\infty [\boldsymbol{V}(\mathbf{x}) - \boldsymbol{V}(\mathbf{x}-t\boldsymbol{\theta})] \cdot \boldsymbol{\theta}\, \frac{\beta dt}{\Gamma(1-\beta)t^{\beta-1}} M(d\boldsymbol{\theta}),$$

and it may be possible to relate this to (5.1a).

6. Concluding remarks

This paper describes an important open problem in fractional calculus: How should one formulate a well-posed fractional diffusion problem on a bounded domain, so that there exists a unique solution that depends continuously on the initial data? A simple example is presented to show the necessity of volume constraints instead of boundary values. Since fractional derivatives are nonlocal operators, it is natural that a "nonlocal boundary condition" has to extend past the boundary. One method of identifying and proving the proper formulation of a fractional diffusion problem on a bounded domain is to apply the recently developed theory of nonlocal diffusion. Since fractional derivatives are a special case nonlocal operators, established results from the theory of nonlocal diffusion can be applied to identify a well-posed formulation.

The connection between nonlocal and fractional theories is not yet complete. Usually, nonlocal diffusion models involve a symmetric interaction

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kernel, with a finite interaction length. The fractional Laplacian, or the Riesz fractional derivative in one dimension, correspond to a nonlocal operator with an infinite interaction length. Riemann-Liouville fractional derivatives are nonlocal operators with an asymmetric power law interaction kernel. Liouville fractional derivatives are nonlocal operators with an asymmetric interaction kernel and an infinite interaction length. Vector fractional derivatives are also nonlocal operators, with an asymmetric interaction kernel in d dimensions, and an infinite interaction length. Research in nonlocal diffusion theory is ongoing, to incorporate asymmetric interaction kernels and infinite interaction lengths, see for example [10].

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