

# A simple solver for the fractional Laplacian in multiple dimensions

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## Abstract

We present a simple solver of the fractional Laplacian based on the hypersingular integral representation. Through singularity subtraction, we obtain a regularized integrand that is amenable to the trapezoidal rule with equispaced nodes. The resulting quadrature scheme gives a discrete operator on a regular grid that is translation-invariant and thus can be applied quickly with the fast Fourier transform. For discretizations of problems related to space-fractional diffusion on bounded domains, we observe that the underlying linear system can be efficiently solved via preconditioned Krylov methods with a preconditioner based on the finite-difference (non-fractional) Laplacian. We show numerical results illustrating the error of our simple scheme as well the efficiency of our preconditioning approach, both for the elliptic (steady-state) fractional diffusion problem and the time-dependent problem.

## 1 Introduction

Fractional powers of the Laplacian operator arise naturally in the study of anomalous diffusion, where the fractional operator plays an analogous role to that of the standard Laplacian for ordinary diffusion (see, e.g., the review articles by Metzler and Klafter [34, 35] and Vázquez [44]). By replacing Brownian motion of particles with Lévy flights [28], whose increments are drawn from the  $\alpha$ -stable Lévy distribution for  $\alpha \in (0, 2)$ , we obtain a fractional diffusion equation (or fractional kinetic equation) in terms of the fractional Laplacian operator of order  $\alpha$  [41], defined for sufficiently nice functions  $u: \mathbf{R}^d \rightarrow \mathbf{R}$  via the Cauchy principal value integral

$$(-\Delta)^{\alpha/2}u(\mathbf{x}) \equiv C_{\alpha,d} \int_{\mathbf{R}^d} \frac{u(\mathbf{x}) - u(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|^{d+\alpha}} d\mathbf{y}, \quad \mathbf{x} \in \mathbf{R}^d \quad (1)$$

with known normalizing constant  $C_{\alpha,d}$  [25].

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For a bounded domain  $\Omega \subset \mathbf{R}^d$  with complement  $\Omega^c \equiv \mathbf{R}^d \setminus \Omega$ , we consider fractional diffusion with homogeneous extended Dirichlet conditions given in terms of (1) by

$$\begin{cases} \partial_t u(\mathbf{x}, t) = -(-\Delta)^{\alpha/2} u(\mathbf{x}, t) + f(\mathbf{x}, t), & \mathbf{x} \in \Omega, & t > 0, \\ u(\mathbf{x}, t) = 0, & \mathbf{x} \in \Omega^c, & t > 0, \\ u(\mathbf{x}, 0) = u_0(\mathbf{x}), & \mathbf{x} \in \Omega. \end{cases} \quad (2)$$

Also of interest is the related elliptic problem

$$\begin{cases} (-\Delta)^{\alpha/2} u(\mathbf{x}) = f(\mathbf{x}), & \mathbf{x} \in \Omega, \\ u(\mathbf{x}) = 0, & \mathbf{x} \in \Omega^c. \end{cases} \quad (3)$$

Somewhat unintuitively, the nonlocality of (1) implies that the solutions of (2) and (3) depend on data prescribed everywhere outside  $\Omega$  [9, 11, 39], though other definitions of the fractional Laplacian on a bounded domain are also in common use [44]. Further, a more general formulation of fractional diffusion involves augmenting (2) by incorporating fractional time derivatives of Caputo or Riemann-Liouville type. We focus in this work on the case of space-fractional diffusion and do not discuss the discretization of time-fractional differential operators, though the latter is of independent interest [26, 31, 49, 50].

## 1.1 Contribution

The contribution of this paper is a simple discretization scheme for (2) and (3) on Cartesian grids, and an efficient algorithm for solving the resulting linear systems. The discretization generalizes easily to domains that can be represented as occluded Cartesian grids, though we focus on regular domains in this work.

Our approach is based on using a Taylor expansion around each point  $\mathbf{x}$  to replace the singular integrand in Eq. (1) with a sufficiently smooth function of  $\mathbf{y}$  on all of  $\mathbf{R}^d$  via singularity subtraction. The resulting integral can be easily discretized using the trapezoidal rule on a regular grid of  $N$  points, leading to a translation-invariant linear operator that can be applied at a cost of  $\mathcal{O}(N \log N)$  using the fast Fourier transform (FFT). The resulting discrete linear system approximating (3) can then be efficiently solved using standard Krylov methods. As  $\alpha \rightarrow 2$ , the resulting linear systems can exhibit the ill-conditioning characteristic of discretizations of the Laplacian operator on a regular grid. To circumvent this, we develop an efficient preconditioning strategy based on the fact that our discrete fractional Laplacian operator may be written as the sum of a standard finite-difference Laplacian and another matrix with mostly small entries.

When the solution  $u$  to (3) is sufficiently smooth, standard results on convergence of the trapezoidal rule and finite-difference operators imply that the error of our approach for computing the fractional Laplacian at a point goes to zero as  $\mathcal{O}(h^2)$ , where  $h$  is the linear spacing between grid points, which we show in Section 2. In general, however, the solution to the fractional Laplace problem on bounded domains is only  $[\alpha/2]$  times continuously differentiable [40], leading to a natural deterioration of the rate of convergence of our simple approach to an observed rate of  $\mathcal{O}(h)$ .

## 1.2 Related work

A discretization scheme similar to that presented here appears in Pozrikidis [38], though without discussion of accuracy or the importance of windowing for singularity subtraction. Huang and

Oberman [22, 23] derive a scheme for the one-dimensional case based on singularity subtraction and finite-difference approximation, but do not tackle the multidimensional case (see also Tian and Du [42], Gao et al. [16], and Duo, Van Wyk, and Zhang [10]). Chen et al. [7] consider a multidimensional discretization and fast preconditioners based on multigrid, but their scheme uses the so-called “coordinate fractional Laplacian” that takes a tensor product of one-dimensional operators and is not equivalent to (1) (see also related finite-difference approaches with different operators [32, 33, 45, 51]).

Other work on efficient solution of fractional Laplacian systems using fast preconditioned iterative methods includes Wang and Du [46], Pang and Sun [37], Fu and Wang [15], and Fu, Ng, and Wang [14], though only in one spatial dimension.

Notable schemes for discretizing the fractional Laplacian based on different ideas include work based on the Caffarelli-Silvestre extension [6, 20, 36], finite-element-based approaches [2, 4, 5, 43], and work on spectral approaches [3, 29, 48]. General references for fractional Laplacians on bounded domains include, e.g., Ros-Oton [39], D’Elia and Gunzburger [9], Felsinger [11], and Lischke et al. [27].

## 2 Spatial discretization of the fractional Laplacian

To begin, we outline our scheme for discretization of (1) in the one-dimensional case where the function  $u$  vanishes outside of some interval. Following that, we give more details in our discussion of the multidimensional case.

### 2.1 Singularity subtraction in one dimension

Concretely, consider the task of approximating the integral

$$(-\Delta)^{\alpha/2}u(x) = C_{\alpha,1} \int_{-\infty}^{\infty} \frac{u(x) - u(y)}{|x - y|^{1+\alpha}} dy \quad (4)$$

where  $u(y) = 0$  for  $|y| > 1$ . For  $\alpha > 1$ , this integral is hypersingular due to the high-order pole at  $x = y$ , which generally leads to large inaccuracies when simple quadrature schemes are applied directly to (4). Therefore, we proceed by regularizing the integrand to remove the singularity and obtain an integral for which simple quadratures are accurate.

Assuming that the function  $u$  is sufficiently smooth, we may write a Taylor series expansion about the point  $x$  to obtain

$$u(y) = u(x) + \frac{1}{2}u''(x)(y - x)^2 + u_{\text{odd}}(y) + R_4(y), \quad (5)$$

where the smooth remainder  $R_4(y) = O(|y - x|^4)$  as  $y \rightarrow x$ . For brevity, we have grouped terms that are odd about  $x$  into  $u_{\text{odd}}$ , as they will not play an explicit role in what follows.

Our regularization strategy is singularity subtraction based on adding and subtracting a calculable integral that matches terms in the Taylor series. Suppose  $w$  is a sufficiently smooth windowing

function with compact support such that  $w(0) = 1$  and  $w(y) = w(-y)$ . Then we may write

$$\begin{aligned}
(-\Delta)^{\alpha/2}u(x) &= C_{\alpha,1} \int_{-\infty}^{\infty} \frac{u(x) - u(y) + w(x-y)[\frac{1}{2}u''(x)(x-y)^2 - u_{\text{odd}}(y)]}{|x-y|^{1+\alpha}} dy \\
&\quad - C_{\alpha,1} \int_{-\infty}^{\infty} \frac{w(x-y)[\frac{1}{2}u''(x)(x-y)^2 - u_{\text{odd}}(y)]}{|x-y|^{1+\alpha}} dy \\
&\equiv \text{(I)} + \text{(II)},
\end{aligned} \tag{6}$$

where we define (I) to be the first integral and (II) to be the second. By construction, (I) is no longer hypersingular, as we see from (5) that the integrand can be equivalently written

$$\frac{[w(x-y) - 1][\frac{1}{2}u''(x)(x-y)^2 - u_{\text{odd}}(y)] + R_4(y)}{|x-y|^{1+\alpha}}.$$

By our smoothness assumptions on  $u$  and  $w$ , this integrand is  $O(|x-y|^{3-\alpha})$  and continuously differentiable as  $y \rightarrow x$  with a second derivative that is integrable. This implies that the standard trapezoidal rule would exhibit second-order convergence when applied to (I); see Cruz-Uribe and Neugebauer [8]. Of course, this requires knowledge of  $u''(x)$  and  $u_{\text{odd}}$  in general, which we do not assume. In the context of discretization of the integral using a uniform grid, however, the situation simplifies.

## 2.2 The first integral in one dimension

Consider discretizing (I) using the trapezoidal rule on a one-dimensional lattice  $\{y_j\}_{j \in \mathbf{Z}} = \{jh\}_{j \in \mathbf{Z}}$  and take  $x = y_i$  to be one of the lattice points. Without loss of generality, we may shift the domain such that  $x = y_0 = 0$ . This discretization yields the second-order accurate approximation

$$\begin{aligned}
\text{(I)} &\approx C_{\alpha,1}h \sum_{j \neq 0} \left[ \frac{u(0) - u(y_j) + w(y_j)[\frac{1}{2}u''(0)(y_j)^2 - u_{\text{odd}}(y_j)]}{|y_j|^{1+\alpha}} \right] \\
&= C_{\alpha,1}h \left[ \sum_{j \neq 0} \frac{u(0)}{|y_j|^{1+\alpha}} - \sum_{j \neq 0} \frac{u(y_j)}{|y_j|^{1+\alpha}} + \frac{u''(0)}{2} \sum_{j \neq 0} \frac{w(y_j)}{|y_j|^{\alpha-1}} - \sum_{j \neq 0} \frac{w(y_j)u_{\text{odd}}(y_j)}{|y_j|^{1+\alpha}} \right] \\
&= C_{\alpha,1}h \left[ A_1 u(0) - \sum_{j \neq 0} \frac{u(y_j)}{|y_j|^{1+\alpha}} + A_2 u''(0) \right],
\end{aligned}$$

where  $A_1 = \sum_{j \neq 0} |y_j|^{-(1+\alpha)}$  and  $A_2 = \sum_{j \neq 0} w(y_j)|y_j|^{1-\alpha}$  are constants independent of  $x$  and  $j$  and the last sum in the second line is identically zero due to oddness considerations. We note that the sum remaining on the final line is over a finite range, as  $u$  is compactly supported. Since  $u$  is assumed to be smooth, we replace  $u''(0)$  with the finite-difference approximation

$$u''(0) \approx L_{\text{FD}}u(0) \equiv \frac{u(h) - 2u(0) + u(-h)}{h^2},$$

which gives our final approximation for (I),

$$\text{(I)} \approx C_{\alpha,1}h \left[ A_1 u(0) - \sum_{j \neq 0} \frac{u(y_j)}{|y_j|^{1+\alpha}} + A_2 L_{\text{FD}}u(0) \right]. \tag{7}$$

### 2.3 The second integral in one dimension and final quadrature

Having established a method for approximating the integral (I) in (6), we turn to (II). Again using oddness considerations, we see that the contribution from  $u_{\text{odd}}$  vanishes such that

$$(II) = -\frac{C_{\alpha,1}u''(0)}{2} \int_{-\infty}^{\infty} \frac{w(y)}{|y|^{\alpha-1}} dy = C_{\alpha,1}hA_3u''(0),$$

where the constant  $A_3$  given by

$$A_3 = -\frac{1}{2h} \int_{-\infty}^{\infty} \frac{w(y)}{|y|^{\alpha-1}} dy$$

is well-defined (since  $w$  is compactly supported) and we again take  $x = 0$  for convenience. We once again replace the second derivative  $u''(0)$  with its finite-difference approximation to obtain  $(II) \approx C_{\alpha,1}hA_3L_{\text{FD}}u(0)$ . Combining this with our quadrature for (I) gives our approximation for  $(-\Delta)^{\alpha/2}u(0)$ ,

$$(-\Delta)^{\alpha/2}u(0) \approx C_{\alpha,1}h \left[ A_1u(0) - \sum_{j \neq 0} \frac{u(y_j)}{|y_j|^{1+\alpha}} + (A_2 + A_3)L_{\text{FD}}u(0) \right],$$

which applies equally well not only to  $x = 0$  but in general to  $x = y_i$  for any grid point  $y_i$ , i.e.,

$$(-\Delta)^{\alpha/2}u(y_i) \approx C_{\alpha,1}h \left[ A_1u(y_i) - \sum_{j \neq i} \frac{u(y_j)}{|y_i - y_j|^{1+\alpha}} + (A_2 + A_3)L_{\text{FD}}u(y_i) \right]. \quad (8)$$

This is our final quadrature for the fractional Laplacian in one dimension.

### 2.4 Singularity subtraction in higher dimensions

We turn now to the multidimensional integral, i.e., (1) with  $d = 2$  or  $d = 3$ . Once again we will assume that the function  $u$  is compactly supported and sufficiently smooth, as we will make explicit. Our basic strategy is the same as in one dimension.

**Lemma 1.** *Suppose that  $u \in C^k(\mathbf{R}^d)$  and let  $w \in C^p(\mathbf{R})$  be a windowing function symmetric about  $z = 0$  such that  $1 - w(z) = \mathcal{O}(|z|^r)$  as  $z \rightarrow 0$ . Let the third-order Taylor approximation of  $u$  about the point  $\mathbf{x} \in \mathbf{R}^d$  be given in multi-index notation by*

$$u(\mathbf{y}) = \sum_{|\beta| \leq 3} \frac{D^\beta u(\mathbf{x})}{\beta!} (\mathbf{y} - \mathbf{x})^\beta + \sum_{|\tilde{\beta}|=4} R_{\tilde{\beta}}(\mathbf{y})(\mathbf{y} - \mathbf{x})^{\tilde{\beta}}, \quad (9)$$

where the remainder is given in explicit form as

$$R_{\tilde{\beta}}(\mathbf{y}) \equiv \frac{|\tilde{\beta}|}{\tilde{\beta}!} \int_0^1 (1-t)^{|\tilde{\beta}|-1} D^{\tilde{\beta}} u(\mathbf{x} + t(\mathbf{y} - \mathbf{x})) dt.$$

Then, defining the function

$$\tilde{u}(\mathbf{y}) \equiv u(\mathbf{y}) - u(\mathbf{x}) - w(|\mathbf{x} - \mathbf{y}|) \sum_{1 \leq |\beta| \leq 3} \frac{D^\beta u(\mathbf{x})}{\beta!} (\mathbf{y} - \mathbf{x})^\beta, \quad (10)$$

we have that  $\tilde{u} \in C^s(\mathbf{R}^d)$  and  $D^\beta \tilde{u}(\mathbf{y}) = \mathcal{O}(|\mathbf{y} - \mathbf{x}|^{t-|\beta|})$  as  $\mathbf{y} \rightarrow \mathbf{x}$  for  $s = \min(k - 4, p)$ ,  $t = \min(1 + r, 4)$ , and  $0 \leq |\beta| \leq \min(s, t)$ .

*Proof.* It is clear that

$$\tilde{u}(\mathbf{y}) = (1 - w(|\mathbf{x} - \mathbf{y}|)) \sum_{1 \leq |\beta| \leq 3} \frac{D^\beta u(\mathbf{x})}{\beta!} (\mathbf{y} - \mathbf{x})^\beta + \sum_{|\beta|=4} R_{\tilde{\beta}}(\mathbf{y}) (\mathbf{y} - \mathbf{x})^{\tilde{\beta}}.$$

By inspection, the order of differentiability of  $\tilde{u}(\mathbf{y})$  is limited by that of  $w(|\mathbf{x} - \mathbf{y}|)$  and of  $R_{\tilde{\beta}}(\mathbf{y})$ . Given the explicit form of  $R_{\tilde{\beta}}(\mathbf{y})$ , it is at least in  $C^{k-4}(\mathbf{R}^d)$  as a function of  $\mathbf{y}$ , whereas  $w \in C^p(\mathbf{R})$  by assumption. Further,  $\tilde{u}(\mathbf{y}) = \mathcal{O}(|\mathbf{y} - \mathbf{x}|^t)$  for  $t = \min(1 + r, 4)$ , since the first summand is  $\mathcal{O}(|\mathbf{y} - \mathbf{x}|^{1+r})$  and the second summand is at least  $\mathcal{O}(|\mathbf{y} - \mathbf{x}|^4)$ . Explicit term-by-term differentiation of  $\tilde{u}(\mathbf{y})$  with the product rule concludes the proof.  $\square$

By subtracting off the windowed multivariate Taylor series we obtain an integral that is no longer hypersingular. In particular, we write

$$\begin{aligned} (-\Delta)^{\alpha/2} u(\mathbf{x}) &= C_{\alpha,d} \int_{\mathbf{R}^d} \frac{u(\mathbf{x}) - u(\mathbf{y}) + w(|\mathbf{x} - \mathbf{y}|) \sum_{1 \leq |\beta| \leq 3} \frac{D^\beta u(\mathbf{x})}{\beta!} (\mathbf{y} - \mathbf{x})^\beta}{|\mathbf{x} - \mathbf{y}|^{d+\alpha}} d\mathbf{y} \\ &\quad - C_{\alpha,d} \int_{\mathbf{R}^d} \frac{w(|\mathbf{x} - \mathbf{y}|) \sum_{1 \leq |\beta| \leq 3} \frac{D^\beta u(\mathbf{x})}{\beta!} (\mathbf{y} - \mathbf{x})^\beta}{|\mathbf{x} - \mathbf{y}|^{d+\alpha}} d\mathbf{y} \\ &\equiv (\text{Id}) + (\text{IIId}), \end{aligned} \quad (11)$$

where we define (Id) to be the first integral and (IIId) to be the second.

## 2.5 The first integral in higher dimensions

To numerically approximate (Id) we use a quadrature rule on a uniform lattice  $\{\mathbf{y}_j\}_{j \in \mathbf{Z}^d} = \{\mathbf{j}h\}_{j \in \mathbf{Z}^d}$ . We assume the lattice is constructed such that the point  $\mathbf{x}$  coincides with with some lattice point  $\mathbf{y}_i$ , which we take to be  $\mathbf{x} = \mathbf{y}_0 = \mathbf{0}$  without loss of generality.

Replacing the integral with a weighted sum over the lattice, we obtain

$$\begin{aligned} (\text{Id}) &\approx C_{\alpha,d} h^d \sum_{\mathbf{j} \neq \mathbf{0}} \frac{u(\mathbf{y}_i) - u(\mathbf{y}_j) + w(|\mathbf{y}_i - \mathbf{y}_j|) \sum_{1 \leq |\beta| \leq 3} \frac{D^\beta u(\mathbf{y}_i)}{\beta!} (\mathbf{y}_j - \mathbf{y}_i)^\beta}{|\mathbf{y}_i - \mathbf{y}_j|^{d+\alpha}} \\ &= C_{\alpha,d} h^d \sum_{\mathbf{j} \neq \mathbf{0}} \frac{u(\mathbf{0}) - u(\mathbf{y}_j) + w(|\mathbf{y}_j|) \sum_{1 \leq |\beta| \leq 3} \frac{D^\beta u(\mathbf{0})}{\beta!} (\mathbf{y}_j)^\beta}{|\mathbf{y}_j|^{d+\alpha}}, \end{aligned}$$

which we note does not include a term for  $\mathbf{j} = \mathbf{0}$ . This corresponds to the standard trapezoidal rule for  $d = 2$  and the punctured trapezoidal rule for  $d = 3$ , though more involved quadrature corrections may be used (see, e.g., Marin, Runborg and Tornberg [30]). Assuming  $w$  is symmetric about the origin, we see that for many values of the multi-index  $\beta$  the corresponding summand vanishes due to oddness considerations. Taking these symmetries into account, we let  $\mathbf{e}_1^T \mathbf{y}_j$  denote the first coordinate of  $\mathbf{y}_j$  and observe that

$$\sum_{\mathbf{j} \neq \mathbf{0}} \sum_{1 \leq |\beta| \leq 3} \frac{w(|\mathbf{y}_j|) \frac{D^\beta u(\mathbf{0})}{\beta!} (\mathbf{y}_j)^\beta}{|\mathbf{y}_j|^{d+\alpha}} = \frac{\Delta u(\mathbf{0})}{2} \sum_{\mathbf{j} \neq \mathbf{0}} \frac{w(|\mathbf{y}_j|) (\mathbf{e}_1^T \mathbf{y}_j)^2}{|\mathbf{y}_j|^{d+\alpha}},$$

which we plug back into our quadrature scheme to obtain

$$\begin{aligned}
(\text{Id}) &\approx C_{\alpha,d} h^d \sum_{\mathbf{j} \neq \mathbf{0}} \frac{u(\mathbf{0}) - u(\mathbf{y}_j) + \frac{\Delta u(\mathbf{0})}{2} w(|\mathbf{y}_j|) (\mathbf{e}_1^T \mathbf{y}_j)^2}{|\mathbf{y}_j|^{d+\alpha}} \\
&= C_{\alpha,d} h^d \left[ \left( \sum_{\mathbf{j} \neq \mathbf{0}} \frac{1}{|\mathbf{y}_j|^{d+\alpha}} \right) u(\mathbf{0}) - \sum_{\mathbf{j} \neq \mathbf{0}} \frac{u(\mathbf{y}_j)}{|\mathbf{y}_j|^{d+\alpha}} + \left( \frac{1}{2} \sum_{\mathbf{j} \neq \mathbf{0}} \frac{w(|\mathbf{y}_j|) (\mathbf{e}_1^T \mathbf{y}_j)^2}{|\mathbf{y}_j|^{d+\alpha}} \right) \Delta u(\mathbf{0}) \right] \\
&\equiv C_{\alpha,d} h^d \left[ A_{1d} u(\mathbf{0}) - \sum_{\mathbf{j} \neq \mathbf{0}} \frac{u(\mathbf{y}_j)}{|\mathbf{y}_j|^{d+\alpha}} + A_{2d} \Delta u(\mathbf{0}) \right]
\end{aligned}$$

with correspondingly defined constants

$$A_{1d} \equiv \left( \sum_{\mathbf{j} \neq \mathbf{0}} \frac{1}{|\mathbf{y}_j|^{d+\alpha}} \right), \quad A_{2d} \equiv \left( \frac{1}{2} \sum_{\mathbf{j} \neq \mathbf{0}} \frac{w(|\mathbf{y}_j|) (\mathbf{e}_1^T \mathbf{y}_j)^2}{|\mathbf{y}_j|^{d+\alpha}} \right). \quad (12)$$

**Theorem 1.** *Suppose the same setup as Lemma 1 with  $k = 6$ ,  $p = 3$ , and  $r = 3$  such that  $t = 4$  and  $s = 2$ . Assume further  $u$  and  $w$  are compactly supported with  $0 \leq w(z) \leq 1$  for all  $z$ . Then the above approximation for (Id) is second-order accurate. That is,*

$$\begin{aligned}
&C_{\alpha,d} \int_{\mathbf{R}^d} \frac{u(\mathbf{0}) - u(\mathbf{y}) + w(|\mathbf{y}|) \sum_{1 \leq |\beta| \leq 3} \frac{D^\beta u(\mathbf{0})}{\beta!} (\mathbf{y})^\beta}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y} \\
&= C_{\alpha,d} h^d \left[ A_{1d} u(\mathbf{0}) - \sum_{\mathbf{j} \neq \mathbf{0}} \frac{u(\mathbf{y}_j)}{|\mathbf{y}_j|^{d+\alpha}} + A_{2d} \Delta u(\mathbf{0}) \right] + \mathcal{O}(h^2),
\end{aligned}$$

with  $A_{1d}$  and  $A_{2d}$  as in (12).

*Proof.* The described approximation is numerically equivalent to the (punctured) trapezoidal rule, so this amounts to bounding the error of the trapezoidal rule applied in  $d$  dimensions with integrand  $\tilde{u}(\mathbf{y})/|\mathbf{y}|^{d+\alpha}$ , where  $\tilde{u}(\mathbf{y})$  is as in Lemma 1 with  $\mathbf{x} = \mathbf{0}$ . Letting  $R > h$  be such that both  $u(\mathbf{y}) = 0$  and  $w(|\mathbf{y}|) = 0$  for  $|\mathbf{y}| > R$ , we proceed by breaking the integral into three contributions: one for the subdomain  $B_h \equiv [-h, h]^d$  “near” the singularity, one for the “mid-range” subdomain  $B_R \setminus B_h \equiv [-R, R]^d \setminus [-h, h]^d$ , and one for the “far” subdomain  $\mathbf{R}^d \setminus B_R$ . We write

$$\int_{\mathbf{R}^d} \frac{\tilde{u}(\mathbf{y})}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y} = \int_{B_h} \frac{\tilde{u}(\mathbf{y})}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y} + \int_{B_R \setminus B_h} \frac{\tilde{u}(\mathbf{y})}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y} + \int_{\mathbf{R}^d \setminus B_R} \frac{\tilde{u}(\mathbf{y})}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y},$$

each piece of which we analyze separately.

Near the singularity, we see due to symmetry considerations that

$$\begin{aligned}
\int_{B_h} \frac{\tilde{u}(\mathbf{y})}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y} &= \sum_{1 \leq |\beta| \leq 3} \frac{D^\beta u(\mathbf{0})}{\beta!} \int_{B_h} \frac{(1 - w(|\mathbf{y}|)) (\mathbf{y})^\beta}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y} + \sum_{|\tilde{\beta}|=4} \int_{B_h} \frac{R_{\tilde{\beta}}(\mathbf{y}) (\mathbf{y})^{\tilde{\beta}}}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y} \\
&= \frac{\Delta u(\mathbf{0})}{2} \int_{B_h} \frac{(1 - w(|\mathbf{y}|)) (\mathbf{e}_1^T \mathbf{y})^2}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y} + \sum_{|\tilde{\beta}|=4} \int_{B_h} \frac{R_{\tilde{\beta}}(\mathbf{y}) (\mathbf{y})^{\tilde{\beta}}}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y} = \mathcal{O}(h^{4-\alpha}),
\end{aligned}$$

where under our assumptions the integrands are both  $O(h^{4-d-\alpha})$  and  $\Delta u$  is bounded. Since  $\tilde{u}(\mathbf{y}) = O(|\mathbf{y}|^t)$ , we see  $\frac{\tilde{u}(\mathbf{y})}{|\mathbf{y}|^{d+\alpha}} = O(|\mathbf{y}|^{t-d-\alpha})$ , which implies that the corresponding (punctured) trapezoidal rule approximation to the integral is  $O(h^{t-\alpha})$ , since we gain a factor of  $h^d$  due to the quadrature weights. Therefore, the contribution to the error from the integral over the near subdomain is  $O(h^{4-\alpha}) = O(h^2)$ , since  $\alpha \in (0, 2)$ .

In the mid-range subdomain, we explicitly use the composite nature of the trapezoidal rule to write

$$\int_{B_R \setminus B_h} \frac{\tilde{u}(\mathbf{y})}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y} = \sum_{\ell} \int_{\Omega_{\ell}} \frac{\tilde{u}(\mathbf{y})}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y},$$

and then consider the error of the trapezoidal rule in approximating the integral over each  $\Omega_{\ell}$  separately, where the square/cubic subdomains  $\{\Omega_{\ell}\}$  in the trapezoidal rule are pairwise disjoint and are such that  $\bigcup_{\ell} \Omega_{\ell} = B_R \setminus B_h$ . Since we are away from the origin, on each subdomain  $\Omega_{\ell}$  the integrand  $\phi(\mathbf{y}) \equiv \frac{\tilde{u}(\mathbf{y})}{|\mathbf{y}|^{d+\alpha}}$  is in  $C^2(\Omega_{\ell})$  which means the standard error bound for the trapezoidal rule on  $\Omega_{\ell}$  gives an error contribution of no more than  $Ch^{d+2} \sum_{|\beta|=2} \|D^{\beta}\phi\|_{L_{\infty}(\Omega_{\ell})}$  for some constant  $C$  independent of  $h$ . However, the term  $\|D^{\beta}\phi\|_{L_{\infty}(\Omega_{\ell})}$  does depend on  $h$ . Since  $D^{\beta}\tilde{u}(\mathbf{y}) = O(|\mathbf{y}|^{t-|\beta|})$  from Lemma 1, the product rule gives  $D^{\beta}\phi(\mathbf{y}) = O(1 + |\mathbf{y}|^{t-|\beta|-d-\alpha})$ . With this we can bound the total error on  $\mathbf{R}^d \setminus B_h$  as

$$\begin{aligned} \sum_{\ell} Ch^{d+2} \sum_{|\beta|=2} \|D^{\beta}\phi\|_{L_{\infty}(\Omega_{\ell})} &\leq C'h^{d+2} \sum_{\ell} \|1 + |\mathbf{y}|^{t-2-d-\alpha}\|_{L_{\infty}(\Omega_{\ell})} \\ &\leq C''h^2 \left(1 + \int_0^R r^{t-3-\alpha} dr\right) = C'''h^2 \end{aligned}$$

where we have bounded

$$h^d \sum_{\ell} \|1 + |\mathbf{y}|^{t-2-d-\alpha}\|_{L_{\infty}(\Omega_{\ell})} \leq c \int_{B_R} (1 + |\mathbf{y}|^{t-2-d-\alpha}) d\mathbf{y} + c'$$

(up to some geometry-dependent factors that are independent of  $h$ ) due to concavity of the summand. Therefore, the error contribution from the mid-range subdomain is  $O(h^2)$ .

Finally, for the far subdomain, we observe that the integrand is in  $C^2(\mathbf{R}^d \setminus B_R)$  and its smoothness is independent of  $h$  in this region, so the standard composite trapezoidal error bound of  $O(h^2)$  applies. Therefore, the overall error is  $O(h^2)$ .  $\square$

## 2.6 The second integral in higher dimensions and final quadrature

We now consider the second integral (II<sub>d</sub>) in (11). Assuming without loss of generality that  $\mathbf{x} = 0$  and using symmetry and oddness considerations as before, we see that

$$\text{(II}_d) = -C_{\alpha,d} \int_{\mathbf{R}^d} \sum_{1 \leq |\beta| \leq 3} \frac{w(|\mathbf{y}|) \frac{D^{\beta} u(\mathbf{0})}{\beta!}(\mathbf{y})^{\beta}}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y} = -\frac{C_{\alpha,d} \Delta u(0)}{2} \int_{\mathbf{R}^d} \frac{w(|\mathbf{y}|) (\mathbf{e}_1^T \mathbf{y})^2}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y}.$$

Defining the constant

$$A_{3d} \equiv -\frac{h^{-d}}{2} \int_{\mathbf{R}^d} \frac{w(|\mathbf{y}|) (\mathbf{e}_1^T \mathbf{y})^2}{|\mathbf{y}|^{d+\alpha}} d\mathbf{y} \quad (13)$$



and combining this with our quadrature for (Id) gives

$$(-\Delta)^{\alpha/2}u(\mathbf{0}) \approx C_{\alpha,d}h^d \left[ A_{1d}u(\mathbf{0}) - \sum_{\mathbf{j} \neq \mathbf{0}} \frac{u(\mathbf{y}_j)}{|\mathbf{y}_j|^{d+\alpha}} + (A_{2d} + A_{3d})\Delta u(\mathbf{0}) \right]$$

or, more generally,

$$(-\Delta)^{\alpha/2}u(\mathbf{y}_i) \approx C_{\alpha,d}h^d \left[ A_{1d}u(\mathbf{y}_i) - \sum_{\mathbf{j} \neq \mathbf{i}} \frac{u(\mathbf{y}_j)}{|\mathbf{y}_i - \mathbf{y}_j|^{d+\alpha}} + (A_{2d} + A_{3d})\Delta u(\mathbf{y}_i) \right].$$

Of course, as written this approximation requires second derivative information in the form of  $\Delta u(\mathbf{y}_i)$ . For smooth  $u$ , however, we may replace this with a finite-difference stencil involving the neighbors of  $\mathbf{y}_i$  in the lattice,

$$\Delta u(\mathbf{y}_i) \approx L_{\text{FD}}u(\mathbf{y}_i) \equiv \frac{1}{h^2} \left( \sum_{\|\mathbf{i}-\mathbf{j}\|_1=1} u(\mathbf{y}_j) - 2^d u(\mathbf{y}_i) \right),$$

just as in the one-dimensional case.

## 2.7 Summary of quadrature for fractional Laplacian

We briefly summarize our complete approach for discretizing the fractional Laplacian applied to a function  $u$ . First, we regularize the integrand of (1) by adding to the numerator a windowed Taylor series approximation of  $u$  about  $\mathbf{x}$  with window function  $w$  to obtain (Id) in (11). This gives an integral that is nice enough to admit discretization with the trapezoidal rule or related schemes. Then, by exploiting symmetries of the problem, we rewrite the discretization in terms of the constants  $A_{1d}$  and  $A_{2d}$  in (12), which do not depend on  $u$ . Finally, we derive an expression for the correction term (IId) in terms of another constant  $A_{3d}$  given in (13), which when combined with (Id) and a finite-difference stencil approximation gives a nice expression for  $(-\Delta)^{\alpha/2}u(\mathbf{y}_i)$  as a linear function of  $u$  evaluated on a regular grid.

A few details of the procedure remain to be discussed. First, there are a number of possibilities for the windowing function  $w$ . In this paper, we use the piecewise-polynomial window

$$w(r) = W_\delta(r) \equiv \begin{cases} 1 - 35 \left(\frac{r}{\delta}\right)^4 + 84 \left(\frac{r}{\delta}\right)^5 - 70 \left(\frac{r}{\delta}\right)^6 + 20 \left(\frac{r}{\delta}\right)^7, & r < \delta, \\ 0, & \text{else.} \end{cases} \quad (14)$$

Of course, this is by no means the only sufficiently smooth choice. Further, we note that the requirement that  $w$  be compactly supported can be relaxed so long as  $W$  decays sufficiently quickly as  $r \rightarrow \infty$  such that the necessary integrals and sums may be computed.

On that note, we also must still compute the constants  $A_{1d}$ ,  $A_{2d}$ , and  $A_{3d}$ . For our choice of polynomial window, the integral defining  $A_{3d}$  can be computed explicitly; for other choices the integral may be numerically computed to high precision offline using, e.g., adaptive quadrature in MATLAB. For compactly supported  $w$ , the sum defining  $A_{2d}$  has a finite number of nonzero terms and is easily computable. Finally, the infinite lattice sum  $A_{1d}$  is given in terms of the Riemann zeta function for  $d = 1$  and may otherwise be well-approximated using far-field compression techniques related to the fast multipole method (FMM) [18, 47]. We use Chebyshev polynomials for far-field compression in the vein of Fong and Darve [13], though we do not require the full FMM machinery as we are interested only in the lattice sum and not a full approximate operator.

### 3 Solving the fractional differential equations on a bounded domain

Having developed our trapezoidal rule scheme for evaluating (1) given  $u$ , we turn now to the fractional differential equations (2) and (3) concerning fractional diffusion on a bounded domain  $\Omega$  with homogeneous extended Dirichlet conditions. We focus on the case  $\Omega = [0, 1]^d$  for simplicity.

#### 3.1 The elliptic case: steady-state fractional diffusion

To solve the elliptic problem (3), we discretize  $\Omega$  using a regular grid of  $N = (n-1)^d$  points  $\{\mathbf{y}_j\}$  with linear spacing  $h = \frac{1}{n+1}$ , where  $\mathbf{j} = (j_1, \dots, j_d)$  and  $\mathbf{y}_j = h\mathbf{j}$ . For notational convenience, we define the index set  $\mathcal{J} \equiv [n]^d \subset \mathbf{Z}^d$ . Then, replacing the fractional Laplacian with our quadrature-based approximation gives

$$C_{\alpha,d}h^d \left[ A_{1d}u_{\mathbf{i}} - \sum_{\substack{\mathbf{j} \in \mathcal{J} \\ \mathbf{j} \neq \{\mathbf{i}\}}} \frac{u_{\mathbf{j}}}{|\mathbf{y}_{\mathbf{i}} - \mathbf{y}_{\mathbf{j}}|^{d+\alpha}} + (A_{2d} + A_{3d})L_{\text{FD}}u_{\mathbf{i}} \right] = f(\mathbf{y}_{\mathbf{i}}) \quad \forall \mathbf{i} \in \mathcal{J}, \quad (15)$$

which is a linear system to be solved for the variables  $\{u_{\mathbf{j}}\} \approx \{u(\mathbf{y}_{\mathbf{j}})\}$ . We remark that the ‘‘boundary conditions’’ affect the system in two ways. First, the center sum has been reduced from an infinite number of terms (in general) to a more manageable finite sum. Second, evaluating the finite-difference stencil  $L_{\text{FD}}$  for  $\mathbf{i}$  near the boundary of the domain will require the prescribed value of  $u(\mathbf{y})$  on the boundary, as in the standard (non-fractional) case.

We write (15) in matrix form as

$$\mathbf{M}\mathbf{u} = \mathbf{f}, \quad (16)$$

where now  $\mathbf{u} \in \mathbf{R}^N$  and  $\mathbf{f} \in \mathbf{R}^N$  are vectors with corresponding entries  $\{u_{\mathbf{j}}\}$  and  $\{f(\mathbf{y}_{\mathbf{j}})\}$  and  $\mathbf{M} \in \mathbf{R}^{N \times N}$  contains the coefficients implied by (15).

#### Forward operator and application with FFT

By construction, the approximate fractional Laplacian operator involved in (15) is translation-invariant, which means that the matrix  $\mathbf{M}$  is block Toeplitz with Toeplitz blocks (BTTB) under any natural ordering of the unknowns. As is well known, this in turn implies that  $\mathbf{M}$  may be applied efficiently using the FFT at a cost of  $O(N \log N)$  FLOPs per application and stored with storage cost  $O(N)$ .

Further, investigation of the constants  $A_{1d}$ ,  $A_{2d}$  and  $A_{3d}$  reveal that  $\mathbf{M}$  is symmetric positive definite. When coupled with the previous observation, this leads naturally to the use of the conjugate gradient method (CG) [19] or related iterative methods for solving (16). However, while the FFT ensures low complexity per iteration, the number of iterations required to achieve a specified iteration can be large unless an effective preconditioner is used. This is of particular concern as  $\alpha \rightarrow 2$ , whereupon we recover the standard (ill-conditioned) Laplacian.

## Preconditioning: Laplacian pattern and fast Poisson solver

To construct an efficient preconditioner for (16), we observe that  $\mathbf{M}$  may be decomposed as the sum of two matrices  $\mathbf{M} = C_{\alpha,d}h^d(\mathbf{K} + \mathbf{L})$ , where

$$\mathbf{K}_{\mathbf{ij}} = \begin{cases} -\frac{1}{|\mathbf{y}_i - \mathbf{y}_j|^{d+\alpha}}, & \mathbf{i} \neq \mathbf{j}, \\ A_{1d}, & \mathbf{i} = \mathbf{j}, \end{cases} \quad \text{and} \quad \mathbf{L}_{\mathbf{ij}} = \begin{cases} \frac{(A_{2d} + A_{3d})}{h^2}, & \|\mathbf{i} - \mathbf{j}\|_1 = 1, \\ -\frac{2^d(A_{2d} + A_{3d})}{h^2}, & \mathbf{i} = \mathbf{j}, \\ 0, & \text{else,} \end{cases}$$

and we note that  $A_{2d} + A_{3d} < 0$ . The sparse matrix  $\mathbf{L}$  is (up to a proportionality constant) the typical finite-difference approximation of the negative Laplacian, whereas the matrix  $\mathbf{K}$  has entries that quickly decay away from  $\mathbf{i} = \mathbf{j}$ , particularly for larger  $\alpha$ . This motivates using  $\mathbf{L}$  itself as a preconditioner when using CG to solve (16). Because  $\mathbf{L}$  is effectively a finite-difference discretization of Poisson's equation on a regular grid with homogeneous Dirichlet boundary conditions, application of  $\mathbf{L}^{-1}$  may be accomplished with the FFT at a cost of  $O(N \log N)$  using typical fast Poisson solver techniques [24, Chapter 12]. For non-rectangular domains, the FFT-based approach is no longer feasible, but the same preconditioner could be used with, e.g., nested dissection [17] or related methods.

We remark that other choices of preconditioner are possible. For example, rather than using  $\mathbf{L}^{-1}$  as our preconditioner we could instead use  $\tilde{\mathbf{M}}^{-1}$ , where  $\tilde{\mathbf{M}}_{\mathbf{ij}} = \mathbf{M}_{\mathbf{ij}}$  if  $\mathbf{L}_{\mathbf{ij}} \neq 0$  and zero otherwise. Preliminary experiments with this approach (not shown) did not seem to show measurable benefit.

### 3.2 The time-dependent case: time-dependent fractional diffusion

We turn now to the full time-dependent problem (2). For spatial discretization we use the approximate fractional Laplacian just as in Section 3.1, which we combine with a Crank-Nicolson scheme for the discretization of temporal derivatives. This leads to the implicit time-stepping method

$$\left( \mathbf{I} + \frac{\Delta t}{2} \mathbf{M} \right) \mathbf{u}^{(k+1)} = \left( \mathbf{I} - \frac{\Delta t}{2} \mathbf{M} \right) \mathbf{u}^{(k)} + \frac{\Delta t}{2} \left( \mathbf{f}^{(k+1)} + \mathbf{f}^{(k)} \right) \quad (17)$$

to be solved for  $\mathbf{u}^{(k+1)} \in \mathbf{R}^N$ , where  $\mathbf{M}$  is as in Section 3.1 and now  $\mathbf{u}^{(k)} \in \mathbf{R}^N$  and  $\mathbf{f}^{(k)} \in \mathbf{R}^N$  have entries  $\{u_{\mathbf{j}}^{(k)}\} \approx \{u(\mathbf{y}_{\mathbf{j}}, t_k)\}$  and  $\{f_{\mathbf{j}}^{(k)}\} = \{f(\mathbf{y}_{\mathbf{j}}, t_k)\}$  for  $t_k = k\Delta t$ .

Just as in Section 3.1, we exploit BTTB structure to apply  $\mathbf{M}$  such that (17) may be solved efficiently with CG at each time step. Compared to the steady-state problem, the system matrix  $(\mathbf{I} + \frac{\Delta t}{2} \mathbf{M})$  here is much better conditioned due to the addition of the identity. However, we still find that the number of iterations is reduced substantially via preconditioning, where we use the matrix  $\mathbf{I} + \frac{\Delta t}{2} C_{\alpha,d} h^d \mathbf{L}$  as preconditioner.

## 4 Numerical results

To demonstrate and profile our approach to discretizing and solving fractional diffusion problems on bounded Cartesian domains, we implemented a number of examples. All computations were performed in MATLAB R2017a on a 64-bit Ubuntu laptop with a dual-core Intel Core i7-7500U processor at 2.70 GHz and 16GB of RAM.

Table 1: Runtimes  $t_{\text{con}}$  for the construction of the operator  $\mathbf{M}$  and  $t_{\text{app}}$  for application via FFT for the one-dimensional elliptic example, as well as relative apply errors for  $\alpha \in \{1.25, 1.50, 1.75\}$ .

$N$	$t_{\text{con}}$	$t_{\text{app}}$	$e_{\text{app},1.25}$	$e_{\text{app},1.5}$	$e_{\text{app},1.75}$	$e_{\text{sol},1.25}$	$e_{\text{sol},1.5}$	$e_{\text{sol},1.75}$
511	1.2e-03	3.2e-04	3.6e-06	9.5e-06	2.0e-05	1.6e-07	5.5e-07	2.0e-06
1023	1.6e-03	6.1e-04	9.6e-07	2.7e-06	5.5e-06	2.6e-08	1.0e-07	4.3e-07
2047	2.4e-03	9.3e-04	2.6e-07	7.7e-07	1.6e-06	4.0e-09	1.8e-08	9.0e-08
4095	3.0e-03	1.5e-03	7.0e-08	2.2e-07	5.0e-07	6.3e-10	3.2e-09	1.9e-08

#### 4.1 Elliptic example: interval in one dimension

We begin with a one-dimensional elliptic example on the interval  $\Omega = [-1, 1]$ , discretizing and solving (3) with right-hand side

$$f(x) = {}_2F_1\left(\frac{1+\alpha}{2}, -2; \frac{1}{2}; x^2\right) \quad (18)$$

given in terms of the Gauss hypergeometric function [1]. In this case, the analytic solution on  $\Omega$  is known and is given up to a known constant of proportionality  $K_\alpha$  by  $u(x) = K_\alpha^{-1} (1-x^2)^{2+\frac{\alpha}{2}}$  [21].

We discretize the interval with regularly-spaced points as in (15) with  $d = 1$ , recording the total time  $t_{\text{con}}$  to construct the discrete operator  $\mathbf{M}$ . We choose  $\delta$  in (14) as a function of the number of discretization points  $N$ , such that  $w$  is supported inside a ball with a radius of 20 discretization points. Using the known solution  $u(x)$  for right-hand side (RHS) (18), we record the time to apply our operator using the FFT,  $t_{\text{app}}$ , and measure the apply error of our discretization as  $e_{\text{app}} \equiv \|\mathbf{M}\mathbf{u}_{\text{true}} - \mathbf{f}\|/\|\mathbf{f}\|$ , where  $\mathbf{u}_{\text{true}}$  is the analytic solution sampled on the discrete grid points and  $\mathbf{f}$  is the discretized RHS. To demonstrate the solution error of our discretization scheme we take the same RHS as before and use CG to solve the resulting linear system (16). This gives a discrete solution  $\mathbf{u}$  that we can compare to  $\mathbf{u}_{\text{true}}$  by computing the relative solution error  $e_{\text{sol}} \equiv \|\mathbf{u} - \mathbf{u}_{\text{true}}\|/\|\mathbf{u}_{\text{true}}\|$ . These metrics are all shown in Table 1 for three different choices of  $\alpha$ , with the error metrics plotted in Fig. 1. Note that  $t_{\text{con}}$  and  $t_{\text{app}}$  do not depend on  $\alpha$ , so we report these quantities only for  $\alpha = 1.50$ .

We show in Table 2 the runtime  $t_{\text{CG}}$  and iterations  $n_{\text{CG}}$  required by CG to solve the linear system (16) for two different choices of tolerance  $\epsilon_{\text{res}}$  in the relative  $\ell_2$ -norm residual. We give results both for the preconditioned system (where the preconditioner  $\mathbf{L}$  is a finite-difference Laplacian as described in Section 3.1) and the unpreconditioned system. Because this is a one-dimensional problem, use of a fast Poisson solver to apply  $\mathbf{L}^{-1}$  is not strictly necessary for efficiency. Instead, we use a sparse Cholesky factorization, with negligible overhead. The corresponding timing results are plotted in Fig. 2 (left), where we see that our simple preconditioning scheme is effective for reducing the time to solution, especially for larger  $\alpha$ .

#### 4.2 Elliptic example: square domain in two dimensions

For the two-dimensional case, we measure construction time  $t_{\text{con}}$  and apply time  $t_{\text{app}}$  just as before and report these in Table 3. However, unlike the one-dimensional case, in two dimensions there is no RHS  $f$  for which (3) has a simple known solution. Instead, we discretize the domain  $\Omega = [0, 1]^2$  with  $N$  DOFs and use standard grid error estimates based on Richardson extrapolation to estimate the rate of convergence.

Table 2: Runtime  $t_{CG}$  and number of iterations  $n_{CG}$  required to solve the one-dimensional elliptic example using CG with/without preconditioning based on the finite-difference Laplacian. The parenthesized quantities indicate the corresponding test did not converge within 1000 iterations.

$\alpha$	$N$	$\epsilon_{\text{res}} = 10^{-6}$		$\epsilon_{\text{res}} = 10^{-9}$	
		$t_{CG}$	$n_{CG}$	$t_{CG}$	$n_{CG}$
1.25	511	4.8e-3 / 1.8e-2	22 / 104	7.2e-3 / 2.0e-2	35 / 123
	1023	1.4e-2 / 5.7e-2	27 / 162	1.5e-2 / 5.0e-2	44 / 190
	2047	2.6e-2 / 1.5e-1	35 / 251	3.9e-2 / 1.8e-1	57 / 295
	4095	6.3e-2 / 4.3e-1	43 / 389	9.5e-2 / 5.1e-1	72 / 457
1.50	511	3.6e-3 / 2.5e-2	15 / 156	6.4e-3 / 2.9e-2	23 / 174
	1023	8.1e-3 / 6.9e-2	20 / 263	1.2e-2 / 8.8e-2	28 / 294
	2047	1.8e-2 / 2.7e-1	22 / 445	2.9e-2 / 3.1e-1	34 / 497
	4095	3.7e-2 / 8.5e-1	26 / 752	5.7e-2 / 9.7e-1	40 / 839
1.75	511	2.7e-3 / 3.3e-2	11 / 216	3.7e-3 / 3.8e-2	15 / 229
	1023	4.5e-3 / 9.9e-2	12 / 397	7.9e-3 / 1.1e-1	17 / 422
	2047	1.1e-2 / 4.3e-1	13 / 731	1.7e-2 / 4.8e-1	18 / 776
	4095	2.7e-2 / (1e+0)	15 / (1000)	4.2e-2 / (1e+0)	21 / (1000)

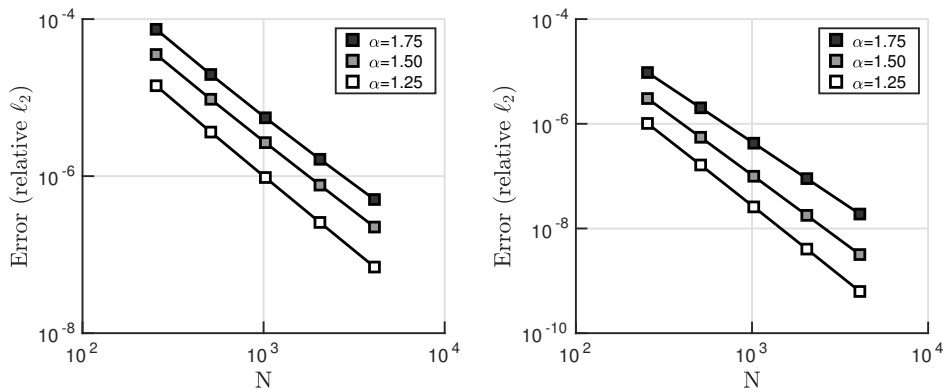


Figure 1: For the one-dimensional example, we plot the relative  $\ell_2$  apply error  $e_{\text{app}}$  (left) and solve error  $e_{\text{sol}}$  (right) as tabulated in Table 1. In each case we see steady convergence, though with differing rates (note the difference in  $y$ -axis scale between figures).

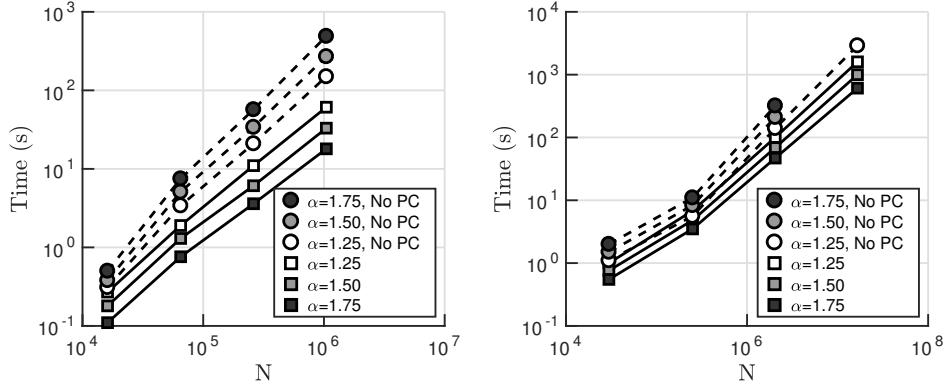


Figure 2: For the two-dimensional (left) and three-dimensional (right) examples, we plot the runtime  $t_{CG}$  required by CG as tabulated in Tables 5 and 8, both with and without preconditioning. Note that some points in the last plot are absent due to excessive runtime.

Concretely, for our application error grid estimate we use the function

$$g_1(\mathbf{x}) = \prod_{i=1}^2 \frac{1}{4} (1 + \cos(2\pi x_i - \pi))^2, \quad (19)$$

which is nice when truncated to  $\Omega = [0, 1]^2$ . Using a coarse grid of size  $255^2$ , a medium-scale grid of size  $511^2$ , and a fine-scale grid of size  $1023^2$ , we obtained three corresponding estimates of the fractional Laplacian of  $g_1$  evaluated on the common coarse grid:  $\{\mathbf{f}_c, \mathbf{f}_m, \mathbf{f}_f\} \subset \mathbf{R}^{255^2}$ . The Richardson error rate estimate is then given by

$$R_p \equiv \frac{\log \|\mathbf{f}_f - \mathbf{f}_m\|_p - \log \|\mathbf{f}_m - \mathbf{f}_c\|_p}{\log 1/2}, \quad (20)$$

where  $\|\cdot\|_p$  is the  $\ell_p$  norm. For solution error, we obtain analogous error rate estimates for the solution  $u$  to the extended Dirichlet problem using RHS  $g_2(\mathbf{x}) = 1$ . These rate estimates can be seen in Table 4, where we observe that the solution error rates are limited to first-order due to the general lack of smoothness of  $u$  near the boundary of  $\Omega$  [40].

In Table 5 and Fig. 2 (left) we give CG convergence results for the two-dimensional example, analogous to the one-dimensional results in Table 2. Note that unlike the one-dimensional case we find it essential to use a fast Poisson solver to apply the preconditioner. While the reduced number of iterations is roughly offset by the cost of applying the preconditioner at each iteration for smaller  $\alpha$  and  $N$ , the utility of our preconditioning approach becomes clear for the larger, more ill-conditioned problems.

### 4.3 Elliptic example: cubic domain in three dimensions

In three dimensions for the case  $\Omega = [0, 1]^3$  we repeat experiments analogous to those in Section 4.2.

To compute our three-dimensional grid error estimates (20), we use the 3D analogue of (19),

$$g_1(\mathbf{x}) = \prod_{i=1}^3 \frac{1}{4} (1 + \cos(2\pi x_i - \pi))^2$$

Table 3: Runtimes  $t_{\text{con}}$  for the construction of the operator  $\mathbf{M}$  and  $t_{\text{app}}$  for application via FFT for the two-dimensional elliptic example.

$N$	$t_{\text{con}}$	$t_{\text{app}}$
$127^2$	8.4e-2	4.5e-3
$255^2$	9.8e-2	3.0e-2
$511^2$	1.9e-1	1.1e-1
$1023^2$	6.1e-1	5.0e-1

Table 4: Grid error estimates  $R_2$  and  $R_\infty$  for both  $\mathbf{u}$  and  $\mathbf{f}$  in (16) for the two-dimensional elliptic example.

$\alpha$	Grid rate, $\mathbf{u}$		Grid rate, $\mathbf{f}$	
	$R_2$	$R_\infty$	$R_2$	$R_\infty$
1.25	0.98	0.87	2.65	2.63
1.50	0.99	0.82	2.38	2.35
1.75	0.99	0.87	2.16	2.15

Table 5: Runtime  $t_{\text{CG}}$  and number of iterations  $n_{\text{CG}}$  required to solve the two-dimensional elliptic example using CG with/without p reconditioning based on the finite-difference Laplacian.

$\alpha$	$N$	$\epsilon_{\text{res}} = 10^{-6}$		$\epsilon_{\text{res}} = 10^{-9}$	
		$t_{\text{CG}}$	$n_{\text{CG}}$	$t_{\text{CG}}$	$n_{\text{CG}}$
1.25	$127^2$	1.7e-1 / 2.2e-1	21 / 61	2.7e-1 / 3.1e-1	33 / 77
	$255^2$	1.1e+0 / 2.3e+0	28 / 95	1.9e+0 / 3.4e+0	43 / 121
	$511^2$	6.5e+0 / 1.6e+1	36 / 148	1.1e+1 / 2.1e+1	57 / 188
	$1023^2$	3.7e+1 / 1.2e+2	47 / 231	6.1e+1 / 1.5e+2	74 / 292
1.50	$127^2$	1.3e-1 / 3.3e-1	15 / 86	1.8e-1 / 3.8e-1	23 / 108
	$255^2$	8.6e-1 / 4.0e+0	18 / 147	1.3e+0 / 5.1e+0	28 / 184
	$511^2$	4.0e+0 / 2.7e+1	21 / 250	6.1e+0 / 3.4e+1	33 / 312
	$1023^2$	2.2e+1 / 2.2e+2	26 / 425	3.3e+1 / 2.7e+2	40 / 528
1.75	$127^2$	8.6e-2 / 4.1e-1	11 / 120	1.1e-1 / 5.0e-1	15 / 149
	$255^2$	5.7e-1 / 6.1e+0	12 / 223	7.6e-1 / 7.5e+0	17 / 278
	$511^2$	2.5e+0 / 4.6e+1	13 / 413	3.6e+0 / 5.7e+1	19 / 516
	$1023^2$	1.2e+1 / 4.0e+2	14 / 766	1.8e+1 / 4.9e+2	21 / 962

Table 6: Runtimes  $t_{\text{con}}$  for the construction of the operator  $\mathbf{M}$  and  $t_{\text{app}}$  for application via FFT for the three-dimensional elliptic example. Table 7: Grid error estimates  $R_2$  and  $R_\infty$  for both  $\mathbf{u}$  and  $\mathbf{f}$  in (16) for the three-dimensional elliptic example.

$N$	$t_{\text{con}}$	$t_{\text{app}}$	Grid rate, $\mathbf{u}$		Grid rate, $\mathbf{f}$		
			$\alpha$	$R_2$	$R_\infty$	$R_2$	$R_\infty$
$31^3$	2.3e-1	3.0e-2	1.25	1.02	0.90	4.35	4.55
$63^3$	3.1e-1	8.7e-2	1.50	1.10	0.87	4.22	4.62
$127^3$	1.3e+0	1.3e+0	1.75	1.30	1.13	3.90	4.99
$255^3$	1.8e+1	2.0e+1					

Table 8: Runtime  $t_{\text{CG}}$  and number of iterations  $n_{\text{CG}}$  required to solve the three-dimensional elliptic example using CG with/without preconditioning based on the finite-difference Laplacian. The parenthesized quantities indicate the corresponding test did not converge within 250 iterations.

$\alpha$	$N$	$\epsilon_{\text{res}} = 10^{-6}$		$\epsilon_{\text{res}} = 10^{-9}$	
		$t_{\text{CG}}$	$n_{\text{CG}}$	$t_{\text{CG}}$	$n_{\text{CG}}$
1.25	$31^3$	6.4e-1 / 7.7e-1	13 / 27	1.0e+0 / 1.1e+0	20 / 37
	$63^3$	4.3e+0 / 4.6e+0	16 / 47	6.8e+0 / 5.6e+0	24 / 63
	$127^3$	6.9e+1 / 1.0e+2	21 / 75	1.0e+2 / 1.4e+2	32 / 100
	$255^3$	1.0e+3 / 2.2e+3	27 / 117	1.6e+3 / 2.9e+3	42 / 156
1.50	$31^3$	5.3e-1 / 1.1e+0	10 / 36	7.6e-1 / 1.5e+0	14 / 50
	$63^3$	3.5e+0 / 5.9e+0	12 / 66	4.8e+0 / 8.3e+0	17 / 91
	$127^3$	4.7e+1 / 1.5e+2	14 / 113	6.9e+1 / 2.1e+2	21 / 154
	$255^3$	7.2e+2 / 3.6e+3	18 / 195	1.0e+3 / (4.6e+3)	26 / (250)
1.75	$31^3$	4.1e-1 / 1.6e+0	7 / 49	5.5e-1 / 2.0e+0	10 / 65
	$63^3$	2.4e+0 / 8.3e+0	8 / 93	3.5e+0 / 1.1e+1	12 / 123
	$127^3$	3.4e+1 / 2.4e+2	10 / 175	4.7e+1 / 3.2e+2	14 / 229
	$255^3$	4.6e+2 / (4.6e+3)	11 / (250)	6.1e+2 / (4.6e+3)	15 / (250)

for the apply error and again  $g_2(\mathbf{x}) \equiv 1$  for the solution error. We use coarse, medium-scale, and fine grids with sizes  $61^3$ ,  $127^3$ , and  $255^3$ , respectively, and give the results in Table 7. We remark that the error rates reported for  $\mathbf{f}$  appear artificially inflated, likely due to the fact that the grid error estimate is an asymptotic approximation that holds in the limit of large  $N$ , and  $N = 63^3$  is not large.

In Table 8 and Fig. 2 (right) we give CG convergence results for the three-dimensional example, just like those for the two-dimensional example. Just as in two dimensions, the utility of our simple preconditioner is clear for larger problems and for larger  $\alpha$ , where iterative approaches to solving the linear system start to become prohibitively expensive without preconditioning.

#### 4.4 Time-dependent example: cubic domain in three dimensions

As described in Section 3.2, our approach to the time-dependent fractional diffusion problem (2) involves first computing the discrete fractional Laplacian operator as before and then using a Crank-Nicolson method to time-step the solution. Here we demonstrate the efficiency of our pre-



Table 9: Grid error estimates  $R_2$  and  $R_\infty$  for the solution at time  $T = 0.25$  to the parabolic problem (2) in both two and three dimensions as described in Section 4.4.

$\alpha$	2D		3D	
	$R_2$	$R_\infty$	$R_2$	$R_\infty$
1.25	0.97	0.87	2.22	3.11
1.50	0.97	0.82	2.30	3.24
1.75	0.97	0.85	3.02	3.39

conditioning scheme for the time-dependent problem and give grid error estimates for  $\Omega = [0, 1]^d$ .

For smooth solutions, the Crank-Nicolson scheme is locally second-order in time and our spatial discretization is locally second-order in space. Thus, we choose our temporal step size in  $d$  dimensions as  $\Delta t = (N^{1/d} + 1)^{-1}$  such that  $\Delta t \approx h$  but the number of time steps required to reach a final time of  $T = 0.25$  is integral. However, we remark that, just as in the elliptic case, we cannot expect better than first-order convergence in general [12].

For our grid error estimates we take  $f \equiv 0$  in (2) and initial condition

$$u_0(\mathbf{x}) = \prod_{i=1}^d \frac{1}{4} (1 + \cos(2\pi\nu_i x_i - \pi))^2,$$

with  $\nu_1 = 3$ ,  $\nu_2 = 11$ , and  $\nu_3 = 2$ . Using (17) to time-step the solution to final time  $T = 0.25$ , we then compute grid error estimates for simultaneous refinement in space and time, which are given in Table 9. For the two-dimensional case we use spatial grids with  $255^2$ ,  $511^2$ , and  $1023^2$  points for the coarse, medium-scale, and fine grids, respectively. For the three-dimensional case we analogously use  $31^3$ ,  $63^3$ , and  $127^3$  points in space, as we are limited by the runtime requirements of solving the largest problems. As in the elliptic setting, we observe an artificial inflation of the Richardson rate in three dimensions.

In Table 10 we give the CG results for a single time time-step with random RHS, i.e., the results for a single linear system. In both two dimensions and three dimensions, we use the preconditioner described in Section 2 applied with a modified fast Poisson solver. Compared to the elliptic setting, we see that the time-dependent system matrix is better conditioned and thus preconditioning for  $\alpha = 1.25$  is not necessary in two dimensions and not helpful in three dimensions. However, for larger  $\alpha$  there is a clear benefit.

We remark that in practical settings with multiple time steps the number of iterations is reduced slightly from the current setting because the old solution  $\mathbf{u}^{(k)}$  can be used as an initial guess for the solution  $\mathbf{u}^{(k+1)}$ , but the difference is not substantial in general.

## 5 Conclusions

We introduced a simple discretization scheme for the fractional Laplacian operator in one, two, and three dimensions based on singularity subtraction combined with the regularly-spaced trapezoidal rule. When applied to sufficiently smooth functions  $u$ , the resulting discretization is provably second-order accurate in the grid spacing  $h$ , whereas for rougher  $u$  we observe first-order accuracy in the  $\ell_2$  solution error.

Table 10: Runtime  $t_{CG}$  and number of iterations  $n_{CG}$  required to perform a single time step for the time-dependent example using CG with/without preconditioning based on the finite-difference Laplacian in both two and three dimensions. In all cases we use  $\epsilon_{res} = 10^{-9}$ .

$\alpha$	2D			3D		
	$N$	$t_{CG}$	$n_{CG}$	$N$	$t_{CG}$	$n_{CG}$
1.25	$255^2$	9.3e-1 / 1.2e+0	12 / 25	$63^3$	4.6e+0 / 3.5e+0	11 / 25
	$511^2$	3.6e+0 / 5.2e+0	12 / 27	$127^3$	6.2e+1 / 6.0e+1	12 / 28
	$1023^2$	1.7e+1 / 2.6e+1	12 / 29	$255^3$	6.3e+2 / 6.1e+2	12 / 30
1.50	$255^2$	9.5e+0 / 2.7e+1	12 / 56	$63^3$	4.2e+0 / 6.6e+0	10 / 47
	$511^2$	3.9e+0 / 1.3e+1	13 / 67	$127^3$	6.2e+1 / 1.3e+2	12 / 60
	$1023^2$	1.9e+1 / 6.6e+1	14 / 79	$255^3$	5.3e+2 / 1.4e+3	13 / 73
1.75	$255^2$	5.2e-1 / 2.9e+0	10 / 121	$63^3$	3.5e+0 / 1.1e+1	8 / 81
	$511^2$	2.1e+0 / 1.6e+1	11 / 162	$127^3$	5.1e+1 / 2.5e+2	9 / 122
	$1023^2$	1.6e+1 / 2.1e+2	12 / 212	$255^3$	4.1e+2 / 3.3e+3	10 / 170

When the order  $\alpha$  of the fractional Laplacian is close to two, the discrete operator is ill conditioned, reflecting the underlying ill-conditioning of the continuous (integer-order) Laplacian. To efficiently solve linear systems with the discrete fractional Laplacian, we demonstrated the utility of a simple preconditioning scheme based on fast Poisson solvers.

For higher-order schemes, it is necessary to forsake the simplicity of our approach to more precisely handle solutions  $u$  that exhibit only fractional-order smoothness near the boundary of  $\Omega$  for both (2) and (3). While we intend to pursue this in future work, we have shown that the scheme presented here provides a fast, simple alternative for situations where lower-order accuracy is amenable.

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