RATIONAL APPROXIMATION TO THE FRACTIONAL LAPLACIAN OPERATOR IN REACTION-DIFFUSION PROBLEMS*

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Abstract. This paper provides a new numerical strategy to solve fractional in space reaction-diffusion equations on bounded domains under homogeneous Dirichlet boundary conditions. Using the matrix transfer technique the fractional Laplacian operator is replaced by a matrix which, in general, is dense. The approach here presented is based on the approximation of this matrix by the product of two suitable banded matrices. This leads to a semi-linear initial value problem in which the matrices involved are sparse. Numerical results are presented to verify the effectiveness of the proposed solution strategy.

Key words. fractional Laplacian operator, matrix functions, Guass-Jacobi rule

AMS subject classifications. 65F60, 35R11, 65D32

1. Introduction.

Fractional-order in space mathematical models, in which an integer-order differential operator is replaced by a corresponding fractional one, are becoming increasingly used since they provide an adequate description of many processes that exhibit anomalous diffusion. This is due to the fact that the non-local nature of the fractional operators enables to capture the spatial heterogeneity that characterizes these processes.

There are however some challenges when facing fractional models. First of all, there is no unique way to define fractional in space derivatives and, in general, these definitions are not equivalent especially when more than one spatial dimension is considered [17]. In addition, considering that the value of the solution at a given point depends on the solution behavior on the entire domain, it is intuitive to understand that the boundary conditions deserve a particular attention and should be appropriately chosen in order to model the phenomenon properly.

In this paper we consider the following fractional in space reaction-diffusion differential equation

$$\frac{\partial u(\mathbf{x},t)}{\partial t} = -\kappa_\alpha \, (-\Delta)^{\alpha/2} u(\mathbf{x},t) + f(\mathbf{x},t,u), \qquad \mathbf{x} \in \Omega \subset \mathbb{R}^n, \quad t \in (0,T), \tag{1}$$

subject to homogeneous Dirichlet boundary conditions

$$u(\mathbf{x},t)|_{\hat{\Omega}} = 0, \qquad \hat{\Omega} = \mathbb{R}^n \setminus \Omega, \tag{2}$$

and the initial condition

$$u(\mathbf{x},0) = u_0(\mathbf{x}), \tag{3}$$

where κ_α represents the diffusion coefficient and the forcing term f and u_0 are sufficiently smooth functions. The symmetric space fractional derivative $-(-\Delta)^{\alpha/2}$ of order α $(1 < \alpha \leq 2)$ is defined through the spectral decomposition of the homogeneous Dirichlet Laplace operator $(-\Delta)$, [9, Definition 2]. Assuming that Ω is a Lipschitz

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domain, the spectrum of $(-\Delta)$ is discrete and positive, and accumulate at infinity. Thus,

$$-(-\Delta)^{\alpha/2}u = \sum_{s=1}^{\infty} \mu_s^{\alpha/2} c_s \varphi_s, \tag{4}$$

where $c_s = \int_\Omega u\,\varphi_s$ are the Fourier coefficients of u, and $\{\mu_s\}$, $\{\varphi_s\}$ are the eigenvalues and the eigenvectors of $(-\Delta)$, respectively.

We remark that the fractional power of the Laplace operator is alternatively defined in the literature using the Fourier transform on an infinite domain [12], with a natural extension to finite domain when the function u vanishes on and outside the boundary of the spatial domain. In this case, in fact, it is possible to consider non-local problems on bounded domains by simply assuming that the solution of fractional problem is equal to zero everywhere outside the domain of interest. Using such definition and assuming to work with homogeneous Dirichlet boundary conditions, in [15, Lemma 1] it has been proved that the one-dimensional fractional Laplacian operator $-(-\Delta)^{\alpha/2}$ as defined in (4) is equivalent to the Riesz fractional derivative. Hence, it can be approximated by the 'fractional centered derivative' introduced by Ortigueira in [11]. Çelik and Duman in [5] have used such a method for solving a fractional diffusion equation with the Riesz fractional derivative in a finite domain. Moreover, by exploiting the decay of the coefficients characterizing the method, in [10] a 'short memory' version of the scheme has been implemented. However, both the original and the modified methods only work for one-dimensional problems.

A mainstay in the numerical treatment of partial differential problems of type (1)–(3) is to apply the method of lines. Discretizing in space with a uniform mesh of stepsize h in each domain direction and using the matrix transfer technique proposed in [8, 9] by Ilić et al., we obtain

$$-(-\Delta)^{\alpha/2}u \approx -\frac{1}{h^\alpha} L^{\alpha/2} u,$$

where $h^{-2}L$ is the approximate matrix representation of the standard Laplacian obtained by using any finite difference method. Consequently, (1) is transformed into a system of ordinary differential equations

$$\frac{d\mathbf{u}}{dt} = -\frac{\kappa_\alpha}{h^\alpha} L^{\alpha/2}\mathbf{u} + \mathbf{f}(t,\mathbf{u}), \tag{5}$$

where $\mathbf{u}$ and $\mathbf{f}(t,\mathbf{u})$ denote the vectors of node values of u and f, respectively. The matrix L raised to the fractional power $\alpha/2$ is, in general, a dense matrix which could be also very large depending on the numbers of mesh points used for the spatial discretization. Therefore, the computational effort for solving (5) could be really heavy, independently of the integrator used. Recently, some authors have developed techniques for reducing this cost. In particular, an approach which can be equally applicable to fractional-in-space problems in two or three spatial dimensions has been considered in [4]. The key point of this approach is the efficient computation of the fractional power of a matrix times a vector.

In this paper, we propose a solution strategy based on a suitable approximation of $L^{\alpha/2}$. In particular, we look for a decomposition of the type

$$L^{\alpha/2} \approx M^{-1}K,$$

where M and K are both banded matrices arising from a rational approximation of the function $z^{\alpha/2-1}$, based on the Gauss-Jacobi rule applied to the integral representation of $L^{\alpha/2}$, cf. [6]. The poles of the formula depends on a continuous parameter whose choice is crucial for a fast and accurate approximation. The above factorization allows to approximate the solution of (5) by solving

$$M\,\frac{d\mathbf{v}}{dt} = -\frac{\kappa_\alpha}{h^\alpha}\,K\mathbf{v} + M\mathbf{f}(t,\mathbf{v}). \tag{6}$$

By virtue of the structure of the matrices M and K the numerical solution of (6) may be computed in a more efficient way with respect to the one of (5). We remark that the approach is independent of the Laplacian working dimension.

The paper is organized as follows. In section 2, the main results about the matrix transfer technique are recalled. Section 3 is devoted to the construction of the rational approximation together with the analysis of the asymptotically optimal choices of the poles. In section 4 a theoretical error analysis is presented. Numerical experiments are carried out in section 5, and the conclusions follow in section 6.

2. Background on the matrix transfer technique. For an independent reading, in this section the basic facts concerning the matrix transfer technique proposed by Ilić et al. in [8, 9] to discretize the one-dimensional fractional Laplacian operator are recalled. In addition, since in this work we also lead with problems in two spatial dimensions, we refer to the results given in [16] as well.

Working with the basic assumption that the fractional Laplacian operator with Dirichlet boundary conditions can be defined as the fractional power of the standard Laplacian, the matrix transfer technique simply consists in approximating the operator $-(-\Delta)^{\alpha/2}$ through the matrix $-h^{-\alpha}L^{\alpha/2}$, where $h^{-2}L$ is any finite-difference approximation of $(-\Delta)$ on a uniform mesh of size h. The only important requirement is that the matrix L is positive definite so that its fractional power is well defined. This requirement is fulfilled by the existing standard central difference schemes. Working like that, the original problem (1)–(3) is then transformed into the semi-linear initial value problem

$$\begin{aligned} \frac{d\mathbf{u}}{dt} &= -\frac{\kappa_\alpha}{h^\alpha}\,L^{\alpha/2}\mathbf{u} + \mathbf{f}(t,\mathbf{u}), \qquad t\in(0,T), \\ \mathbf{u}(0) &= \mathbf{u}_0, \end{aligned} \tag{7}$$

where $\mathbf{u}_0$ denotes the vector of node values of u_0.

It is important to remark that while L is typically sparse, when $\alpha \neq 2$, the matrix $L^{\alpha/2}$ loses its sparsity and becomes dense. Observe moreover that the stiffness property of (7) for $\alpha = 2$ is essentially inherited by the fractional counterpart so that an implicit scheme or an exponential integrator is generally needed for solving this initial value problem. In both cases the density of $L^{\alpha/2}$ may lead to a computational demanding integrator when the discretization is sharp. In order to overcome the limitations in terms of computational efficiency, we propose a strategy based on a suitable approximate factorization of $L^{\alpha/2}$. In the next section we focus on the construction of such approximation.

3. Approximation to the matrix fractional power. From the theory of matrix functions (see [7] for a survey) we know that the fractional power of a generic

matrix A can be written as a contour integral

$$A^\beta = \frac{A}{2\pi i}\int_\Gamma z^{\beta-1}(zI-A)^{-1}dz,$$

where Γ is a suitable closed contour enclosing the spectrum of A, $\sigma(A)$, in its interior. The following known result (see, e.g., [2]) expresses A^β in terms of a real integral. The proof is based on a particular choice of Γ and a subsequent change of variable.

PROPOSITION 1. *Let $A \in \mathbb{R}^{m\times m}$ be such that $\sigma(A) \subset \mathbb{C}\backslash(-\infty, 0]$. For $0 < \beta < 1$ the following representation holds*

$$A^\beta = \frac{A\sin(\beta\pi)}{\beta\pi}\int_0^\infty (\rho^{1/\beta}I + A)^{-1}d\rho.$$

In order to confine the dependence of β to a weight function, we consider the change of variable

$$\rho^{1/\beta} = \tau\frac{1-t}{1+t}, \qquad \tau > 0, \tag{8}$$

which yields

$$\begin{aligned}
&\frac{1}{\beta}\int_0^\infty (\rho^{1/\beta}I + A)^{-1}d\rho \\
&= 2\int_{-1}^1 \left(\tau\frac{1-t}{1+t}\right)^{\beta-1}\left(\tau\frac{1-t}{1+t}I + A\right)^{-1}\frac{\tau}{(1+t)^2}dt \\
&= 2\tau^\beta\int_{-1}^1 (1-t)^{\beta-1}(1+t)^{-\beta}\left(\tau(1-t)I + (1+t)A\right)^{-1}dt,
\end{aligned}$$

and hence

$$A^\beta = A\frac{\sin(\beta\pi)}{\pi}2\tau^\beta\int_{-1}^1 (1-t)^{\beta-1}(1+t)^{-\beta}\left(\tau(1-t)I + (1+t)A\right)^{-1}dt. \tag{9}$$

The above formula naturally suggests the use of the k-point Gauss-Jacobi rule and consequently a rational approximation of the type

$$A^\beta \approx R_k(A) := A\sum_{j=1}^k \gamma_j(\eta_j I + A)^{-1}, \tag{10}$$

where the coefficients γ_j and η_j are given by

$$\gamma_j = \frac{2\sin(\beta\pi)\tau^\beta}{\pi}\frac{w_j}{1+\vartheta_j}, \qquad \eta_j = \frac{\tau(1-\vartheta_j)}{1+\vartheta_j},$$

in which w_j and ϑ_j are, respectively, the weights and nodes of the Gauss-Jacobi quadrature rule with weight function $(1-t)^{\beta-1}(1+t)^{-\beta}$. Of course, the above approximation can be used in our case with $\beta = \alpha/2$ whenever $A = h^{-2}L$ represents the discrete Laplacian operator with Dirichlet boundary conditions, whose spectrum is contained in $\mathbb{R}^+$. At this point, denoting by $z\,P_{k-1}(z)$ and $Q_k(z)$ the polynomials of degree k such that $R_k(z) = (z\,P_{k-1}(z))/Q_k(z)$, we can approximate the solution of (7) by solving (6) with $M = Q_k(L)$ and $K = LP_{k-1}(L)$. We remark that the use

of the Gauss-Jacobi rule ensures that $\gamma_j > 0$ and $\eta_j > 0$ for each j, and hence it is immediate to verify that the spectrum of $R_k(L)$ is strictly contained in the positive real axis. This condition is fundamental to preserve the stability properties of (7) whenever $L^{\alpha/2}$ is replaced by $R_k(L)$.

We need to mention that in the field of fractional calculus the approximation (10) has already been used in [1] for the approximation of the Caputo's fractional derivative. Here, however, the definition of τ in (8), and the subsequent error analysis will be completely different because of the spectral properties of the Laplacian operator with respect to the ones of the first-derivative.

3.1. Choice of τ. The choice of the parameter τ in the change of variable (8) is crucial for the quality of the approximation attainable by (10). Assuming that the generic matrix A is symmetric and positive definite, let $\lambda_{\min}$ and $\lambda_{\max}$ be its smallest and largest eigenvalue, respectively. Let moreover $\Lambda = [\lambda_{\min}, \lambda_{\max}]$. It is well known that

$$\left\| A^\beta - R_k(A) \right\|_2 \leq \max_{\Lambda} \left| \lambda^\beta - R_k(\lambda) \right|. \tag{11}$$

In this view, looking at (9), a good choice of τ is the one that minimizes, uniformly with respect to $\lambda \in \Lambda$, the error of the Gauss-Jacobi formula when applied to the computation of

$$\int_{-1}^{1} (1-t)^{\beta-1} (1+t)^{-\beta} \left(\tau (1-t) + (1+t)\lambda\right)^{-1} dt, \qquad \lambda \in \Lambda.$$

From the theory of best uniform polynomial approximation and its application to the analysis of the Gauss quadrature rules (see e.g. [14] for a recent study) it is known that the position of the poles of the integrand function with respect to the interval of integration defines the quality of the approximation. In our case, we observe that for each $\tau \in \Lambda$ the poles of the integrand function

$$f_{\tau,\lambda}(t) = \left(\tau (1-t) + (1+t)\lambda\right)^{-1},$$

are functions of λ defined by

$$p_\tau(\lambda) = \frac{\tau + \lambda}{\tau - \lambda},$$

and we clearly have $p_\tau(\lambda) > 1$ for $\lambda < \tau$, and $p_\tau(\lambda) < -1$ for $\lambda > \tau$. Our aim is to define τ in order to maximize the distance of the set

$$Q_\tau = \{\, p_\tau(\lambda), \lambda \in \Lambda \,\}$$

from the interval of integration $[-1, 1] \subset \mathbb{R} \backslash Q_\tau$. We observe that for $\lambda_{\min} < \tau < \lambda_{\max}$ the worst case is given by $\lambda = \lambda_{\min}$ or $\lambda = \lambda_{\max}$ since we have respectively

$$\min_{\lambda \in \Lambda} \operatorname{dist}(p_\tau(\lambda), [-1,1]) = p_\tau(\lambda_{\min}) - 1,$$

or

$$\min_{\lambda \in \Lambda} \operatorname{dist}(p_\tau(\lambda), [-1,1]) = -p_\tau(\lambda_{\max}) - 1.$$

As consequence, the idea is to set τ such that

$$p_\tau(\lambda_{\min}) - 1 = -p_\tau(\lambda_{\max}) - 1,$$

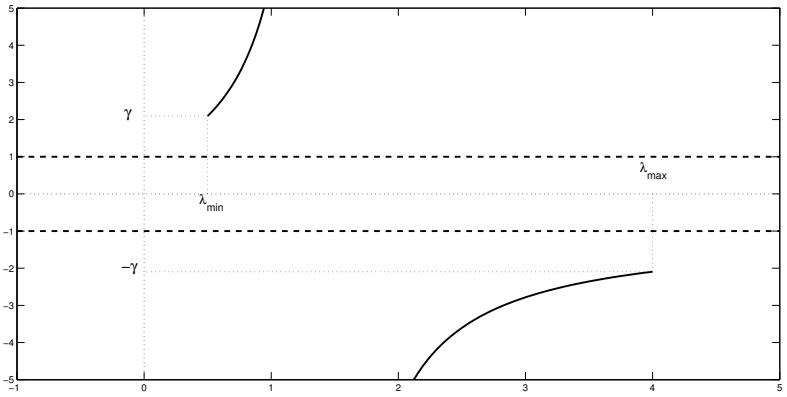

FIG. 1. *Example of function $p_\tau(\lambda)$ for $\lambda_{\min} = 0.5$, $\lambda_{\max} = 4$. The choice of τ as in (12) ensures the symmetry of the set Q_τ. The minimum distance of the curve $p_\tau(\lambda)$ from the set $[-1, 1]$ is given by $\gamma - 1$ and is attained either in $\lambda = \lambda_{\min}$ or $\lambda = \lambda_{\max}$.*

that leads directly to the equation

$$\frac{\tau + \lambda_{\min}}{\tau - \lambda_{\min}} = -\frac{\tau + \lambda_{\max}}{\tau - \lambda_{\max}},$$

whose solution is

$$\tau_{opt} = \sqrt{\lambda_{\min}\lambda_{\max}}. \tag{12}$$

Formally, τ_{opt} is given by

$$\tau_{opt} = \arg \max_{\lambda_{\min} < \tau < \lambda_{\max}} \min_{\lambda \in \Lambda} |p_\tau(\lambda)| .$$

In this way, the set $Q_{\tau_{opt}}$ is symmetric with respect to the origin, that is $Q_{\tau_{opt}} = (-\infty, -\gamma) \cup (\gamma, +\infty)$, where

$$\gamma = \frac{\sqrt{\kappa(A)} + 1}{\sqrt{\kappa(A)} - 1}, \tag{13}$$

in which $\kappa(A)$ denotes the spectral condition number of A. This situation is summarized in an example reported in Figure 1.

4. Error analysis. In this section we analyze the error of the rational approximation (10) with the choice of $\tau = \tau_{opt}$ in (8). We start with the following result, whose proof is given in [14, Theorems 4.3 and 4.4].

THEOREM 2. *Let $g(z)$ be a function analytic in an open subset of the complex plane containing the ellipse*

$$\Gamma_\rho = \left\{ z = \frac{1}{2}\left(\rho e^{i\theta} + \frac{1}{\rho e^{i\theta}}\right), \rho > 1, \theta \in [0, 2\pi) \right\}.$$

Let moreover $p_k^*[g]$ be the polynomial of degree $\leq k$ of best uniform approximation of g in $[-1, 1]$ and

$$E_k^*[g] = \max_{t \in [-1,1]} |g(t) - p_k^*[g](t)| .$$

Then

$$E_k^*[g] \leq \frac{2M(\rho)}{(\rho-1)\rho^k}, \tag{14}$$

where

$$M(\rho) = \max_{z\in\Gamma_\rho} |g(z)|\,.$$

THEOREM 3. *Let A be a symmetric positive definite matrix and $0<\beta<1$. Then for k sufficiently large, the error of the rational approximation (10), generated by the Gauss-Jacobi rule applied to the integral (9) for $\tau=\tau_{opt}$, is given by*

$$\left\|A^\beta - R_k(A)\right\|_2 \leq C\,\|A\|_2\,\tau^\beta \frac{(\rho_M+1)}{(\rho_M-1)\,(\rho_M-\gamma)}\frac{k}{\rho_M^{2k}},$$

where C is a constant independent of k, and

$$\rho_M = \gamma + \sqrt{\gamma^2-1}.$$

Proof. For $\lambda\in\Lambda$ let

$$f_\lambda(t) = \left(\tau_{opt}\,(1-t) + (1+t)\,\lambda\right)^{-1},$$

and

$$I(f_\lambda) = \int_{-1}^{1} (1-t)^{\beta-1}\,(1+t)^{-\beta}\,f_\lambda(t)dt.$$

Let moreover $I_k(f_\lambda)$ be the corresponding k-point Gauss-Jacobi approximation with weights w_j, $j=1,\ldots,k$. By standard arguments we have that

$$\begin{aligned} |I(f_\lambda) - I_k(f_\lambda)| &\leq \left|I(f_\lambda - p_{2k-1}^*[f_\lambda])\right| + \left|I_k(f_\lambda - p_{2k-1}^*[f_\lambda])\right| \\ &\leq 2C_\beta E_{2k-1}^*[f_\lambda], \end{aligned} \tag{15}$$

where, since $w_j>0$,

$$C_\beta = \sum_{j=1}^k |w_j| = \sum_{j=1}^k w_j = \int_{-1}^{1} (1-t)^{\beta-1}\,(1+t)^{-\beta}\,dt.$$

Now, independently of $\lambda\in\Lambda$, the choice of $\tau=\tau_{opt}$ makes possible to use the bound (14) for each $1<\rho<\rho_M$ where ρ_M solves

$$\frac{1}{2}\left(\rho_M + \frac{1}{\rho_M}\right) = \gamma,$$

since $Q_{\tau_{opt}} = (-\infty,-\gamma)\cup(\gamma,+\infty)$. Thus by (15), (14) and using

$$M(\rho) = \max_{z\in\Gamma_\rho} |f_\lambda(z)| \leq \frac{1}{\gamma - \frac{1}{2}\left(\rho+\frac{1}{\rho}\right)},$$

we obtain

$$|I(f_\lambda) - I_k(f_\lambda)| \leq \frac{4C_\beta}{(\rho-1)\rho^{2k-1}\left(\gamma - \frac{1}{2}\left(\rho+\frac{1}{\rho}\right)\right)}, \quad 1<\rho<\rho_M. \tag{16}$$

Now, neglecting the factor $1/(\rho-1)$ and then minimizing with respect to ρ yields

$$\begin{aligned}\overline{\rho} &= \frac{2k-1}{2k}\left(\gamma+\sqrt{\gamma^2-1+\frac{1}{(2k-1)^2}}\right)\\ &\approx \frac{2k-1}{2k}\rho_M =: \rho^*.\end{aligned}$$

Hence, for k large enough (we need $\rho^*>1$), we can use ρ^* in (16), obtaining

$$|I(f_\lambda)-I_k(f_\lambda)| \le \frac{8keC_\beta\,(\rho_M+1)}{(\rho_M-1)\,\rho_M^{2k}\,(\rho_M-\gamma)}. \tag{17}$$

Indeed, defining k^* such that

$$\frac{2k-1}{2k} \ge \frac{2}{\rho_M+1} \quad \text{for } k \ge k^*$$

we have

$$\frac{1}{\frac{2k-1}{2k}\rho_M-1} \le \frac{\rho_M+1}{\rho_M-1}.$$

Moreover, in (17) we have used the inequalities

$$\begin{aligned}\frac{1}{\left(\frac{2k-1}{2k}\rho_M\right)^{2k-1}} &\le \frac{e}{\rho_M^{2k-1}},\\ \gamma-\frac{1}{2}\left(\frac{2k-1}{2k}\rho_M+\frac{2k}{2k-1}\frac{1}{\rho_M}\right) &\ge \frac{\rho_M\,(\rho_M-\gamma)}{2k}.\end{aligned}$$

Finally, since by (9)

$$\left\|A^\beta-R_k(A)\right\|_2 \le \frac{\|A\|_2\sin(\beta\pi)}{\pi}2\tau^\beta \max_{\lambda\in\Lambda}\left|I(f_\lambda)-I_k(f_\lambda)\right|,$$

using (17) we obtain the result. ∎

COROLLARY 4. *The asymptotic convergence factor fulfills*

$$\overline{\lim_{k\to\infty}}\left\|A^\beta-R_k(A)\right\|_2^{1/k} \le \left(\frac{\sqrt[4]{\kappa(A)}-1}{\sqrt[4]{\kappa(A)}+1}\right)^2.$$

Proof. By (13)

$$\rho_M = \gamma+\sqrt{\gamma^2-1} = \frac{\sqrt[4]{\kappa(A)}+1}{\sqrt[4]{\kappa(A)}-1}.$$

∎

REMARK 5. *From the above analysis it is easy to observe that for the Laplacian operator $h^{-2}L$, discretized with standard central differences (3-points or 5-points in one or two dimensions, respectively), we have*

$$\left(\frac{\sqrt[4]{\kappa(L)}+1}{\sqrt[4]{\kappa(L)}-1}\right)^2 \approx 1+\frac{2\pi}{N},$$

where N represents the number of discretization points in one dimension.

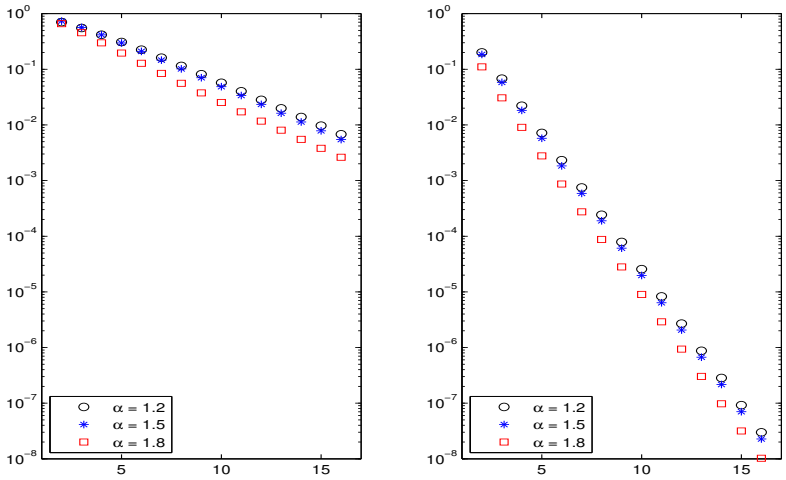

FIG. 2. *Relative error of the rational approximation versus k, the number of points of the Gauss-Jacobi rule, for some values of α. The one- and the two-dimensional cases are on the left and on the right, respectively. In the first case the dimension of the problem is* 200 *and in the second one it is* 400.

In Figure 2 we plot the relative error for the one- and two-dimensional Laplacian discretized as in the previous remark for some values of α. The geometric convergence theoretically proved in this section is clear in the pictures, together with the substantial independence of α, which is absorbed by the weight function. It is also quite evident that the method is particularly effective for the two-dimensional case; this represents an important feature since most of the standard techniques for the discretization of the fractional Laplacian only works in one dimension.

5. Solving fractional in space reaction-diffusion problems. As already said in Section 2, if we discretize on a uniform mesh the fractional Laplacian operator occurring in (1), we obtain the initial value problem

$$\frac{d\mathbf{u}}{dt} = -\frac{\kappa_\alpha}{h^\alpha} L^{\alpha/2}\mathbf{u} + \mathbf{f}(t,\mathbf{u}), \quad \mathbf{u}(0) = \mathbf{u}_0. \tag{18}$$

Therefore, the application of the rational approximation (10) of $L^{\alpha/2}$, based on the k-point Gauss-Jacobi rule and given by $R_k(L) \equiv M^{-1}K$, leads to the following initial value problem

$$\frac{d\mathbf{v}}{dt} = -\frac{\kappa_\alpha}{h^\alpha} R_k(L)\mathbf{v} + \mathbf{f}(t,\mathbf{v}), \quad \mathbf{v}(0) = \mathbf{u}_0. \tag{19}$$

Denoting by

$$E_k = R_k(L) - L^{\alpha/2}$$

the error of the rational approximation, (19) can be equivalently written as

$$\frac{d\mathbf{v}}{dt} = -\frac{\kappa_\alpha}{h^\alpha}\left(L^{\alpha/2} + E_k\right)\mathbf{v} + \mathbf{f}(t,\mathbf{v}), \quad \mathbf{v}(0) = \mathbf{u}_0. \tag{20}$$

The solution $\mathbf{v}(t)$ is therefore the solution of the perturbed version of (18). Setting

$$g(t,\mathbf{u}) = -\frac{\kappa_\alpha}{h^\alpha} L^{\alpha/2}\mathbf{u} + \mathbf{f}(t,\mathbf{u}),$$

we assume that g satisfies the one-sided Lipschitz condition

$$\langle g(t,\mathbf{u}_1) - g(t,\mathbf{u}_2), \mathbf{u}_1 - \mathbf{u}_2\rangle \le m \|\mathbf{u}_1 - \mathbf{u}_2\|_2^2, \qquad m < 0, \quad \mathbf{u}_1, \mathbf{u}_2 \in \mathbb{R}^N, \tag{21}$$

where $\langle\cdot,\cdot\rangle$ denotes the scalar product corresponding to the Euclidean norm $\|\cdot\|_2$. We are interested in an a priori upper bound on the distance of $\mathbf{u}$ and $\mathbf{v}$. The difference $\mathbf{w}(t) = \mathbf{u}(t) - \mathbf{v}(t)$ is the solution of the initial value problem

$$\begin{aligned} \frac{d\mathbf{w}}{dt} &= g(t,\mathbf{u}) - g(t,\mathbf{v}) + \frac{\kappa_\alpha}{h^\alpha} E_k \mathbf{v}, \qquad t \in (0,T), \\ \mathbf{w}(0) &= \mathbf{0}. \end{aligned}$$

Calculating the scalar product of $\mathbf{w}(t)$ with both sides of the differential equation, we find for the left-hand side

$$\left\langle \frac{d\mathbf{w}(t)}{dt}, \mathbf{w}(t) \right\rangle = \frac{1}{2}\frac{d}{dt}\langle \mathbf{w}(t), \mathbf{w}(t)\rangle = \frac{1}{2}\frac{d}{dt}\|\mathbf{w}(t)\|_2^2 = \|\mathbf{w}(t)\|_2 \frac{d}{dt}\|\mathbf{w}(t)\|_2 .$$

From (21) and Schwarz' inequality we obtain for the right-hand side

$$\begin{aligned} \left\langle g(t,\mathbf{u}) - g(t,\mathbf{v}) + \frac{\kappa_\alpha}{h^\alpha} E_k \mathbf{v}, \mathbf{w}(t) \right\rangle &= \langle g(t,\mathbf{u}) - g(t,\mathbf{v}), \mathbf{w}(t)\rangle + \frac{\kappa_\alpha}{h^\alpha}\langle E_k\mathbf{v}, \mathbf{w}(t)\rangle \\ &\le m\|\mathbf{w}\|_2^2 + \frac{\kappa_\alpha}{h^\alpha}\|E_k\mathbf{v}\|_2 \|\mathbf{w}\|_2 . \end{aligned}$$

Combining these results we find for the scalar function $\|\mathbf{w}(t)\|_2$:

$$\frac{d}{dt}\|\mathbf{w}(t)\|_2 \le m\|\mathbf{w}(t)\|_2 + \frac{\kappa_\alpha}{h^\alpha}\|E_k\mathbf{v}(t)\|_2 .$$

Now, since $\mathbf{w}(0) = \mathbf{0}$, by the Grönwall inequality we obtain

$$\|\mathbf{w}(t)\|_2 \le \frac{\kappa_\alpha}{h^\alpha}\|E_k\|_2 \int_0^t e^{m(t-s)}\|\mathbf{v}(s)\|_2 \, ds. \tag{22}$$

This immediately provides the proof of the following result.

PROPOSITION 6. *If $\mathbf{u}$ and $\mathbf{v}$ are solutions of (18) and (19), respectively, and m is the one-sided Lipschitz constant introduced in (21), assuming that $\|\mathbf{v}(s)\|_2 \le c$ for each $s \in [0,t]$, then*

$$\|\mathbf{u}(t) - \mathbf{v}(t)\|_2 \le \frac{\kappa_\alpha}{h^\alpha}\|E_k\|_2 \frac{c}{m}\left(e^{mt} - 1\right). \tag{23}$$

A more sharper condition estimate may be derived if also the right-hand side of (20) satisfies a one-sided Lipschitz condition.

PROPOSITION 7. *Assume that there exists $\overline{m} < 0$ such that for each $\mathbf{u}_1, \mathbf{u}_2 \in \mathbb{R}^N$*

$$\left\langle g(t,\mathbf{u}_1) - g(t,\mathbf{u}_2) - \frac{\kappa_\alpha}{h^\alpha}E_k(\mathbf{u}_1 - \mathbf{u}_2), \mathbf{u}_1 - \mathbf{u}_2 \right\rangle \le \overline{m}\|\mathbf{u}_1 - \mathbf{u}_2\|_2^2 . \tag{24}$$

Moreover, assume that the zero solution is an equilibrium point for (18), that is, $\mathbf{f}(t,\mathbf{0}) = \mathbf{0}$. Then there exists $\widetilde{m} < 0$ such that

$$\|\mathbf{u}(t) - \mathbf{v}(t)\|_2 \le \frac{\kappa_\alpha}{h^\alpha}\|E_k\|_2 \|\mathbf{v}(0)\|_2 \, t\, e^{\widetilde{m}t}. \tag{25}$$

Proof. Condition (24) ensures that for each $\mathbf{z}(t)$, solution of (19) with initial condition $\mathbf{z}(0) = \mathbf{z}_0$, we have

$$\|\mathbf{v}(t) - \mathbf{z}(t)\|_2 \leq e^{\bar{m}t} \|\mathbf{v}(0) - \mathbf{z}(0)\|_2 .$$

Since we have assumed that $\mathbf{z} \equiv \mathbf{0}$ is a solution, we have

$$\|\mathbf{v}(t)\|_2 \leq e^{\bar{m}t} \|\mathbf{v}(0)\|_2 .$$

Now, let $\tilde{m} := \max(m, \bar{m})$. Replacing m with $\tilde{m}$ in (22) and $\bar{m}$ with $\tilde{m}$ in the above inequality, (25) immediately follows. ∎

5.1. Choice of k. The above propositions can easily be adopted to select a value of k that allows to keep the error below a given tolerance. Indeed, for using (23) one can consider the approximation

$$m \approx -\frac{k_\alpha}{h^\alpha} \left(\lambda_{\min}(L)\right)^{\alpha/2} \tag{26}$$

and define $c := \|\mathbf{v}(0)\|_2$. If $\mathbf{v}(0) = \mathbf{0}$ some information about $\mathbf{v}$ can be obtained working in small dimesion. The approximation (26) can also be used for $\tilde{m}$ whenever it is possible to employ (25). Finally, since (see (11))

$$\|E_k\|_2 \leq \left| R_k(\lambda_{\min}(L)) - \left(\lambda_{\min}(L)\right)^{\alpha/2} \right|,$$

working scalarly we can easily select k such that

$$\|\mathbf{u}(t) - \mathbf{v}(t)\|_2 \leq C\, tol,$$

where tol is a given tolerance and the constant C plays the role of a scaling factor that should be set equal to c or $\|\mathbf{v}(0)\|_2$ when using (23) or (25), respectively (this to avoid the dependence of k on the magnitude of the solution). Anyway, we remark that this procedure may provide a conservative value of k, because of the bounds used for obtaining the estimate.

5.2. Numerical examples. In this subsection, we provide the results of some numerical experiments we have conducted to prove the effectiveness of the proposed approach with respect to the matrix transfer technique. In order to take the advantage in terms of computational work and memory saving of the sparse structure of the matrices M and K, instead of (19), we solve the equivalent initial value problem

$$M \frac{d\mathbf{v}}{dt} = -\frac{\kappa_\alpha}{h^\alpha} K\mathbf{v} + M\,\mathbf{f}(t, \mathbf{v}), \quad \mathbf{v}(0) = \mathbf{u}_0. \tag{27}$$

In particular, we first focus on a fractional in space diffusion equation. Then, we consider two reaction-diffusion equations; in the second one the forcing term is dependent on the solution and we choose an initial data that does not satisfy the boundary conditions. All of these examples are in one spatial dimension. In each case, discretizing the spatial domain $\Omega = (a, b)$ with a uniform mesh having stepsize $h = (b - a)/(N + 1)$, we consider the standard 3-points central difference discretization of the Laplacian $h^{-2}L = h^{-2}\text{tridiag}(-1, 2, -1) \in \mathbb{R}^{N\times N}$. Finally, we also report the results obtained by applying our approach for the numerical solution of a fractional reaction-diffusion example in two space dimensions. In this case, we discretize in space the problem via the 5-points finite difference stencil. The matrix L is therefore a block tridiagonal

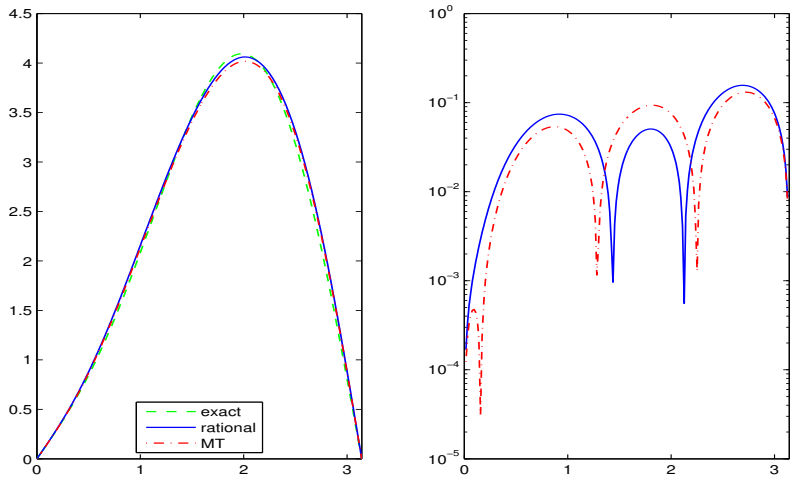

FIG. 3. *Comparison of the analytic solution of the problem in Example 1 with the numerical solutions provided by the rational approach and the matrix transfer technique at $t = 0.4$ (left) and corresponding errors (right).*

matrix of size N^2 having the following form $L = \text{tridiag}(-I, B, -I)$, with I denoting the identity matrix of size N and $B = \text{tridiag}(-1, 4, -1) \in \mathbb{R}^{N\times N}$.

In all examples, we solve (18) and (27) by the MATLAB routine `ode15s`. Moreover, we indicate by *'exact'* the analytical solution, by *'MT'* the solution of the problem (18), obtained by applying the matrix transfer technique, and by *'rational'* the solution arising from (27).

EXAMPLE 1. *Consider the problem (1) on the spatial domain $\Omega = (0, \pi)$, with $\kappa_\alpha = 0.25$ and $f = 0$. According to [15, Section 3.1], the analytic solution corresponding to the initial condition $u_0(x) = x^2(\pi - x)$ is given by*

$$u(x,t) = \sum_{n=1}^{\infty} \frac{8(-1)^{n+1} - 4}{n^3} \sin(nx) \exp(-\kappa_\alpha n^\alpha t).$$

Setting $\alpha = 1.8$, at time $t = 0.4$ in the left-hand side of Figure 3 the exact solution is compared with the numerical solutions of the semi-discrete problems (18) and (27) with $h = \pi/201$ (that is $h = 0.0157$) and $k = 4$. On the right picture, the step-by-step maximum norm of the difference between the analytic solution and the numerical ones is reported. As one can see, the numerical solution provided by the rational approximation is in good agreement with the one obtained by the matrix transfer technique. For this choice of t, the bounds (23) and (25) essentially coincide and an error comparable to the one obtained experimentally is predicted by choosing $k = 20$. Of course, a smaller value of k would be obtained for $t > 0.4$ since the bound (25) rapidly goes to zero as t grows.

EXAMPLE 2. *Consider the problem (1) on the spatial domain $\Omega = (-1, 1)$, with $u_0(x) = (1 - x^2)^{1+\alpha/2}$ and the source term fixed such that the exact solution is given by*

$$u(x,t) = (t+1)^\gamma (1 - x^2)^{1+\alpha/2}, \qquad \gamma < 0.$$

In our experiments, we select the model parameters $\kappa_\alpha = 0.1, \alpha = 1.2, \gamma = -1$ and we

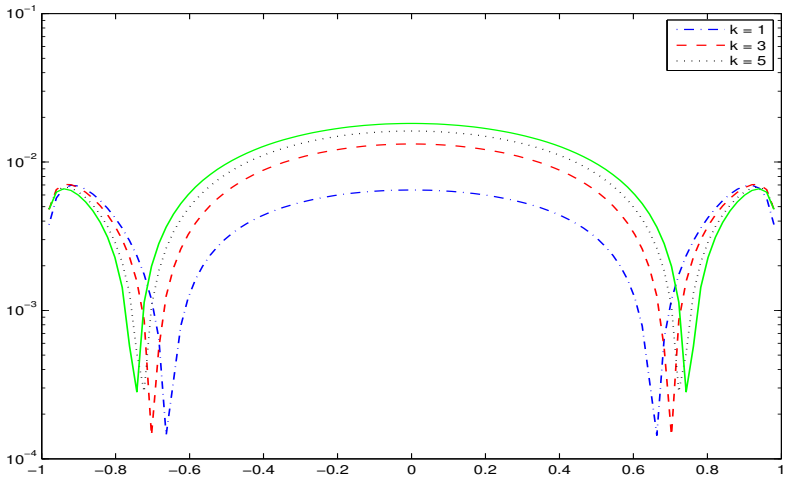

FIG. 4. *Comparison of the errors provided by solving the problem of the Example 2 using both rational with $k = 1$ (blue dashed-dot-line), $k = 3$ (red dashed-line) and $k = 5$ (black dot-line) and MT (green solid-line).*

discretize the spacial domain using $N = 100$. In Figure 4 we report the step-by-step error provided by the numerical solutions obtained by applying the Gauss-Jacobi rule with $k = 1, 3, 5$ at $t = 0.1$ compared with the one obtained by solving directly (18). As expected, the solution provided by the rational approach is able to mimic, as k increases, the one derived by applying the matrix transfer technique. In particular, when $k = 5$ the corresponding error $\|\mathbf{u} - \mathbf{v}\|_2 = O(10^{-2})$ while, by the theoretical estimate (23), we would obtain this bound for $k = 7$.

EXAMPLE 3. *Consider now equation (1) in the one-dimensional case with non-linear source term*

$$f(x, t, u) = u(1 - u),$$

known in the literature as the fractional Fisher-KPP reaction-diffusion equation. In this example, we set $\kappa_\alpha = 1$, $\alpha = 1.5$ and $\Omega = (-100, 100)$. We use $N = 500$ and we compute the numerical solutions provided by the matrix transfer technique and the rational approximation with $k = 3$. In particular, in the two pictures on the top of Figure 5 we have drawn the solutions profiles corresponding to the initial condition $u_0(x) = 0.5$ while, in the ones on the bottom, the solutions profiles corresponding to $u_0(x) = (100 + x)^2(100 - x)^2$ at time $t = 1$ (left) and $t = 10$ (right), respectively. As one can see, the two numerical solutions match very well and behave similarly with the theoretical one as t grows, cf. [13].

EXAMPLE 4. *We solve the fractional reaction-diffusion equation in two space dimensions*

$$\frac{\partial u(x, y, t)}{\partial t} = -\kappa_\alpha \, (-\Delta)^{\alpha/2} u(x, y, t) + f(x, y, t, u), \qquad (x, y) \in (0, 1) \times (0, 1),$$

with

$$f(x, y, t, u) = t^\alpha \frac{\kappa_\alpha}{16} \sum_{j=1}^{4} (1 + \mu_j^{\alpha/2}) v_j + \alpha t^{\alpha-1} \sin^3(\pi x) \sin^3(\pi y) - \kappa_\alpha u,$$

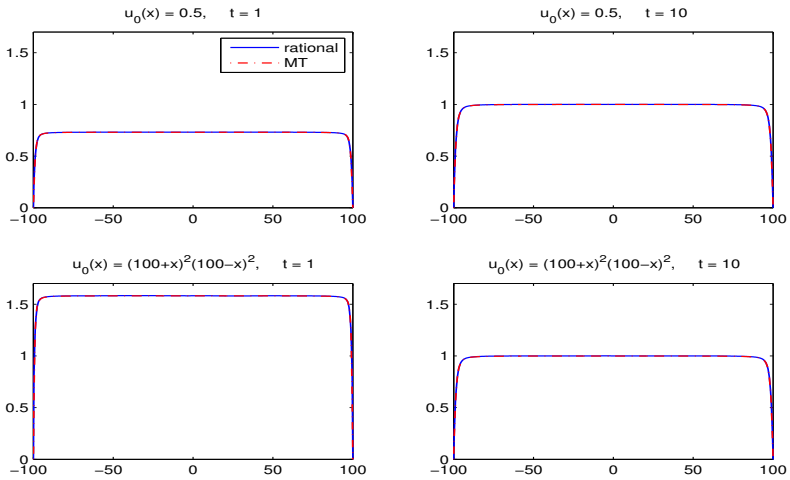

FIG. 5. *Comparison of the numerical solutions of the problem in Example 3 provided by MT and rational at $t = 1$ (left) and $t = 10$ (right) for two different choice of u_0.*

where

$$
\begin{aligned}
v_1 &= 9\sin(\pi x)\sin(\pi y), & \mu_1 &= 2\pi^2,\\
v_2 &= -3\sin(\pi x)\sin(3\pi y), & \mu_2 &= 10\pi^2,\\
v_3 &= -3\sin(3\pi x)\sin(\pi y), & \mu_3 &= 10\pi^2,\\
v_4 &= \sin(3\pi x)\sin(3\pi y), & \mu_4 &= 18\pi^2,
\end{aligned}
$$

subject to $u(x, y, 0) = 0$ and homogeneous Dirichlet boundary conditions [3].

The exact solution to this problem is

$$u(x, y, t) = t^{\alpha}\sin^3(\pi x)\sin^3(\pi y).$$

The numerical solution provided by the rational approach based on the Gauss-Jacobi rule with $k = 7$ and the matrix transfer technique are drawn at $t = 1$ in Figure 6 using $\alpha = 1.5$, $\kappa_\alpha = 10$ and $N = 40$ points in each domain direction. It is worth noting that in order to obtain the same accuracy, the matrix transfer technique costs three times the rational approach.

6. Conclusions. In this paper we have proposed a rational approximation to the discrete fractional Laplacian. When applied for solving the reaction-diffusion equations this leads to a semi-discrete problem which can be solved in an efficient way due to the band structure of the matrices occurring in the definition of the approximation. With respect to the existing approaches based on the discretization of the Riesz derivative the main advantages are the ones of the matrix transfer technique itself, that is: the approach can be generalized to work in more than one dimension without modifying the overall solution methodology, it does not require to work with a uniform grid in space, all linear algebra tasks are with sparse matrices.

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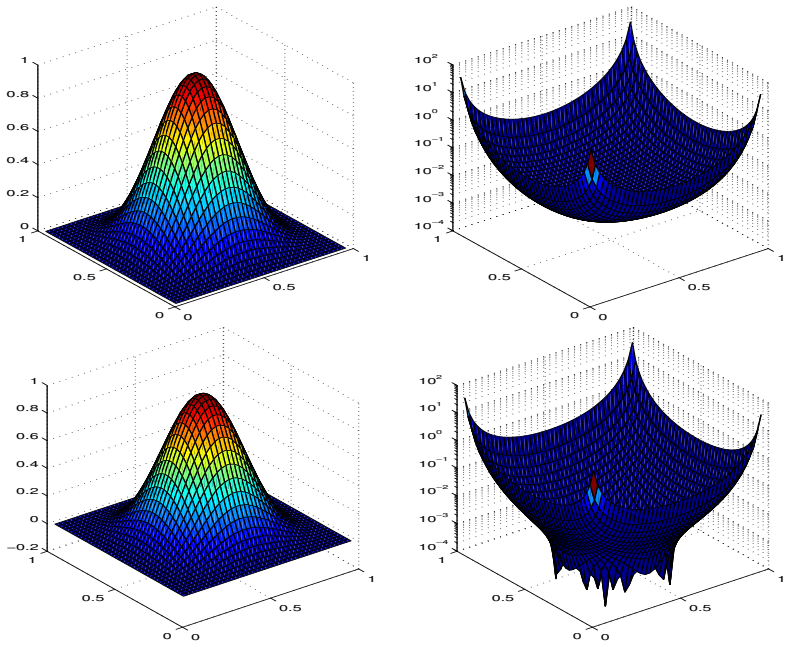

FIG. 6. *Comparison of the analytical solution of the problem in Example 4 with the numerical solution provided at $t = 1$ by rational (top) and MT (bottom) and corresponding relative errors (right) for $\alpha = 1.5$ and $\kappa_\alpha = 10$.*

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