Fast Numerical Methods for Fractional Diffusion Equations

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Fractional diffusion equation

- Standard diffusion equation

$$\partial_t u(x,t) = \partial_x^2 u(x). \tag{1}$$

- Time fractional

$$\partial_t^\alpha u(x,t) = \partial_x^2 u(x), \quad 0 < \alpha \le 2. \tag{2}$$

- Space fractional

$$\partial_t u(x,t) = \partial_x^\beta u(x), \quad 1 < \beta \le 2. \tag{3}$$

- Time-Space fractional

$$\partial_t^\alpha u(x,t) = \partial_x^\beta u(x). \tag{4}$$

  Generalization of integer order differential equations, which can be seen from the Fourier and Laplace transform

$$s^\alpha \mathcal{L}\hat{u}(s,k) = -|k|^\beta \hat{u}(s,k). \tag{5}$$

- stochastic interpretation, anomalous diffusion, random walk

$$E|X(t)|^\beta \propto t^\alpha$$

- We are interested $\alpha < 2$ and $1 < \beta < 2$. When $\beta = 2$, if $0 < \alpha < 1$ we call it slow or sub-diffusion and if $1 < \alpha < 2$, fast or super-diffusion.
- nonlocal operators, memory, long range interaction, heavy tail
- fractal geometry, highly heterogeneous aquifer and underground environmental problem, wave propagation in viscoelastic media, turbulence, finance etc.
- monograph: Oldham and Spanier,1974, Samko et al. 1993, Podlubny 1999, Kilbas et al. 2006, M. M. Meerschaert and Sikorskii 2010 or 2012 etc.
- Journal, Fractional Calculus and Applied Analysis, 1998-present

Definition

The left- and right-sided Riemann-Liouville fractional integrals are defined as

$$ {}_aD_x^{-\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x \frac{f(\xi)}{(x-\xi)^{1-\alpha}} d\xi, \quad x > a, \quad \alpha > 0, $$

and

$$ {}_xD_b^{-\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_x^b \frac{f(\xi)}{(\xi-x)^{1-\alpha}} d\xi, \quad x < b, \quad \alpha > 0. $$

respectively. Let $g(x) = \frac{1}{\Gamma(\alpha)} x^{\alpha-1}$,

$$ {}_aD_x^{-\alpha} f(x) = \int_a^x f(\xi) g(x-\xi) d\xi. $$

Denote

$$ D_\theta^{-\alpha} = \theta \, {}_aD_x^{-\alpha} + (1-\theta) \, {}_xD_b^{-\alpha}, \quad \theta \in [0,1]. $$

In particular, $\theta = 1/2$, Reisz potential

$$ D_{1/2}^{-\alpha} = \frac{1}{\Gamma(\alpha)} \int_a^b \frac{f(\xi)}{|\xi - x|^{1-\alpha}} d\xi, \quad a < x < b, \quad \alpha > 0. $$

Definition

For $0 < \alpha < 1$,

$$ {}_aD_x^\alpha f(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_a^x \frac{f(\xi)}{(x-\xi)^\alpha} d\xi, $$

$$ {}_xD_b^\alpha f(x) = \frac{-1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_x^b \frac{f(\xi)}{(\xi-x)^\alpha} d\xi. $$

- Left side and right side Riemann-Liouville (RL) derivative are defined as

$$ {}_aD_x^\alpha f(x) = {}_aD_x^n \, {}_aD_x^{\alpha-n} f(x), \quad x > a, $$

$$ {}_xD_b^\alpha f(x) = {}_xD_b^n \, {}_xD_b^{\alpha-n} f(x), \quad x < b $$

for $n-1 < \alpha < n$. If $\alpha = n$, then

$$ {}_aD_x^\alpha f(x) = \frac{d^n}{dx^n} f(x), \text{ and } {}_xD_b^\alpha f(x) = (-1)^n \frac{d^n}{dx^n} f(x). $$

Definition for fractional Laplacian operator for space

- Reisz derivative:

$$\partial_x^\alpha f(x) = -\frac{1}{2\cos(\alpha\pi/2)}\left({}_aD_x^\alpha f(x) + {}_xD_b^\alpha f(x)\right)$$

- Hyper-singular integral form

$$(-\Delta)^{\alpha/2} f(x) = c_{d,\alpha}\int_{\mathbb{R}^d}\frac{f(x)-f(y)}{|x-y|^{d+\alpha}}\,dy, \quad c_{d,\alpha} = \frac{2^\alpha\Gamma(\frac{\alpha+d}{2})}{\pi^{d/2}|\Gamma(-\alpha/2)|}$$

- In one dimensional, under suitable conditions, they are equivalent; but high dimensional, isotropic vs anisotropic

$$\sum_{i=1}^d \partial_{x_i}^\alpha \neq (-\Delta)^{\alpha/2}$$

Fourier symbol $-|k_1|^\alpha - |k_2|^\alpha \neq -\|k\|^\alpha$ with $\|k\|^2 = |k_1|^2 + |k_2|^2$ in 2D.

Caputo derivative for time

- Consider the initial value problem

$$ {}_0D_t^{\alpha} u(t) + Au(t) = f(t), \quad t > 0, $$

Here, A is standard second order differential operator. The initial condition is taken as ${}_0D_t^{\alpha-k} u(t)$ for $k = 0, 1, \cdots, n-1$.

- Left side Caputo derivative (1967) is defined as

$$ {}_0^C D_t^{\alpha} u(t) = {}_0D_t^{\alpha-n} \frac{d^n}{dt^n} u(t), \quad t > 0, $$

for $n - 1 < \alpha < n$.

- ${}_0D_t^{\alpha-n} \frac{d^n}{dt^n} \neq \frac{d^n}{dx^n} {}_0D_t^{\alpha-n} = {}_0D_t^{\alpha}$

Motivation

Computational issues

- nonlocal and thus high storage cost
- weakly singular solutions; boundary singularity, low-order convergence
- dense matrix

Goals

- long time simulation, high accuracy and efficient methods

Model equation

- Consider two-term time fractional diffusion equation [1]

$$K_1 \, {}_0^C D_t^\alpha u(x,t) + K_2 \, {}_0^C D_t^\beta u(x,t) = \partial_x^2 u(x,t) + f(x,t)$$

where $x \in \Omega = (0, L), 0 < t \le T$, $K_1, K_2 > 0$, and $0 < \alpha < 1 < \beta \le 2$.

- The single term version by Ford and Yan (2017) FCAA
- Special case is Bagley-Torvik equation (1984)

$$u_{tt} + {}_0D_t^\alpha u + Au = f.$$

- Kai Diethlm and Ford, Luchko (2002) (2004) (2005), Esmaeili (2017).
- fractional telegraph equation, $\beta = 2\alpha$ with α or $\beta = 1 + \alpha$
- Finite difference method: L1, L2 approximation in time, compact finite difference in space

[1] Z Hao, G Lin, Finite difference schemes for multi-term time-fractional mixed diffusion-wave equations arXiv:1607.07104, 2016

Fast direct solver

- The difference scheme can be equivalently reformulated as

$$(K_1\tau^{\beta-\alpha}\mathbf{M}_t^{\alpha} + K_2\mathbf{M}_t^{\beta})\mathbf{u}\mathbf{M}_x + \frac{\tau^{\beta}}{h^2}\mathbf{u}\mathbf{S}_x = \mathbf{b}\mathbf{M}_x \tag{6}$$

- Partial diagonalization with $O(M\log M)$ in space leads to

$$\begin{pmatrix} c_0 & 0 & 0 & \cdots & 0 & 0 \\ c_1 & d_1 & 0 & \cdots & 0 & 0 \\ c_2 & d_2 & d_1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ c_{N-2} & d_{N-2} & d_{N-3} & \cdots & d_1 & 0 \\ c_{N-1} & d_{N-1} & d_{N-2} & \cdots & d_2 & d_1 \end{pmatrix} \begin{pmatrix} e_0 \\ e_1 \\ e_2 \\ \vdots \\ e_{N-2} \\ e_{N-1} \end{pmatrix} = \begin{pmatrix} g_0 \\ g_1 \\ g_2 \\ \vdots \\ g_{N-2} \\ g_{N-1} \end{pmatrix}.$$

- The divide and conquer strategy (Commenges1984) and (Ke2015) in time direction as $\Theta_N = O(N\log^2 N)$, which has great advantage than the forward substitution method with operations $O(N^2)$.

Fast direct solver

A, x and b can be partitioned as follows:

$$\begin{pmatrix} A^{(1)} & 0 \\ C^{(1)} & A^{(1)} \end{pmatrix} \begin{pmatrix} x^{(1)} \\ x^{(2)} \end{pmatrix} = \begin{pmatrix} b^{(1)} \\ b^{(2)} \end{pmatrix}. \tag{8}$$

Thus the original linear system can be equivalently transformed into two half size linear systems

$$\left\{ \begin{array}{l} A^{(1)}x^{(1)} = b^{(1)} \\ A^{(1)}x^{(2)} = b^{(2)} - C^{(1)}x^{(1)} \end{array} \right. . \tag{9}$$

The computation cost can be estimated below

$$\Theta_N = 2\Theta_{N/2} + \frac{N}{2}\log(\frac{N}{2}).$$

By this formula, we can derive the total operations in space and time is $O(MN \log M \log^2 N)$, which enjoys linearithmic complexity.

Numerical examples

Table: Temporal convergence orders, errors and CPU time of the scheme with fixed stepsize $h = 1/16$

	$\alpha_1 = 0.2,\ \alpha_2 = 1.2$			$\alpha_1 = 0.5,\ \alpha_2 = 1.5$		
N	$E(h,\tau)$	*Order*	CPU(s)	$E(h,\tau)$	*Order*	CPU(s)
16	4.4722e-2	–	0.0411	5.7604e-2	–	0.0216
32	2.2796e-2	0.9722	0.0694	2.8439e-2	1.0183	0.0402
64	1.1489e-2	0.9885	0.0802	1.3953e-2	1.0273	0.0810
128	5.7626e-3	0.9955	0.1596	6.8480e-3	1.0268	0.1555

Table: Spatial convergence orders, errors and CPU time the scheme with fixed stepsize $\tau = 1/2^{20}$

	$\alpha_1 = 0.2,\ \alpha_2 = 1.2$			$\alpha_1 = 0.5,\ \alpha_2 = 1.5$		
M	$E(h,\tau)$	*Order*	CPU(s)	$E(h,\tau)$	*Order*	CPU(s)
4	1.0743e-3	–	378.44	1.0073e-3	–	365.83
6	2.1008e-4	4.0248	564.18	1.9709e-4	4.0234	544.93
8	6.6644e-5	3.9910	701.06	6.2494e-5	3.9927	714.85

Standard diffusion equation

The mass balance equation

$$\partial_t u(x,t) + \partial_x F = f(x,t),$$

and the Fick's first law

$$F = -k(x)\partial_x u(x,t).$$

leads to classical diffusion equation

$$\partial_t u(x,t) - \partial_x[k(x)\partial_x u(x,t)] = f(x,t),$$

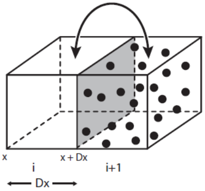

Figure: Eulerian picture for standard diffusion, Schumer et al. 2001

Fractional diffusion equation

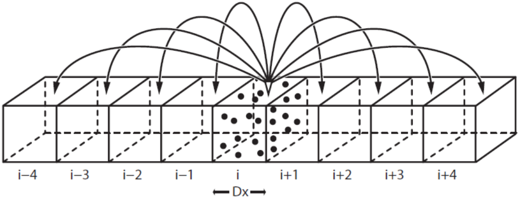

Figure: Eulerian picture for fractional diffusion, Schumer et al. 2001

- A fractional Fick's law

$$F = -k(x)\ \partial_x^{\alpha-1} u(x,t).$$

- Space fractional diffusion equation

$$\partial_t u(x,t) = \partial_x (k(x) \partial_x^{\alpha-1} u(x,t)) + f(x,t)$$

- When $k(x) = 1$,

$$\partial_t u(x,t) = \partial_x^{\alpha} u(x,t)$$

Finite difference method

- Model equation

$$\partial_t u(x,t) = \partial^\alpha_{x,\theta} u(x,t) + f(x,t) \quad \alpha \in (1,2),\, \theta \in (0,1)$$

with $\partial^\alpha_{x,\theta} = \theta\,{}_aD^\alpha_x u(x,t) + (1-\theta)\,{}_xD^\alpha_b u(x,t)$

- Finite difference method for two-sided fractional differential equations
- Shifted Grunwald-Letinkov formula, Meerschaert and Tadjeran (2004),

$$A^\alpha_{h,r} f(x) = \frac{1}{h^\alpha} \sum_{k=0}^{[x-a]/h} g_k^{(\alpha)} f(x-(k-r)h)$$

Lemma

(Tuan and Gorenflo 1995) Let $1 < \alpha < 2$, $f(x)$ is smooth enough. For any integer $r \geq 0$, we can obtain

$${}_aD^\alpha_x f(x) = A^\alpha_{h,r} f(x) - \sum_{l=1}^{n-1} c_l^{\alpha,r}\,{}_aD^{\alpha+l}_x f(x) h^l + O(h^n)$$

Structure of the matrix

- For finite difference method, we can have Toeplitz matrices. (Hong Wang (2010), Hai-wei Sun (2012))

$$A = \begin{pmatrix} a_0 & a_1 & a_2 & \cdots & a_{M-1} \\ a_{-1} & a_0 & a_1 & \ddots & \vdots \\ a_{-2} & a_{-1} & \ddots & \ddots & a_2 \\ \vdots & \ddots & \ddots & a_0 & a_1 \\ a_{1-M} & \cdots & a_{-2} & a_{-1} & a_0 \end{pmatrix}.$$

♢ computational cost $Mlog(M)$ and storage $O(M)$

What we do [2]

- high accuracy finite difference scheme
- stability and convergence analysis

[2] Z. Hao, Z. Sun, W. Cao, A fourth-order approximation of fractional derivatives with its applications, Journal of Computational Physics 281, 787-805, 2015

Where does the singularity come from?

After time discretization, we get

$$\alpha u - \theta \; {}_aD_x^{\alpha} u - (1-\theta) \; {}_xD_b^{\alpha} u = f(x), \quad x \in (a,b),$$
$$u(a) = u(b) = 0,$$

When $\theta = 1$, the equation reduces to

$$- \; {}_aD_x^{\alpha} u = f - \alpha u.$$

Let $\widetilde{f} = f - \alpha u$. Then integrating on both sides twice reads

$$- \; {}_aD_x^{\alpha-2} u = \; {}_aD_x^{-2} \widetilde{f} + C_1(x-a) + C_2,$$

where C_1 and C_2 are coefficients to be determined. Taking $x \to a^+$ leads to $C_2 = 0$ in above identity. Since $u(a) = 0$, performing the fractional derivative operator ${}_0D_x^{2-\alpha}$ on both sides gives

$$u = - \; {}_aD_x^{-\alpha} \widetilde{f} - \frac{C_1}{\Gamma(\alpha)}(x-a)^{\alpha-1}.$$

Improved algorithm based on finite difference scheme

The kernel of the fractional differential operator is $(x-a)^{\alpha-1}$

$$ {}_aD_x^\alpha[(x-a)^{\alpha-1}] = 0. $$

- It is reasonable to assume

$$ u(x) = u_r(x) + \xi_s u_s(x), $$

where $u_s(x) = (x-a)^{\alpha-1}(b-x)$ and $f_s = \alpha u_s - {}_aD_x^\alpha u_s$.

- traditional approach: adapative nonuniform step-size, enriched basis like enriched finite element method, singularity reconstruction
- improved algorithm [3]: extrapolation and error correction

[3] Z. Hao and W. Cao, An improved algorithm based on finite difference schemes for fractional boundary value problems with nonsmooth solution, Journal of Scientific Computing 73 (1), 395-415, 2017

Variable coefficient

- Recall the steady space fractional diffusion equation [4]

$$-D(k(x)D_x^{\alpha-1}u(x)) = f(x)$$

The corresponding weak formulation

$$a(u,v) = (kD_x^{\alpha-1}u, Dv) = (f,v) \tag{10}$$

- To develop well-posed weak formulation, Mao and Shen (2016) consider variant problem

$$\partial_t u(x,t) = {}_a\partial_x^\alpha[k_1(x)\, {}_b\partial_x^\alpha u(x,t)] + {}_x\partial_b^\alpha[k_2(x)\, {}_a\partial_x^\alpha u(x,t)]$$

where $1/2 \le \alpha \le 1$.

Mathematical theory

- wellposedness, V. J. Ervin and J. P. Roop (2006)
- rigorous regularity analysis for two side case is still missing

[4] Z. Hao, M. Park, G. Lin, Z. Cai, Finite element method for two-sided fractional differential equations with variable coefficients: Galerkin approach, Journal of Scientific Computing, 2018 (accepted)

Reformulation of problem

- Consider

$$-D(k(x)D_\theta^{-\beta}Du) = f(x), \quad x \in (0,1),$$

where $D_\theta^{-\beta} := \theta\ {}_0D_x^{-\beta} + (1-\theta)\ {}_xD_1^{-\beta}$.

- By using the product rule and dividing by $k(x)$, the above equation can be transformed into the following equivalent form

$$-D(D_\theta^{-\beta}Du) + K(x)D_\theta^{-\beta}Du = g, \quad x \in (0,1),$$
$$u(0) = u(1) = 0,$$

where $K = -k'/k \in L^\infty(0,1), \quad g = f/k$.

- Define the bilinear form

$$a(u,v) := (D_\theta^{-\beta}Du, Dv) + (KD_\theta^{-\beta}Du, v).$$

Finite element method

Then the variational formulation is given by: find $u \in H_0^{1-\frac{\beta}{2}}(0,1)$ such that

$$a(u,v) = (g,v), \quad \forall v \in H_0^{1-\frac{\beta}{2}}(0,1).$$

- We show the well-posedness of continuous problem
- We use piecewise linear finite element method.
- The coefficient matrix of the derived linear system, $AU = b$, is

$$A = \theta S_D + (1-\theta)S_D^T + \bar{K}[\theta S_C - (1-\theta)S_C^T],$$

where $U = (u_i)$, $\bar{K} = diag(K(x_1), K(x_2), \cdots, K(x_{N-1}))$, $b = (b_i)$, $b_i = (g, \phi_i)$, and T means the transpose.

Regularity

Consider the model equation with $\alpha \in (1,2)$

$$(-\Delta)^{\alpha/2}u + \mu_1 Du + \mu_2 u = f(x), \quad x \in \Omega, \tag{11}$$

$$u(x) = 0, \quad x \in \Omega^c. \tag{12}$$

- Grubb (2016) showed standard Sobolev spaces $u \in H^s$ with $s = \alpha + \min(1/2 - \alpha/2 - \varepsilon, r)$
- When $\mu_1 = \mu_2 = 0$ Acosta et al (2018), Zhang (2018) show $\tilde{u} = u/(1-x^2)^{\alpha/2} \in B^s_{\omega^{\alpha/2}}$ weighted Sobolev space with $s = \alpha + r$
- When $\mu_1 = 0$ Zhang (2018) show $\tilde{u} \in B^s_{\omega^{\alpha/2}}$ weighted Sobolev space with $s = \alpha + \min(\alpha + 1 - \varepsilon, r)$
- When $\mu_1 \neq 0$ Hao and Zhang (2018) show $\tilde{u} \in B^s_{\omega^{\alpha/2}}$ weighted Sobolev space with $\alpha + \min(3\alpha/2 - 1 - \varepsilon, r)$
- When $\mu_1 = 0$ Hao and Zhang (2018) show $\tilde{u} \in B^s_{\omega^{\alpha/2}}$ weighted Sobolev space with $\alpha + \min(3\alpha/2 + 1 - \varepsilon, r)$

Spectral Galerkin method

The following *pseudo-eigenfunctions* for fractional diffusion operator are essential to carry out the analysis and implement the spectral Galerkin method.

Lemma

(Acosta 2018, Zhang 2018) For the n-th order Jacobi polynomial $P_n^{\alpha/2}(x)$, it holds that

$$(-\Delta)^{\alpha/2}[\omega^{\alpha/2}P_n^{\alpha/2}(x)] = \lambda_n^{\alpha}P_n^{\alpha/2}(x), \tag{13}$$

where $\lambda_n^{\alpha} = \frac{\Gamma(\alpha+n+1)}{n!}$.

- $A = \Lambda + M$, the diagonal matrix λ is dominating and the condition number is $|\alpha - 1|$
- show sharp regularity estimate.
- prove optimal error estimates for the spectral Galerkin method both in $H^{\alpha/2}$ norm and negative weighted L^2 norm.

Pseudo eigenfunction relation

Denote $\mathcal{L}_\theta^\alpha = -[\theta\, {}_aD_x^\alpha + (1-\theta)\, {}_xD_b^\alpha]$

Lemma (Ervin et al. 2016, Mao and Karniadakis 2018)

For the n-th order Jacobi Polynomial $\{P_n^{\sigma,\sigma^*}(x)\}$, *it holds that*

$$\mathcal{L}_\theta^\alpha[\omega^{\sigma,\sigma^*}(x)P_n^{\sigma,\sigma^*}(x)] = \lambda_{\theta,n}^\alpha P_n^{\sigma^*,\sigma}(x) \qquad (14)$$

where

$$\lambda_{\theta,n}^\alpha = -\frac{\sin(\pi\alpha)}{\sin(\pi\sigma)+\sin(\pi\sigma^*)}\frac{\Gamma(\alpha+n+1)}{n!},$$

$\sigma^* = \alpha - \sigma \in (0,1]$ *and* $\sigma \in (0,1]$ *is determined by the following equation:*

$$\theta = \frac{\sin(\pi\sigma^*)}{\sin(\pi\sigma^*)+\sin(\pi\sigma)}. \qquad (15)$$

In particular, we can see that $\sigma = 1$ and $\sigma^* = \alpha - 1$ for $\theta = 1$; $\sigma = \sigma^* = \frac{\alpha}{2}$ for $\theta = 1/2$.

Spectral Petrov-Galerkin method

Define the finite dimensional space

$$V_N := \omega^{\sigma^*,\sigma}\mathbb{P}_N = \text{Span}\{\varphi_0, \varphi_1, \ldots, \varphi_N\},\ \varphi_k(x) := \omega^{\sigma^*,\sigma} P_k^{\sigma^*,\sigma}(x)$$

The spectral Petrov-Galerkin method is to find $u_N \in U_N = \omega^{\sigma,\sigma^*}\mathbb{P}_N$ such that

$$(\mathcal{L}_\theta^\alpha u_N, v_N) + \mu(u_N, v_N) = (f, v_N), \quad \forall v_N \in V_N. \tag{16}$$

Denote $\phi_n(x) = \omega^{\sigma,\sigma^*} P_n^{\sigma,\sigma^*}(x)$. For implementation, plugging $u_N = \sum_{n=0}^N \hat{u}_n \phi_n(x)$ in (16) and taking $v_N = \varphi_k(x)$, we obtain from Lemma 3 and the orthogonality of Jacobi polynomials that

$$\lambda_{\theta,k}^\alpha h_k^{\sigma^*,\sigma} \hat{u}_k + \mu \sum_{n=0}^N M_{k,n}\hat{u}_n = (f, \varphi_k), \quad k = 0, 1, 2, \cdots, N, \tag{17}$$

where $\lambda_{\theta,k}^\alpha$ is defined in Lemma 3 and

$$M_{k,n} = \int_{-1}^1 (1-x^2)^\alpha P_n^{\sigma,\sigma^*}(x) P_k^{\sigma^*,\sigma}(x)\, dx. \tag{18}$$

Here $M_{k,n}$ and $f_k = (f, \phi_k)$ can be found as Galerkin version.

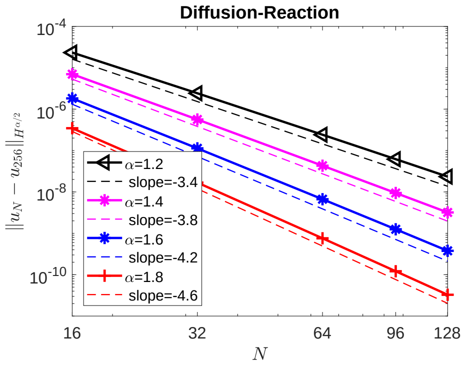

Figure: The convergence order of the spectral Galerkin methods is $2\alpha + 1$ in $H^{\alpha/2}$.

Two-sided case [5] and fractional Laplace (2018) [6]

[5]Z. Hao, G. Lin and Z. Zhang, Regularity in weighted Sobolev spaces and spectral methods for two-sided fractional reaction-diffusion equations (2017) submitted to FCAA.

[6]Z. Hao and Z. Zhang, Optimal regularity and error estimate for a spectral Galerkin method for (1D) fractional advection-diffusion-reaction equations,

Summary

- Two-term time fractional diffusion equations
- Space fractional diffusion equations
  - Finite difference method
  - Finite element method
  - Spectral method
  - Regularity

Ongoing work: high dimensional problems, irregular domain.

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