Efficient Monte Carlo Method for fractional PDEs in High Dimensions

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Outline

- **Motivation**
- **Monte Carlo method for IFL**
- **Analysis and error estimates**
- **Numerical results**

Integral Fractional Laplacian (IFL)

Let $s > 0$, and $u : \mathbb{R}^d \to \mathbb{R}$ be a smooth function with rapidly decaying derivatives (i.e., of Schwartz class)[1]

- Pseudo-differential operator via Fourier transform

$$(-\Delta)^s u(x) = \mathscr{F}^{-1}\{|\xi|^{2s}\mathscr{F}[u](\xi)\}(x), \quad x \in \mathbb{R}^d$$

- Point-wise integral representation: for $s \in (0,1)$,

$$(-\Delta)^s u(x) = C_{d,s}\,\mathrm{p.v.}\int_{\mathbb{R}^d} \frac{u(x)-u(y)}{|x-y|^{d+2s}}\mathrm{d}y, \quad x \in \mathbb{R}^d$$

where $C_{d,s}$ is a normalisation constant.

[1] M. Kwasnicki. *Ten equivalent definitions of fractional Laplace operator,* FCAA'17.

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PDEs with IFL: Challenges

$$(-\Delta)^s u(x) = f(x) \ \text{ in } \ \Omega; \quad u(x) = 0 \ \text{ on } \ \Omega^c := \mathbb{R}^d \backslash \Omega.$$

- Nonlocality — dense matrix even for local basis
- Singularity — nonstandard basis and/or ad hoc quadrature
- Regularity — Low or slow decaying

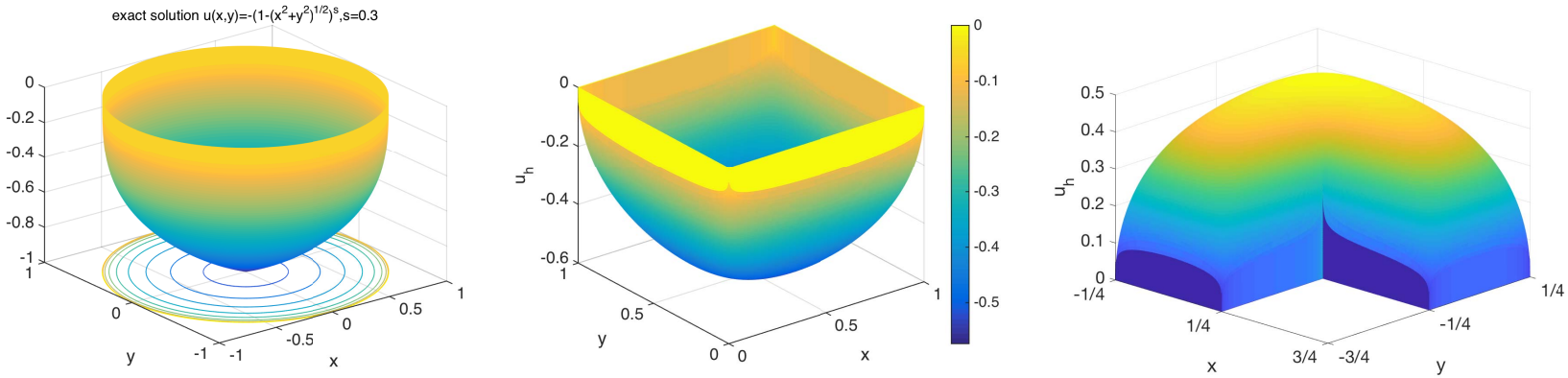

Figure: Exact or numerical solutions with $s = 0.3$. Note: $u \in H^{s+\frac{1}{2}-\epsilon}(\Omega)$ (cf. Vishik-Eskin'65; Grubb'15).

Some existing works

- Caffarelli-Silvestre Extension'07: $(d+1)$-dimensional "local" singular problem (Cheng-Xu-Yamamoto'01)
  - FD: Li et al.'21,$\cdots$
  - FEM: Nochetto et al.'15,$\cdots$
  - SM: Chen-Shen'20
- Finite Difference: Huang-Oberman'14; Dou-Zhang'18'19, Dou-Wang-Zhang'19; Minden-Ying'20; Hao-Zhang-Du'20; Xu-Cheng-Leung-Qian'20 (spherical means),$\cdots$
- Finite Element: Acosta et al'17; Ainsworth-Glusa'18; Bonito-Lei-Pasciak'19 (Dunford-Taylor formula), Wu-Xu et. al.'22, S.-Wang-Chen-Li'22, Deng et al'21, Chen et al'21 $\cdots$, many on FEM analysis
- Radial Basis/Meshless Method: Burkardt-Wu-Zhang'21
- Spectral Method in 1D or unit disk: Mao-Chen-Shen'16; Hao-Zhang'20; Hao-Li-Zhang-Zhang'20; Mao-Chen-Shen'16; Chen-Mao-Li'19;$\cdots$

Existing works: spectral method on $\mathbb{R}^d$

- Mao-Shen'17; Tang-Yuan-Zhou'18; Tang-Wang-Yuan-Zhou'19; Shen-Wang'22;
- **Generalised Hermite function (GHF)**[2]

  Fractional Sobolev orthogonality: if $i \neq j$,

$$\left((-\Delta)^{s/2} H_i,\, (-\Delta)^{s/2} H_j\right)_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^d} |\xi|^{2s} \mathscr{F}[H_i](\xi)\, \overline{\mathscr{F}[H_j](\xi)}\, \mathrm{d}\xi = 0$$

  Then $S =$ diagonal.

- **Mapped Chebyshev function (MCF)**[3]

  Fourier-like bi-orthogonality: if $p \neq q$,

$$(\widehat{\mathbb{T}}_p, \widehat{\mathbb{T}}_q)_{L^2(\mathbb{R}^d)} = 0\,; \quad \left(\nabla\widehat{\mathbb{T}}_p, \nabla\widehat{\mathbb{T}}_q\right)_{L^2(\mathbb{R}^d)} = 0$$

  Based on the **Dumford-Taylor formulation**, $S \approx S_N =$ diagonal.

[2] S.-Ma-Li-Wang-Jia. *Nontensorial generalised Hermite spectral methods for PDEs with fractional Laplacian and Schrodinger operators.* ESAIM M2AN, 2021.

[3] S.-Shen-Tang-Wang-Yuan. *Fast Fourier-like mapped Chebyshev spectral Galerkin methods for PDEs with IFL in unbounded domains.* SINUM, 2020.

Other existing works

- **Deep neural networks:**
  - Gulian-Raissi-Perdikaris-Karniadakis'2019
  - Mao-Li-Karniadakis'2019
  - Pang-D'Elia-Parks-Karniadakis'2019
  - Guo-Wu-Yu-Zhou'2022
- **Monte Carlo Method:**
  - Kyprianou-Osojnik-Shardlow'2018: Unbiased walk-on-spheres Monte Carlo methods: 2D case
  - Shardlow'2019: fields and first eigenvalue: 2D case

Feynman-Kac formula (FKf)

- **FKf** is a link between PDEs and stochastic processes.
- The first example of **FKf** is for the following PDEs

$$\begin{cases} \partial_t u + \mu \partial_x u + \frac{1}{2}\sigma^2 \partial_x^2 u - Vu + f = 0, & (x,t) \in \mathbb{R} \times [0,T], \\ u(x,T) = \psi(x), & \text{on } x \in \mathbb{R}, \end{cases}$$

where μ, σ, V, ψ, and f are known functions. Then, the **FKf** tells us that the solution u can be written as

$$u(x,t) = E\Big[\int_t^T e^{-\int_t^\tau V(X_\tau,\tau)\mathrm{d}\tau} f(X_\tau, r)\mathrm{d}r + e^{-\int_t^\tau V(X_\tau,\tau)\mathrm{d}\tau}\psi(X_T)\Big| X_t = x\Big]$$

where X is an Itó process driven by the equation

$$\mathrm{d}X = \mu(X,t)dt + \sigma(X,t)\mathrm{d}W^Q,$$

with $W^Q(t)$ is a Wiener process (i.e., Brownian motion) under Q, and the initial condition for $X(t)$ is $X(t) = x$.

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Preliminaries

- The classical Poisson equations

$$-\Delta u(\boldsymbol{x}) = f(\boldsymbol{x}) \quad \text{in } \Omega; \quad u(\boldsymbol{x}) = g(\boldsymbol{x}) \quad \text{on } \partial\Omega,$$

which is governed by Brownian motion and the solution has a **FKf** , expressed as an expectation at first exit from Ω of the associated Wiener process.

- Remarkably, the **FKf** was extended to fractional Laplacian:

$$\begin{cases} (-\Delta)^{\frac{\alpha}{2}} u(x) = f(x), & \text{in } \Omega, \\ u(x) = g(x), & \text{on } \Omega^c := \mathbb{R}^n \backslash \Omega. \end{cases} \tag{1.1}$$

where Brownian motion was replaced by α-stable Lévy process.

Feynman-Kac Formula (FK)

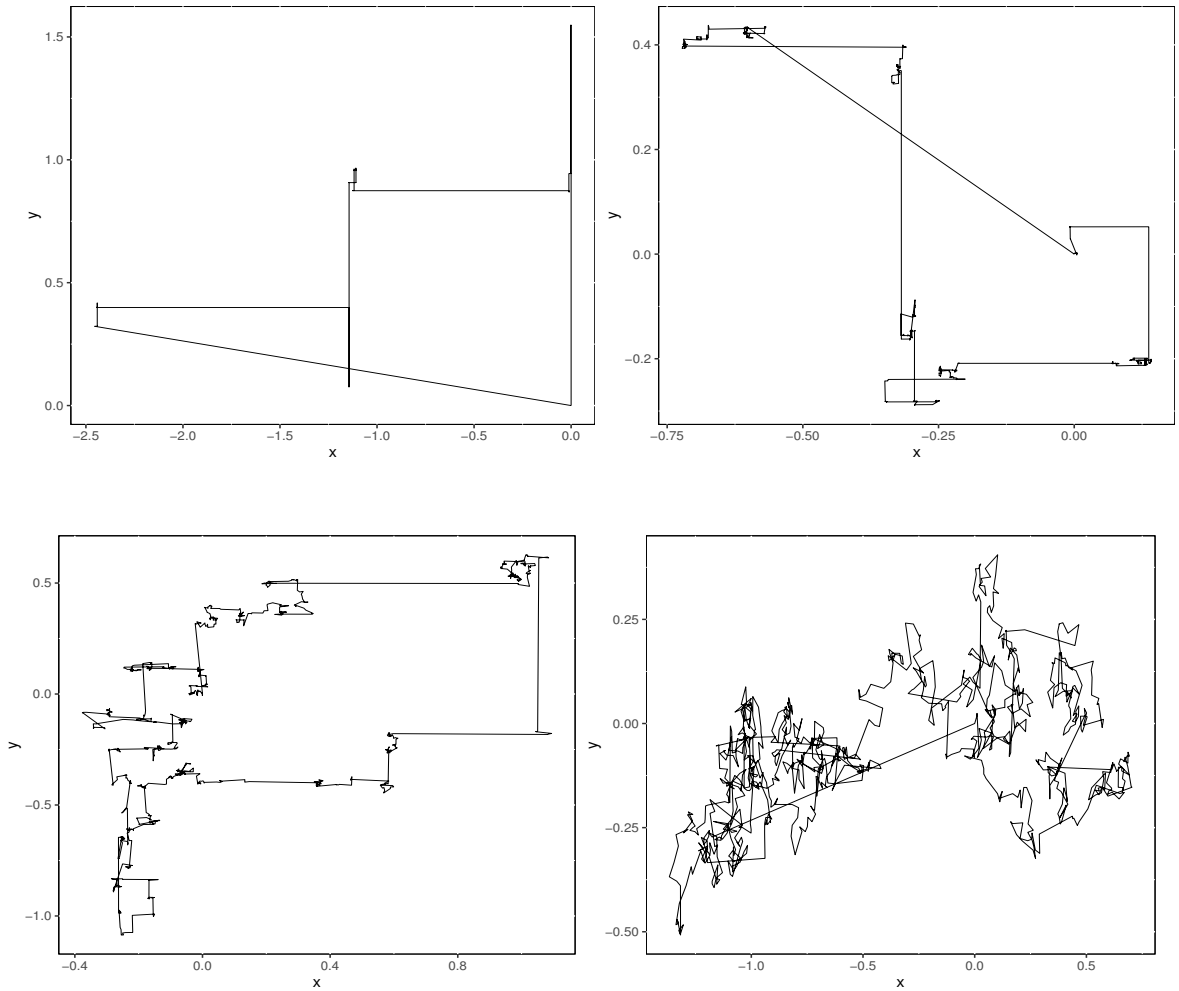


Figure: The motion trajectory of α-stable process with $\alpha = 0.4, 0.8, 1.2, 1.6$

Feynman-Kac Formula

- For any $\alpha \in (0,2)$ and a Borel set $\Lambda \subset \mathbb{R}^n$, we denote

$$L^1_\alpha(\Lambda) = \Big\{ u \in L^1(\Lambda) \ \text{ s.t. } \int_\Lambda \frac{|u(x)|}{1+|x|^{n+\alpha}}\,\mathrm{d}x < \infty \Big\}.$$

- **FKf for (1.1):** Suppose that $g(x) \in L^1_\alpha(\Omega^c)$ and $f(x) \in C^{\alpha+\epsilon}(\Omega)$ for some $\epsilon > 0$. Then there exists a unique continuous solution to problem (1.1) in $L^1_\alpha(\mathbb{R}^n)$, which is given by

$$u(x) = \mathbb{E}_{X^\alpha_0 = x}\Big[\int_0^{\tau_\Omega} f(X^\alpha_s)\,\mathrm{d}s\Big] + \mathbb{E}_{X^\alpha_0 = x}\big[g(X^\alpha_{\tau_\Omega})\big], \quad x \in \Omega,$$

where $\tau_\Omega = \inf\{t > 0 | X^\alpha_t \notin \Omega\}$, and $\{X^\alpha_t\}_{t\geq 0}$ is a symmetric α-stable Lévy process with $X^\alpha_0 = x$.

Feynman-Kac representation in a ball

- We define $\mathbb{B}_r^{n,\boldsymbol{c}_0} = \{\boldsymbol{x} \in \mathbb{R}^n : |\boldsymbol{x} - \boldsymbol{c}_0| \leq r\}$, with $\boldsymbol{c}_0 \in \mathbb{R}^n$ and $r > 0$. Let $\mathbb{B}_r^n = \mathbb{B}_r^{n,\mathbf{0}}$ for simplicity.

Lemma

Let $r > 0$, and assume that $f \in L^1_\alpha(\mathbb{B}_r^n) \cap C(\overline{\mathbb{B}}_r^n)$, $g \in L^1_\alpha(\mathbb{R}^n \setminus \mathbb{B}_r^n)$, then the solution can be represented as [a]

$$u(\boldsymbol{x}) = \begin{cases} \displaystyle\int_{\mathbb{B}_r^n} f(\boldsymbol{y}) Q_r(\boldsymbol{x}, \boldsymbol{y})\, \mathrm{d}\boldsymbol{y} + \int_{\mathbb{R}^n \setminus \mathbb{B}_r^n} g(\boldsymbol{z}) P_r(\boldsymbol{x}, \boldsymbol{z}) \mathrm{d}\boldsymbol{z}, & \text{in } \mathbb{B}_r^n, \\ g(\boldsymbol{x}), & \text{on } \mathbb{R}^n \setminus \mathbb{B}_r^n, \end{cases}$$

[a] C. Bucur *Some observations on the Green function for the ball in the fractional Laplace framework,* CPAA'16.

Feynman-Kac representation in a ball

- $P_r(\boldsymbol{x},\boldsymbol{z})$ is the Poisson kernel defined by

$$P_r(\boldsymbol{x},\boldsymbol{z}) = \widetilde{C}_n^{\alpha}\Big(\frac{r^2-|\boldsymbol{x}|^2}{|\boldsymbol{z}|^2-r^2}\Big)^{\alpha/2}\frac{1}{|\boldsymbol{x}-\boldsymbol{z}|^n}, \quad \boldsymbol{x}\in\mathbb{B}_r^n, \quad \boldsymbol{z}\in\mathbb{R}^n\setminus\overline{\mathbb{B}}_r^n,$$

- For $\boldsymbol{x}\neq\boldsymbol{y}$,

$$Q_r(\boldsymbol{x},\boldsymbol{y}) = \begin{cases} \widehat{C}_n^{\alpha}|\boldsymbol{y}-\boldsymbol{x}|^{\alpha-n}\displaystyle\int_0^{\varrho(\boldsymbol{x},\boldsymbol{y})}\frac{t^{\frac{\alpha}{2}-1}}{(t+1)^{\frac{n}{2}}}\,\mathrm{d}t, & \alpha\neq n,\\ \widehat{C}_1^{\frac{1}{2}}\log\Big(\frac{r^2-\boldsymbol{x}\boldsymbol{y}+\sqrt{(r^2-\boldsymbol{x}^2)(r^2-\boldsymbol{y}^2)}}{r|\boldsymbol{y}-\boldsymbol{x}|}\Big), & \alpha=n, \end{cases}$$

with

$$\varrho(\boldsymbol{x},\boldsymbol{y}) = \frac{(r^2-|\boldsymbol{x}|^2)(r^2-|\boldsymbol{y}|^2)}{r^2|\boldsymbol{x}-\boldsymbol{y}|^2},$$

$$\widetilde{C}_n^{\alpha} = \frac{\Gamma(n/2)\sin(\pi\alpha/2)}{\pi^{\frac{n}{2}+1}}, \quad \widehat{C}_n^{\alpha} = \frac{\Gamma(n/2)}{2^{\alpha}\pi^{\frac{n}{2}}\Gamma^2(\alpha/2)}.$$

Feynman-Kac representation in a ball

- The following alternative formulation with explicit expression for the solution of (1.1) is more convenient for computation, where we transform the expression of the original solution into an expectation form.

Theorem

The solution of problem (1.1) *can also be expressed as*

$$u(\boldsymbol{x}) = \zeta(\boldsymbol{x})\mathbb{E}_{\tilde{Q}_r}[f(Y)] + \mathbb{E}_{P_r}[g(Z)], \quad Y \in \mathbb{B}_r,\ Z \in \mathbb{R}^n \backslash \mathbb{B}_r^n,$$

where $\zeta(\boldsymbol{x})$ *is the weight function of the form*

$$\zeta(\boldsymbol{x}) = \int_{\mathbb{B}_r^n} Q_r(\boldsymbol{x}, \boldsymbol{y})\, \mathrm{d}\boldsymbol{y}.$$

Feynman-Kac representation in a ball

- A comparison with existing one:
  - with $\widetilde{Q}_r$ and P_r are the probability density functions

$$u(\boldsymbol{x}) = \zeta(\boldsymbol{x})\mathbb{E}_{\tilde{Q}_r}[f(Y)] + \mathbb{E}_{P_r}[g(Z)], \quad Y \in \mathbb{B}_r,\ Z \in \mathbb{R}^n \setminus \mathbb{B}_r^n,$$

  - associated with the α-stable Lévy process

$$u(\boldsymbol{x}) = \mathbb{E}_{X_0^\alpha = \boldsymbol{x}}\left[\int_0^{\tau_\Omega} f(X_s^\alpha)\,\mathrm{d}s\right] + \mathbb{E}_{X_0^\alpha = \boldsymbol{x}}\left[g(X_{\tau_\Omega}^\alpha)\right], \quad \boldsymbol{x} \in \Omega.$$

- It is difficult to directly solve problems in complex regions, as the Green's function and Poisson kernel in the complex domain is not easy to find.

A new representation for the irregular domain

- We aim to develop an efficient algorithm with easy to implement for a bounded domain in high dimensions.
- For bounded domain Ω, the solution of (1.1) can be simulated by an α-stable process, that is, the solution to (1.1) at the point $\boldsymbol{x}$:

$$u(\boldsymbol{x}) = \mathbb{E}_{X_0^\alpha = \boldsymbol{x}}\Big[\int_0^{\tau_\Omega} f(X_s^\alpha)\,\mathrm{d}s\Big] + \mathbb{E}_{X_0^\alpha = \boldsymbol{x}}\big[g(X_{\tau_\Omega}^\alpha)\big], \quad \boldsymbol{x} \in \Omega.$$

  This process stops when it reaches the outside of the region Ω.

- The movement path in the complex domain can still be simulated according to the random way, and the path is composed of a series of balls, P_r and Q_r in the balls are known, so the approximate value of the function in the domain can be obtained.

A new representation for the irregular domain

- Since the Markov process will leave the given domain at a finite time, the discrete point sequence can reach outside the domain Ω after a limited number of steps. Therefore, at each jump, the probability of this point leaving the given region at the next move always be positive, that is, $P(m^* < \infty) = 1$, where we denoted by

$$m^* = \inf\{m \in \mathbb{N} : X_m \notin \Omega\},$$

the stopping step for the random walk.

Irregular domain

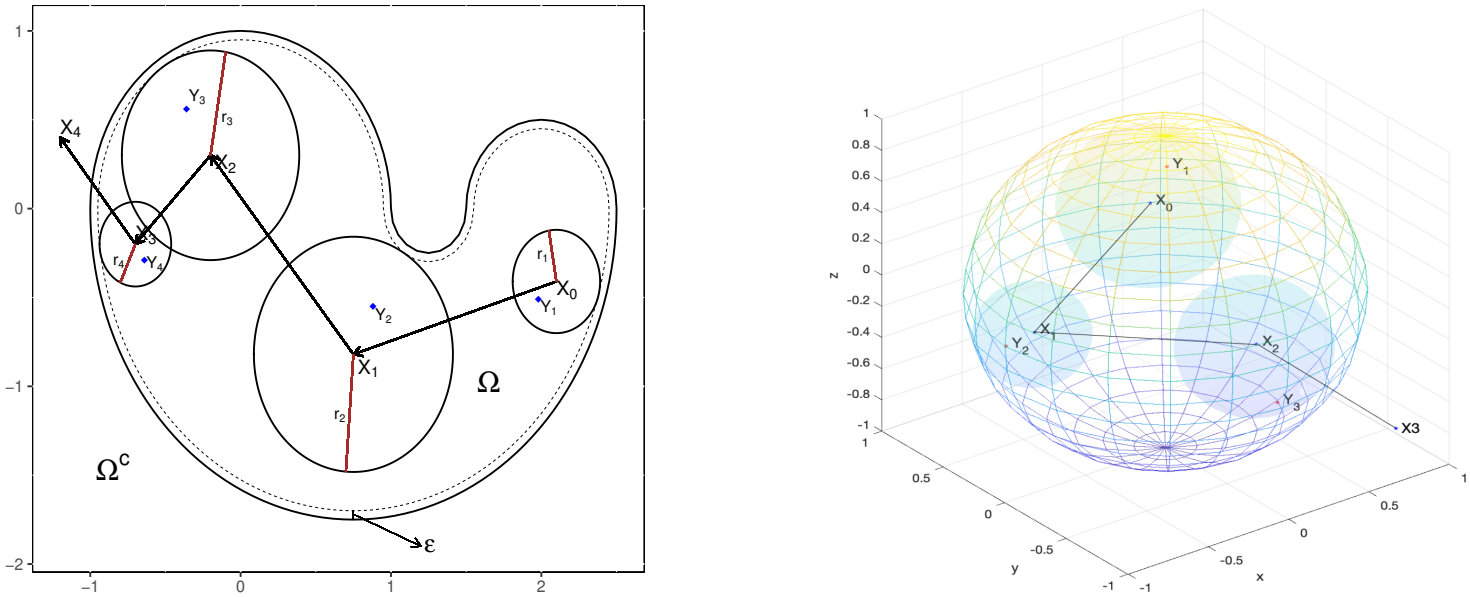


Figure: The path of walk; Left: on 2-D irregular domain; Right: on the unit ball in 3-D.

A new representation for the irregular domain

Theorem

Let $\alpha \in (0, 2]$ *and* Ω *be an open bounded domain, and assume that* $f \in L^1_\alpha(\Omega) \cap C(\overline{\Omega})$ *and* $g \in L^1_\alpha(\mathbb{R}^n \setminus \Omega)$*, then the solution of* (1.1) *in* $L^1_\alpha(\mathbb{R}^n)$ *can be expressed as*

$$u(\boldsymbol{x}) = \sum_{k=1}^{m^*-1} \zeta(X_k)\mathbb{E}_{\tilde{Q}_{r_k}}[f(Y_k)] + \mathbb{E}_{P_{r_{m^*-1}}}[g(Z_{m^*})], \quad Y_k \in \mathbb{B}_{r_k}, \ Z_k \in \mathbb{R}^n \setminus \mathbb{B}^n_{r_k},$$

where $\zeta(X_k)$ *is the weight function in* k*-th ball,*

$$\zeta(X_k) = \int_{\mathbb{B}^n_{r_k}} Q_{r_k}(X_k, \boldsymbol{y})\, \mathrm{d}\boldsymbol{y}.$$

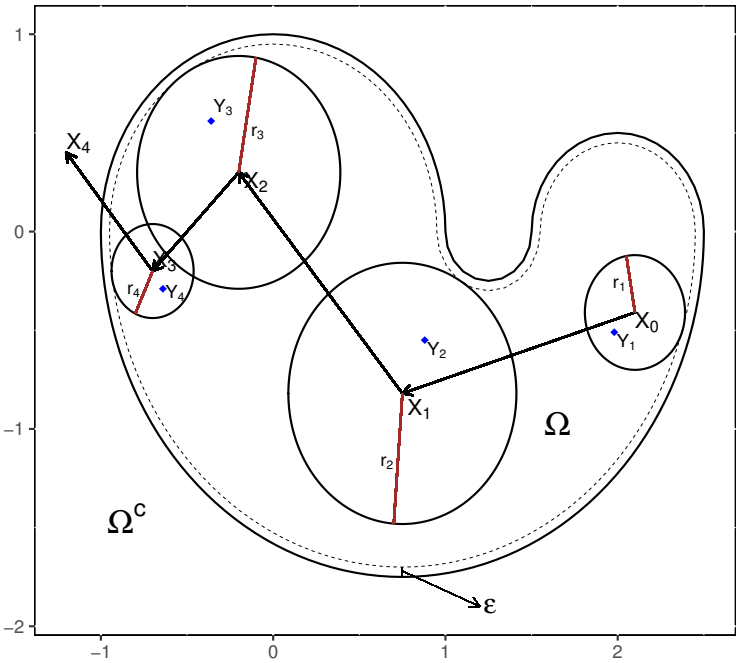
Efficient algorithm

- Instead of simulating the irregular trajectories of symmetric α-stable processes, we take advantage of the explicit expressions of $\widetilde{Q}_r$ and P_r as the probability density functions, which gives the transition probability of the symmetric α-stable process trajectory inside the ball during its passage from the center to the boundary $\partial\Omega$ or outside the domain Ω.

- Given an accuracy threshold $\varepsilon > 0$, we define an inwardly 'thickening' the boundary $\partial\Omega$ as

$$\Gamma_\varepsilon = \{\boldsymbol{x} \in \Omega : \mathrm{dist}(\boldsymbol{x}, \partial\Omega) < \varepsilon\},$$

where $\mathrm{dist}(\boldsymbol{x}, \partial\Omega)$ denotes the distance from $\boldsymbol{x} \in \Omega$ to $\partial\Omega$.



The path of walk on 2-D irregular domain

Efficient algorithm

- In each experiment, we need to simulate several important quantities as below
  1. The coordinates of the center of i-th ball;
  2. The jump distance from the i-th ball to $(i+1)$-th ball;
  3. The weight of the expectation $\zeta(\boldsymbol{x}_i)$;
- To simplify the implementation, we recommend proceeding with this calculation in spherical coordinates.

Computation of the jump distance γ

- We can evaluate the jump distance (denoted by γ) from the current ball to the next ball by using the following formula, which indicates the jump distance is a uniformly distributed random number.

Lemma

Let $\alpha \in (0, 2]$ and let the radius of the current ball $r > 0$. Assume that the ball jumps in the region Ω, then the jump distance γ from the current ball to the next ball is given by

$$\gamma(\omega; r, n, \alpha) = \sqrt{\frac{r^2}{B(1-\frac{\alpha}{2}, \frac{\alpha}{2}) - B^{-1}(\frac{\pi\,\omega}{\sin(\pi\alpha/2)}; 1-\frac{\alpha}{2}, \frac{\alpha}{2})}}, \quad \omega \in (0, 1),$$

where $B^{-1}(\cdot\,; a, b)$ denote the inverse function of incomplete Beta function $B(\cdot\,; a, b)$, and $B(a, b) := B(1; a, b)$ denote the Beta function.

Computation of the weight function $\zeta(x)$

We reformulate Green's function into a concise form, which helps us evaluate the weight function $\zeta(\boldsymbol{x})$ of each ball more easily.

Lemma

For $r > 0$, $\zeta(\boldsymbol{x})$ in Theorem 2 can be computed by

$$\zeta(\boldsymbol{x}) = \widehat{C}_n^{\alpha} \int_{\mathbb{B}_r^n} |\boldsymbol{y} - \boldsymbol{x}|^{\alpha-n} \Big[B\Big(\frac{n-\alpha}{2}, \frac{\alpha}{2}\Big) - B\Big(\varrho^*(\boldsymbol{x}, \boldsymbol{y}); \frac{n-\alpha}{2}, \frac{\alpha}{2}\Big) \Big] \, \mathrm{d}\boldsymbol{y}.$$

In particular, if $\boldsymbol{x} = \mathbf{0}$, we have

$$\zeta(\mathbf{0}) = \frac{r^{\alpha}}{2^{\alpha-1}\Gamma^2(\frac{\alpha}{2})} \int_0^1 \tilde{\rho}^{\alpha-1} \Big[B\Big(\frac{n-\alpha}{2}, \frac{\alpha}{2}\Big) - B\Big(\tilde{\rho}^2; \frac{n-\alpha}{2}, \frac{\alpha}{2}\Big) \Big] \, \mathrm{d}\tilde{\rho}.$$

The Monte Carlo simulation

The density $\widetilde{Q}(\boldsymbol{x}, \boldsymbol{y})$ can be used to construct transition probabilities for a discrete sequence of points. When calculating the value of a point x_0 in the region Ω, namely $u(\boldsymbol{x}_0)$,

(1) First calculate the shortest distance $r_1 = \mathrm{dist}(\boldsymbol{x}_0, \Gamma_\varepsilon)$ from x to the boundary Γ_ε, and draw a sphere $\mathbb{B}_{r_1}^n$ tangent to the boundary with $\boldsymbol{x}_0$ as the center and r_1 as the radius.

(2) Next, construct a random variable X_1 that is evaluated outside sphere $\mathbb{B}_{r_1}^n$, and its density function is $P_{r_1}(\boldsymbol{x}_0, \boldsymbol{x}_1)$, and then construct another random variable Y_1 that is evaluated inside the sphere $\mathbb{B}_{r_1}^n$ which is follow the density function $\widetilde{Q}(\boldsymbol{x}_0, \boldsymbol{y}_1)$.

The Monte Carlo simulation

(3) If $X_1 = \boldsymbol{x}_1$ is taken outside the region Ω, then, the value of $u(\boldsymbol{x}_0)$ can be expressed as:

$$u(\boldsymbol{x}_0) = \zeta(\boldsymbol{x}_0)\mathbb{E}_{\boldsymbol{x}_0}[f(Y_1)] + \mathbb{E}_{\boldsymbol{x}_0}[g(X_1)].$$

If $X_1 = \boldsymbol{x}_1$ is taken inside the region Ω, we compute $r_2 = \mathrm{dist}(\boldsymbol{x}_1, \Gamma_\varepsilon)$ which is the shortest distance from x_1 to the region boundary Γ_ε, and draw a sphere $\mathbb{B}^n_{r_2}$ tangent to the boundary with $\boldsymbol{x}_1$ as the center and r_2 as the radius.

(4) Next, construct a random variable X_2 that is evaluated outside sphere $\mathbb{B}^n_{r_2}$, and its density function is $P_{r_2}(\boldsymbol{x}_1, \boldsymbol{x}_2)$, and then construct another random variable Y_2 that is evaluated inside the sphere $\mathbb{B}^n_{r_2}$ which is follow the density function $\widetilde{Q}(\boldsymbol{x}_1, \boldsymbol{y}_2)$.

The Monte Carlo simulation

(5) If $X_2 = \boldsymbol{x}_2$ is taken outside the region Ω, Then, the value of $u(\boldsymbol{x}_0)$ can be expressed as:

$$u(\boldsymbol{x}_0) = \zeta(\boldsymbol{x}_0)\mathbb{E}_{\boldsymbol{x}_0}[f(Y_1)] + \zeta(\boldsymbol{x}_1)\mathbb{E}_{\boldsymbol{x}_1}[f(Y_1)|X_1] + \mathbb{E}_{\boldsymbol{x}_0}[g(X_2)].$$

Then, we let

$$u(X_k) = \zeta(X_k)\mathbb{E}_{\boldsymbol{x}}[f(Y_{k+1})|X_k] + \mathbb{E}_{\boldsymbol{x}}[u(X_{k+1})|X_k].$$

(6) By an induction argument, we suppose that the process exist the region Ω on m step, then the solution of problem (1.1) is

$$u(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{x}}[u(X_0)] = \mathbb{E}_{\boldsymbol{x}}[u(X_m)] + \sum_{k=0}^{m-1} \mathbb{E}_{\boldsymbol{x}}[u(X_k) - u(X_{k+1})]$$

$$= \mathbb{E}_{\boldsymbol{x}}[u(X_m)] + \sum_{k=0}^{m-1} \mathbb{E}_{\boldsymbol{x}}\left[u(X_k) - \mathbb{E}_{\boldsymbol{x}}[u(X_{k+1})|X_k]\right].$$

The Monte Carlo simulation

Therefore, we can construct a Monte Carlo procedures based on the random sample

$$S_i = g(X^i_{m^*}) + \sum_{k=0}^{m^*-1} \zeta(X^i_k) f(Y^i_{k+1}),$$

where i denotes the i-th experiment, and we have $E(S_i) \approx u(\boldsymbol{x}_0)$.

Corollary

Let $r > 0$, and assume that $f, g \in L^1_\alpha(\mathbb{B}^n_r) \cap C(\overline{\mathbb{B}}^n_r)$, for $\boldsymbol{x} \in \Omega$, the estimate for $u(\boldsymbol{x})$ is given by

$$u(\boldsymbol{x}) = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} S_i = \mathbb{E}_{\boldsymbol{x}} \Big[g(X_{m^*}) + \sum_{k=0}^{m^*-1} \zeta(X_k) f(Y_{k+1}) \Big].$$

A comparison with existing work

- Kyprianou-Osojnik-Shardlow'2018: Unbiased walk-on-spheres Monte Carlo methods
  - The simulation in [KOS'18] involves α-stable Lévy process:

$$u(x) = \mathbb{E}_{X_0^\alpha = x}\left[g(X_{\tau_\Omega}^\alpha)\right] + \mathbb{E}_{X_0^\alpha = x}\left[\int_0^{\tau_\Omega} f(X_s^\alpha)\,\mathrm{d}s\right], \quad x \in \Omega,$$

    Then, the discretization in the time direction requires saving massive historical data including the whole stochastic process.

  - It is difficult to analyze the high-dimensional problem.
- Our method overcomes all the above two problems!

The analysis of the error

Lemma

For any $\varepsilon > 0$, *and let* $u \in L^1_\alpha(\mathbb{R}^n)$, $f \in L^1_\alpha(\mathbb{B}^n_r) \cap C(\overline{\mathbb{B}}^n_r)$ *and* $g \in L^1_\alpha(\mathbb{R}^n \setminus \mathbb{B}^n_r)$ *with* $r > 0$ *and* $\alpha \in (0, 2]$, *there holds*

$$\left|\mathbb{E}[g(X'_{m^*})] - \mathbb{E}[u(X_{m^*})]\right| \leq \frac{2^{1-\alpha} M}{\alpha \Gamma^2(\alpha/2)} \varepsilon^\alpha, \quad X_{m^*} \in \mathbb{R}^n \setminus \mathbb{B}^n_{r-\varepsilon},$$

where

$$X'_{m^*} = \begin{cases} X_{m^*}, & \text{if } X_{m^*} \in \mathbb{R}^n \setminus \mathbb{B}^n_r, \\ \inf\limits_{\chi \in \partial \mathbb{B}^n_r} \{|\chi - X_{m^*}|\}, & \text{if } X_{m^*} \in \mathbb{B}^n_r \setminus \mathbb{B}^n_{r-\varepsilon}. \end{cases}$$

The error bound

Lemma

For any $\varepsilon > 0$, *and assume that* $u \in L^1_\alpha(\mathbb{R}^n)$, $f \in L^1_\alpha(\mathbb{B}^n_r) \cap C(\overline{\mathbb{B}}^n_r)$ *and* $g \in L^1_\alpha(\mathbb{R}^n \setminus \mathbb{B}^n_r)$ *with* $r > 0$ *and* $\alpha \in (0, 2]$, *then we have*

$$\mathbb{E}_{\boldsymbol{x}}[\bar{S} - u(\boldsymbol{x})]^2 \leq \mathcal{O}(N^{-1} + \varepsilon^{2\alpha}).$$

An estimate of the average computation

Lemma

For any $\varepsilon > 0$, $\alpha \in (0, 2]$, and given initial point $\boldsymbol{x} \in \mathbb{B}_r^n$ with $r > 0$, then the probability of the point $\boldsymbol{x}$ leaving the domain $\mathbb{B}_r^n$ is positive, that is,

$$\mathbb{E}_{\boldsymbol{x}}(m^*) < 1 + \frac{q_*}{(1 - p_*)^2},$$

where the constants

$$p_* := p_*(n, \alpha, r, \varepsilon) = \frac{\pi^{n/2}}{\Gamma(n/2)} \widetilde{C}_n^{\alpha} \Big[B\Big(\frac{\alpha}{2}, 1 - \frac{\alpha}{2}\Big) - B\Big(\frac{\varepsilon^2}{r^2}; \frac{\alpha}{2}, 1 - \frac{\alpha}{2}\Big)\Big],$$

$$q_* := q_*(n, \alpha, r, \varepsilon) = 1 - \frac{\pi^{n/2}}{\Gamma(n/2)} \widetilde{C}_n^{\alpha} \Big[B\Big(\frac{\alpha}{2}, 1 - \frac{\alpha}{2}\Big) - B\Big(\frac{(r - \varepsilon)^2}{r^2}; \frac{\alpha}{2}, 1 - \frac{\alpha}{2}\Big)\Big].$$

with $\widetilde{C}_n^{\alpha}$ is a positive constant.

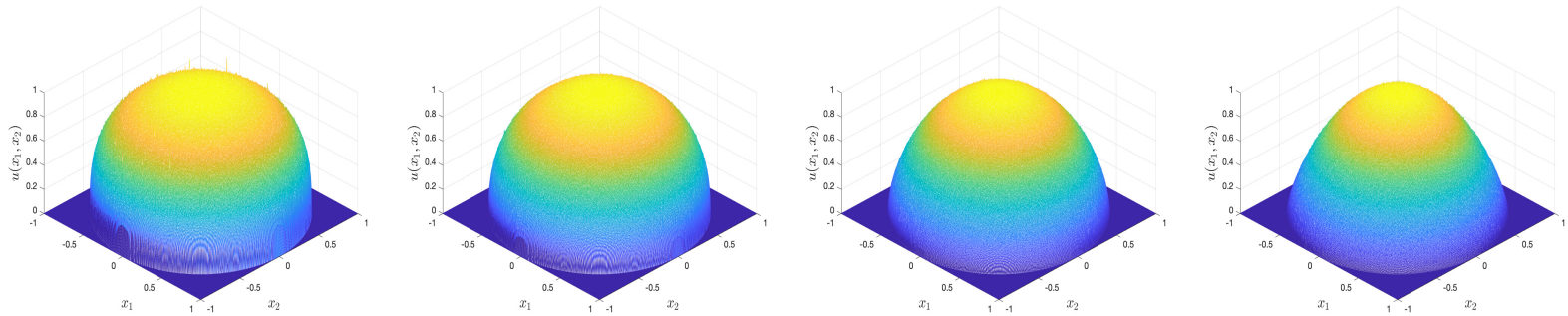
2D with homogeneous BCs

- Consider (1.1) on a unit disk $\mathbb{B}_1^2$ with the following exact solutions:

$$u(\boldsymbol{x}) = (1 - |\boldsymbol{x}|^2)_+^{\frac{\alpha}{2}},$$

where $a_+ = \max\{a, 0\}$.

- The source term $f = 2^\alpha \Gamma^2(\frac{\alpha}{2} + 1)$, and the nonlocal boundary condition becomes homogeneous, that is, $g(\boldsymbol{x}) = 0$ in Ω^c.



(a) $\alpha = 0.4$ (b) $\alpha = 0.8$ (c) $\alpha = 1.2$ (d) $\alpha = 1.6$

Figure: Profiles of the numerical solutions zoomed in $\mathbb{B}_1^2$ with various α.

2D with homogeneous BCs

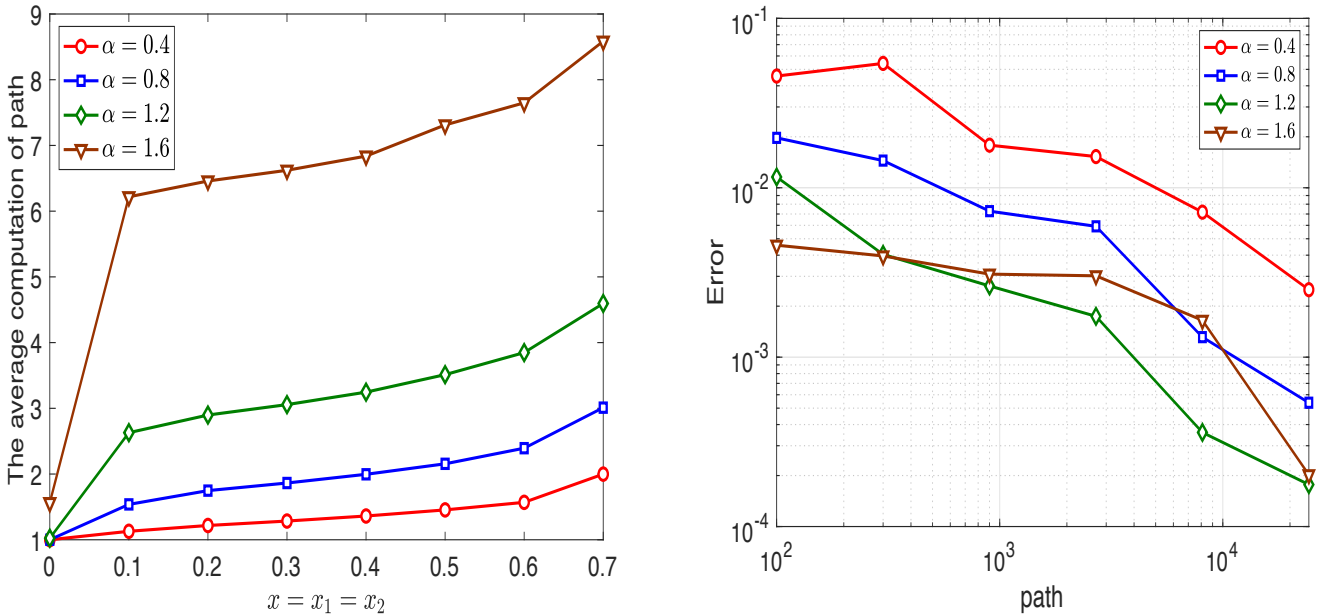


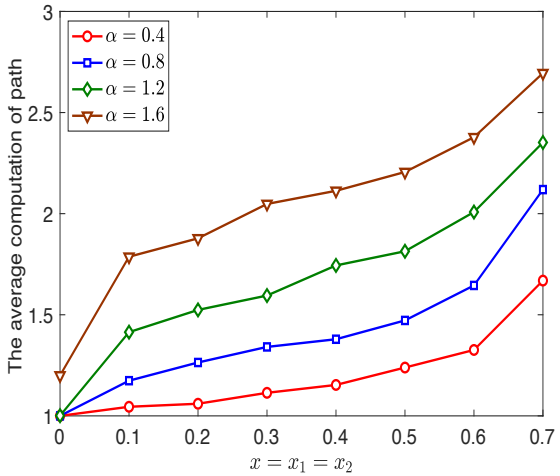
Figure: Simulation for two-dimension. Left: the average number of steps for fixed point with various α; Right: numerical errors against ε.

2D with non-homogeneous BCs

- Consider (1.1) with the following source functions:

$$f(\boldsymbol{x}) = \Gamma(2+\alpha)\,{}_2F_1\Big(\frac{2+\alpha}{2}, \frac{3+\alpha}{2}; 1; -|\boldsymbol{x}|^2\Big), \quad \text{on } \Omega = \mathbb{B}_1^2, \tag{2.2}$$

then we have the exact solution $u(\boldsymbol{x}) = (1+|\boldsymbol{x}|^2)^{-\frac{3}{2}}$ on $\mathbb{R}^2$, and the nonhomegeneous boundary condition $g(\boldsymbol{x}) = u(\boldsymbol{x})$ on Ω^c.



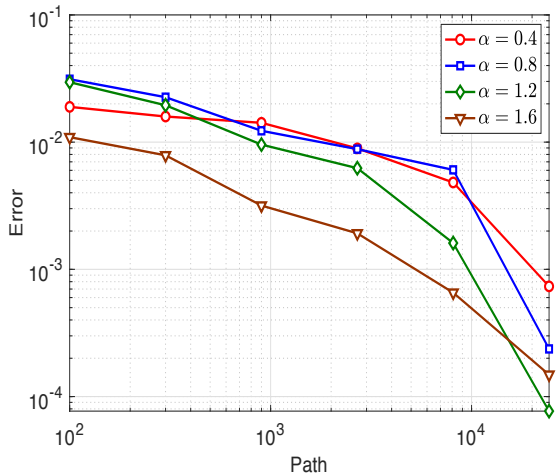


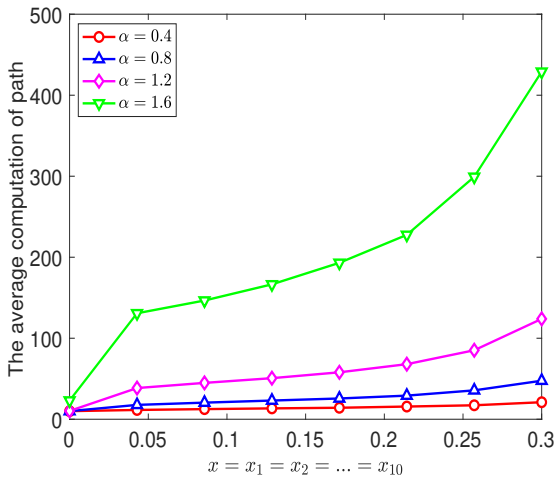
Figure: Simulation for two-dimension. Left: the average number of steps for fixed point with various α; Right: numerical errors against the number of path with various α.

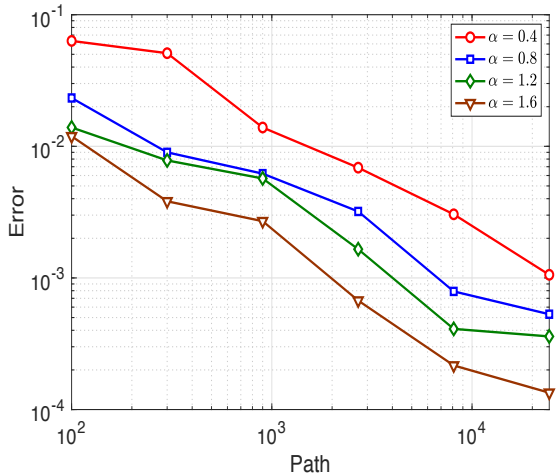
10 dimensional problem with homogeneous BCs

- Consider the following exact solutions in 10-dimensions:

$$u(\boldsymbol{x}) = (1 - |\boldsymbol{x}|)_+^{\frac{\alpha}{2}}, \quad \boldsymbol{x} \in \Omega = \mathbb{B}^{10}, \tag{2.3}$$

then $f(\boldsymbol{x}) = 2^\alpha \Gamma(1 + \frac{\alpha}{2})\Gamma(\frac{n+\alpha}{2})/\Gamma(\frac{n}{2})$ and $g(\boldsymbol{x}) = 0$ in Ω^c.





IFL on complex domains

We further consider the following three cases:

(i) For the stripe domain, we take

$$f(\boldsymbol{x}) = 2^{\alpha}\Gamma(1+\frac{\alpha}{2})(\cos^{\frac{\alpha}{3}}(c_2\boldsymbol{x}) + \sin^{\frac{\alpha}{2}}(c_1\boldsymbol{x}))\cos(-|\boldsymbol{x}|^2) \ \text{ on } \Omega,$$

where $c_1 = (\frac{\pi}{3}, -\frac{\pi}{4})$, $c_2 = (-\frac{\pi}{2}, \frac{2\pi}{3})$, $\boldsymbol{x} = (x_1, x_2)^T$, $g(\boldsymbol{x}) = 0$.

(ii) For regular hexagon domain, we take

$$f(\boldsymbol{x}) = \sin^2(c_1\boldsymbol{x}) + \cos^2(c_2\boldsymbol{x}) - (\alpha x_1 x_2)^3, \ \text{ on } \Omega,$$

where Ω is the regular hexagon domain on $[-1,1]^2$, $g(\boldsymbol{x}) = 0$.

(iii) For the annulus domain, we take

$$f(\boldsymbol{x}) = \cos(x_2^2 - 2x_1x_2) - \sin(x_1^2 + 2x_1x_2), \ \text{ on } \Omega,$$

where $\Omega = \{\boldsymbol{x} \in \mathbb{R}^2 : 0.3 < |\boldsymbol{x}|^2 < 1\}$ is the annulus domain, $g(\boldsymbol{x}) = 0$.

IFL on complex domains

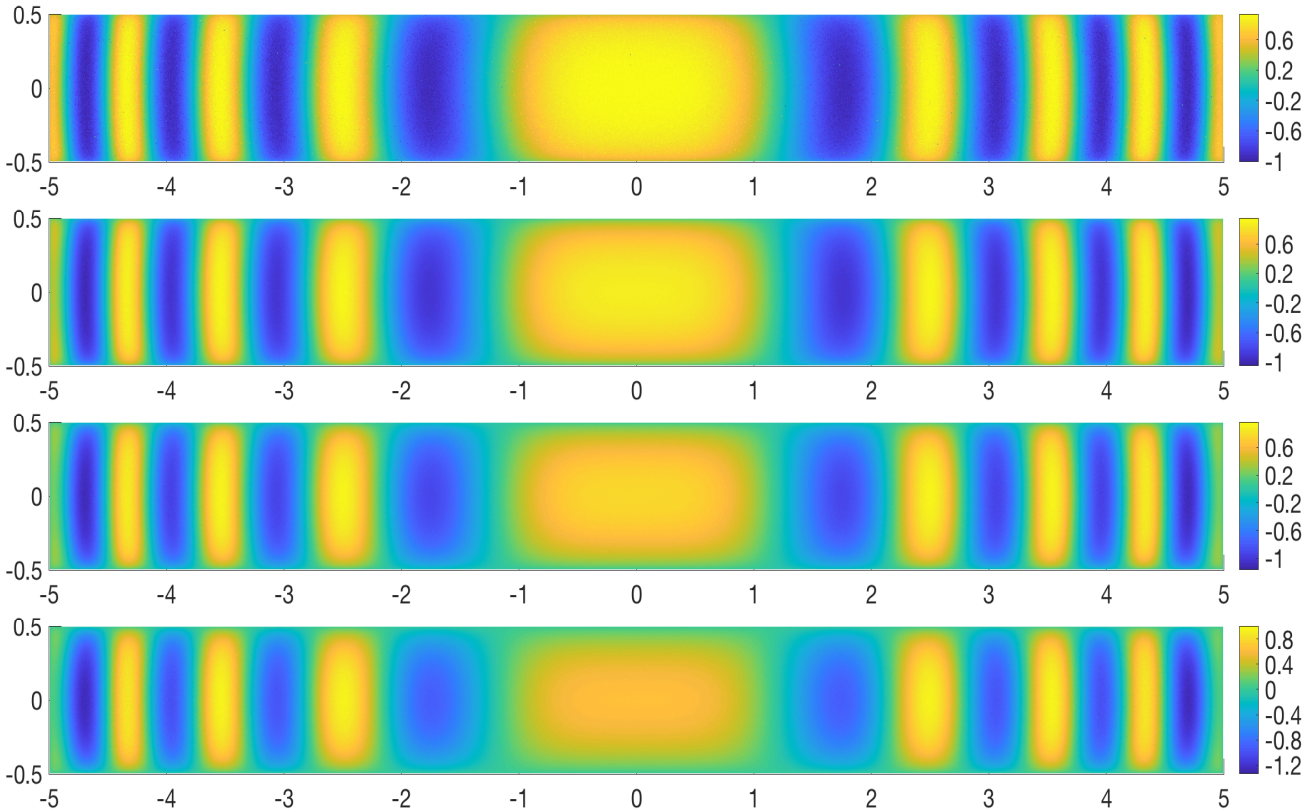
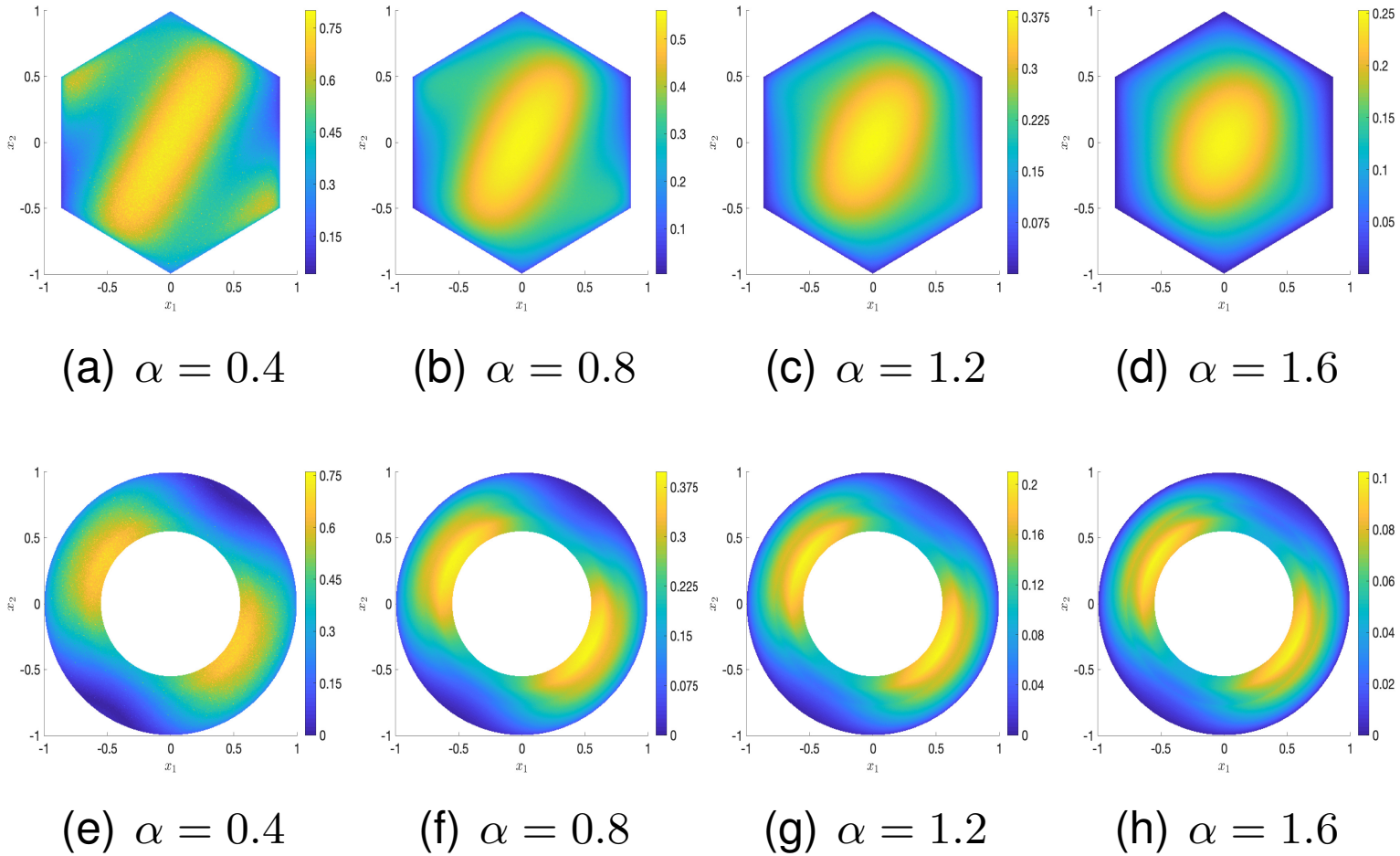


Figure: Profiles of the numerical solutions zoomed in the stripe domain $[-5, 5] \times [-0.5, 0.5]$ with $\alpha = 0.4, 0.8, 1.2, 1.6$ (from top to bottom).

IFL on complex domains



(a) $\alpha = 0.4$ (b) $\alpha = 0.8$ (c) $\alpha = 1.2$ (d) $\alpha = 1.6$

(e) $\alpha = 0.4$ (f) $\alpha = 0.8$ (g) $\alpha = 1.2$ (h) $\alpha = 1.6$

Figure: Profiles of the numerical solutions with various α. Top: the hexagon domain; Botton: the annulus domain.

Further extension

- time dependent PDEs involving IFL on Ω

$$\begin{cases} \partial_t u(\boldsymbol{x},t) + (-\Delta)^{\frac{\alpha}{2}} u(\boldsymbol{x},t) = V(\boldsymbol{x})u(\boldsymbol{x},t) + r(\boldsymbol{x}), & (\boldsymbol{x},t) \in \Omega \times (0,\infty), \\ u(\boldsymbol{x},0) = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega; \qquad u(\boldsymbol{x},t) = g(\boldsymbol{x},t), & \boldsymbol{x} \in \Omega^c \times (0,\infty). \end{cases}$$

- time dependent semilinear PDEs involving nonlocal operator

$$\begin{cases} \partial_t u(\boldsymbol{x},t) + \mathcal{L}_\delta u(\boldsymbol{x},t) = f(u(\boldsymbol{x},t),\boldsymbol{x},t), & (\boldsymbol{x},t) \in \Omega \times (0,\infty), \\ u(\boldsymbol{x},0) = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega; \qquad u(\boldsymbol{x},t) = g(\boldsymbol{x},t), & \boldsymbol{x} \in \Omega_\delta \times (0,\infty), \end{cases}$$

  where $\mathcal{L}_\delta$ is a general nonlocal operator.

- fractional Eigenvalue problem

$$\begin{cases} (-\Delta)^{\frac{\alpha}{2}} u(\boldsymbol{x}) = \lambda u(\boldsymbol{x}), & \boldsymbol{x} \in \Omega, \\ u(\boldsymbol{x}) = 0, & \boldsymbol{x} \in \Omega^c. \end{cases}$$

Conclusion

- We propose an efficient Monte Carlo method for solving PDEs with IFL on bounded domains in high dimensions.
- We provide a new **FKf** for the solution of fractional Poisson equations on the ball and the irregular domain in high dimensions.
- We establish the error analysis with the aid of the explicit expression of Green's function and Poisson's kernel.
- It only requires the solution belong to $L^1_\alpha(\Omega)$, and the algorithm seems more efficient with smaller α!

Reference:

1. **C. Sheng, B. Su, and C. Xu.** *Efficient Monte Carlo Method for Integral Fractional Laplacian in Multiple Dimensions.* arXiv preprint arXiv:2204.08860, 2022 Apr.

Thank you !