

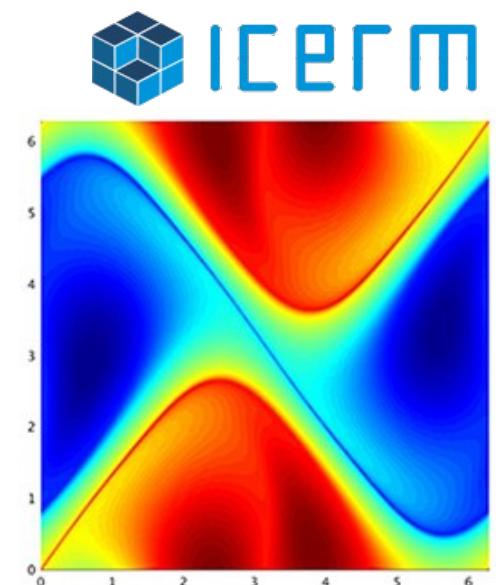
NON-SYMMETRIC FRACTIONAL DIFFUSION AS A SPECIAL CASE OF NONLOCAL CONVECTION-DIFFUSION

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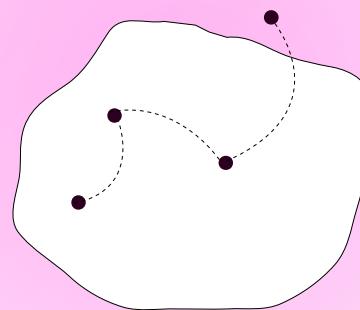


Fractional PDEs: Theory, Algorithms and Applications
ICERM, Providence, RI – June 20th 2018

Introduction

NONLOCAL MODELS

our interest: nonlocal diffusion operators describing jump processes



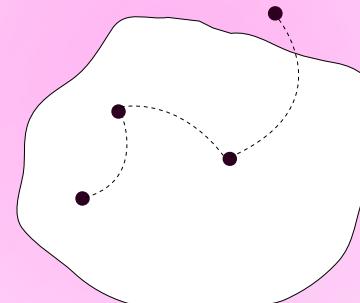
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nonlocal equation = **master equation**

solution = **pdf** of a stochastic process

$$\begin{cases} u_t + \mathcal{L}u = f & \text{in } \Omega, t > 0 \\ u = 0 & \text{in } \mathbb{R} \setminus \Omega, t > 0 \\ u(\mathbf{x}, 0) = u_0(\mathbf{x}) & \text{in } \Omega \end{cases}$$



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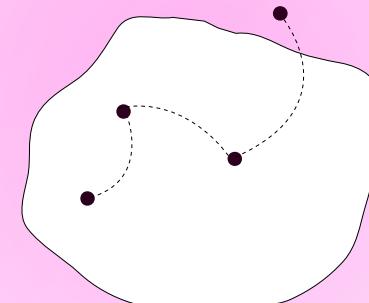
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how do they look like?

$$\mathcal{L}u(\mathbf{x}) = \int_{\mathbb{R}^n} (u(\mathbf{y}) - u(\mathbf{x})) \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{y}$$



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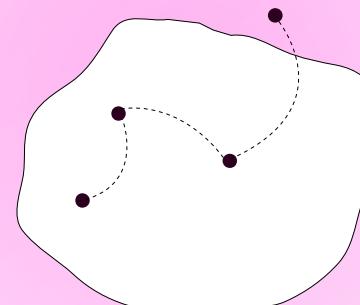
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extensively studied using the
nonlocal vector calculus
(note: finite interaction radius)



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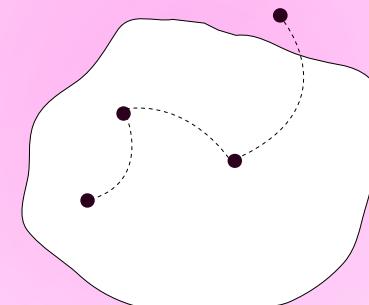
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FRACTIONAL (NONLOCAL) MODELS

Nonlocal **symmetric** diffusion

$$\mathcal{L}u(\mathbf{x}) = \int_{\mathbb{R}^n} (u(\mathbf{y}) - u(\mathbf{x})) \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{y}$$

$\exists \gamma$ s.t. $\mathcal{L}u(\mathbf{x}) = (-\Delta)^s u = c \int_{\mathbb{R}^n} \frac{u(\mathbf{x}) - u(\mathbf{y})}{|\mathbf{y} - \mathbf{x}|^{n+2s}} d\mathbf{y}, \quad 0 < s < 1$

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**nonlocal convection =
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integration on an
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truncation
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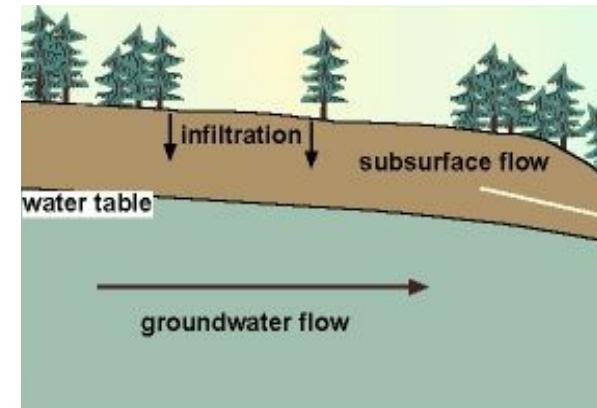
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NOT ONLY STOCHASTIC PROCESSES

this analysis is applicable also to

- nonlocal models for continuum mechanics
- nonlocal heat conduction
- subsurface flow/porous media



Outline

- Why **truncated** kernels:
the fractional Laplacian as a special case of the nonlocal operator
- **Non-symmetric** nonlocal operators:
analysis and applications

NONLOCAL VECTOR CALCULUS

- generalization of the classical vector calculus to nonlocal operators
- allows us to study nonlocal diffusion similarly to the classical, local, counterpart in a **variational setting**
- based on the concept of nonlocal fluxes

NONLOCAL VECTOR CALCULUS

analyzing **symmetric diffusion**

- divergence of ν : $\mathcal{D}(\nu)(\mathbf{x}) = \int_{\mathbb{R}^n} (\nu(\mathbf{x}, \mathbf{y}) + \nu(\mathbf{y}, \mathbf{x})) \cdot \boldsymbol{\alpha}(\mathbf{x}, \mathbf{y}) d\mathbf{y}$
- gradient of u : $-\mathcal{D}^*(u)(\mathbf{x}, \mathbf{y}) = (u(\mathbf{y}) - u(\mathbf{x})) \boldsymbol{\alpha}(\mathbf{x}, \mathbf{y})$
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question 1: how to obtain this form??

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the operator $\mathcal{D}(\mathcal{D}^*\cdot)$
is not enough

let's get back to this later...

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question 0: how to deal with infinite domains??

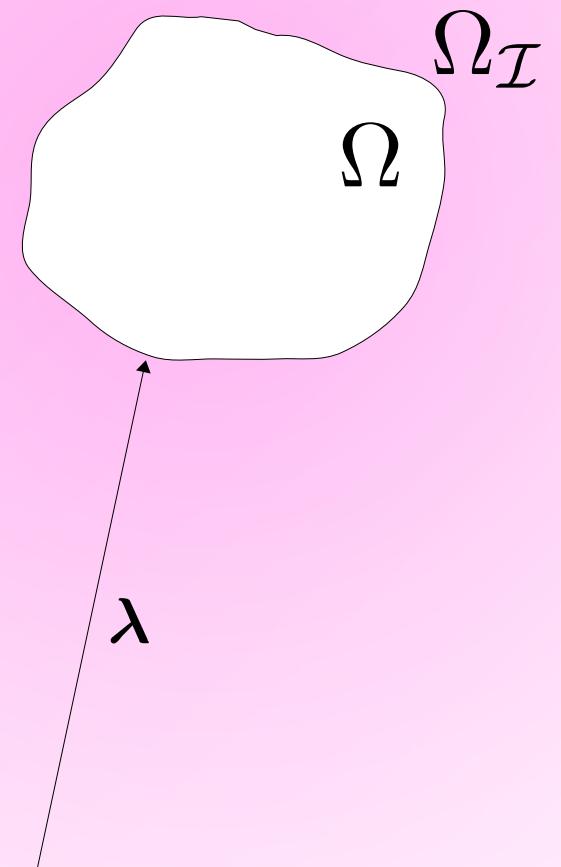
recall: we analyzed nonlocal problems with finite-interaction radius

⇒ what happens to the nonlocal solution when we truncate the kernel?

NONLOCAL VECTOR CALCULUS

Interaction domain of an open bounded region $\Omega \in \mathbb{R}^d$

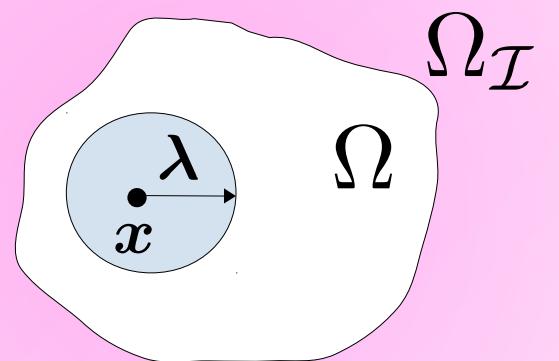
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Kernel: we assume

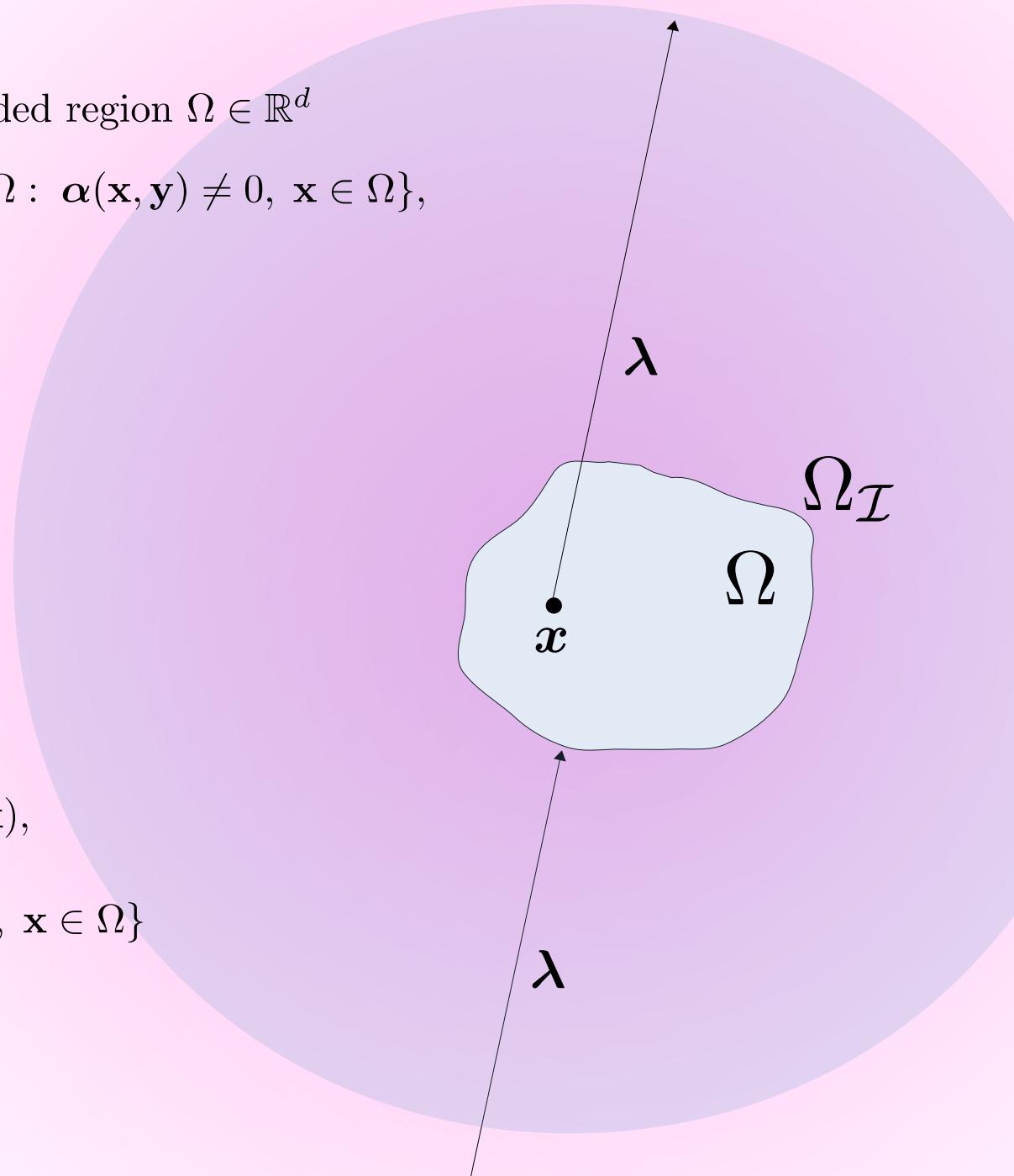
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$$B_\lambda(\mathbf{x}) = \{\mathbf{y} \in \Omega : |\mathbf{x} - \mathbf{y}| \leq \lambda, \mathbf{x} \in \Omega\}$$

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THE FRACTIONAL LAPLACIAN AS A *NONLOCAL* OPERATOR

- M.D., M. Gunzburger, The fractional Laplacian operator on bounded domains as a special case of the nonlocal diffusion operator, *Computers and Mathematics with applications*, 66, 1245–1260, 2013

FRACTIONAL and TRUNCATED FRACTIONAL

Fractional Laplacian $\mathcal{L}u = (-\Delta)^s u = c \int_{\mathbb{R}^n} \frac{u(\mathbf{x}) - u(\mathbf{y})}{|\mathbf{y} - \mathbf{x}|^{n+2s}} d\mathbf{y}$

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want to compare

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result

$$\|u - \tilde{u}\|_{H^s(\Omega \cup \Omega_{\mathcal{I}})} \leq \frac{K_n}{s(\lambda - I)^{2s}} \|u\|_{L^2(\Omega)}$$

(approaches 0 as $\lambda \rightarrow \infty$)

NUMERICAL APPROXIMATION

- the **efficient** numerical solution of fractional differential equations is an **open problem**
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truncation error + numerical error

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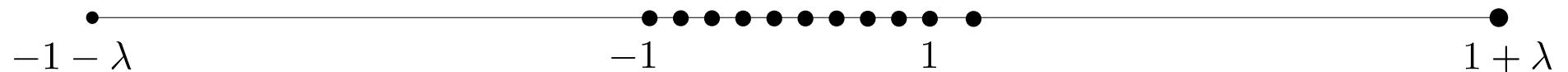
truncation error + numerical error

analysis of **Asymptotically Compatible**
schemes [Du, Tian] tells the whole story

NUMERICAL APPROXIMATION

computational domain

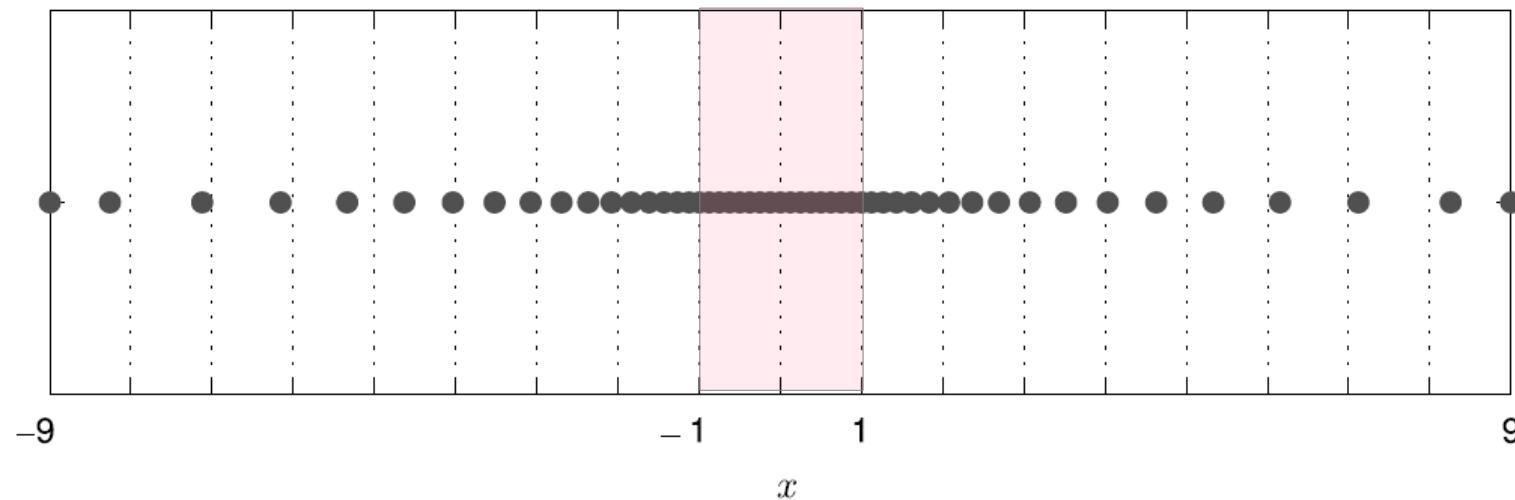
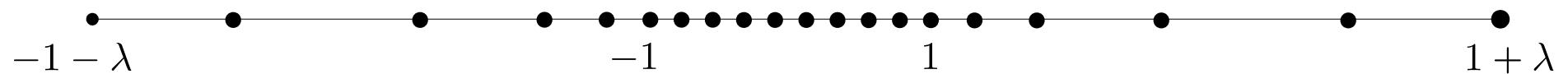
$$\Omega = (-1, 1), \Omega_{\mathcal{I}} = (-1 - \lambda, -1) \cup (1, 1 + \lambda) \Rightarrow \Omega \cup \Omega_{\mathcal{I}} = (-1 - \lambda, 1 + \lambda)$$



NUMERICAL APPROXIMATION

computational domain

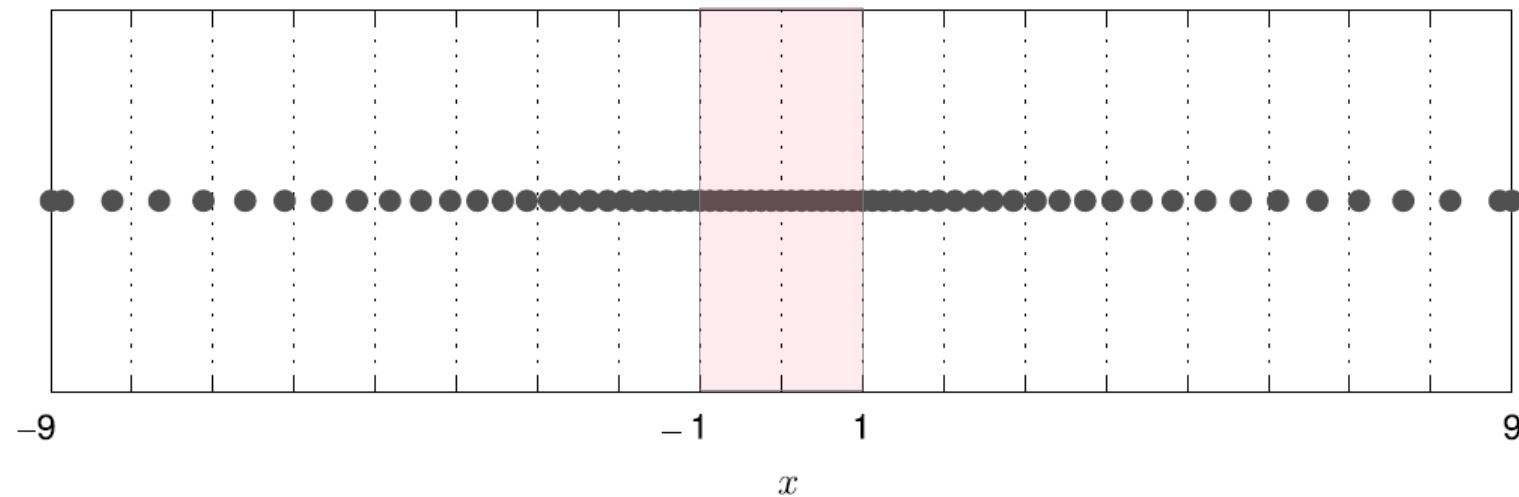
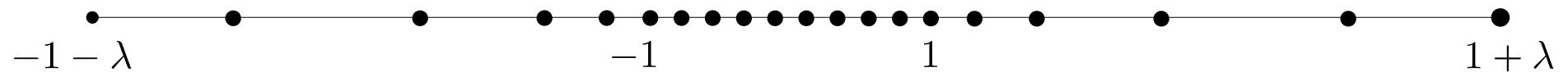
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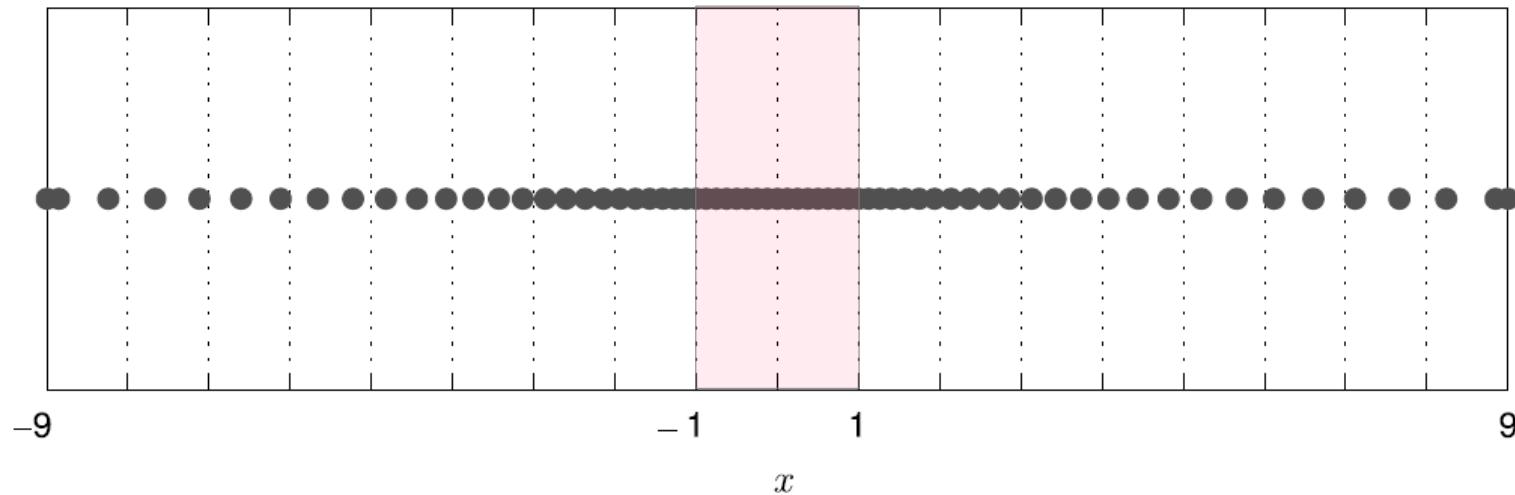
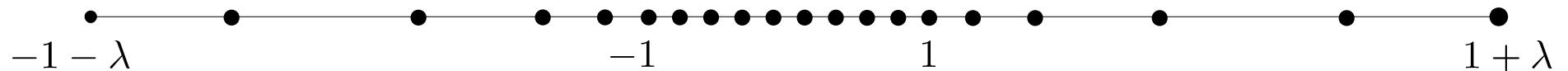
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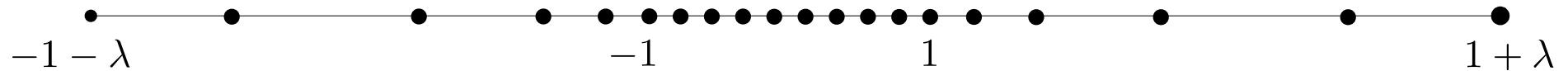


note: it affects the accuracy of the quadrature!

NUMERICAL APPROXIMATION

computational domain

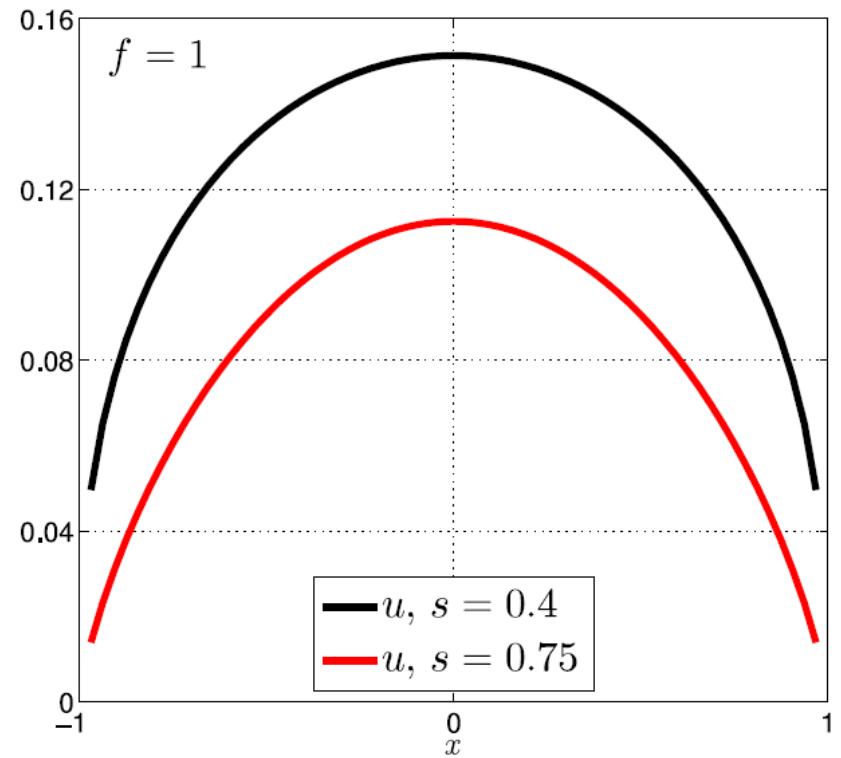
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compare

$$\begin{cases} -\mathcal{L}u = f & \text{in } \Omega \\ u = 0 & \text{in } \mathbb{R}^n \setminus \Omega \end{cases} \quad \begin{cases} -\tilde{\mathcal{L}}u = f & \text{in } \Omega \\ u = 0 & \text{in } \Omega_{\mathcal{I}} \end{cases}$$

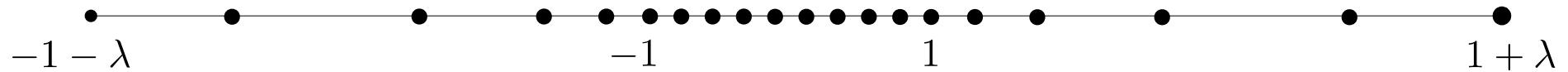
$$f = \{1, x\} \text{ and } s = 0.75$$



NUMERICAL APPROXIMATION

computational domain

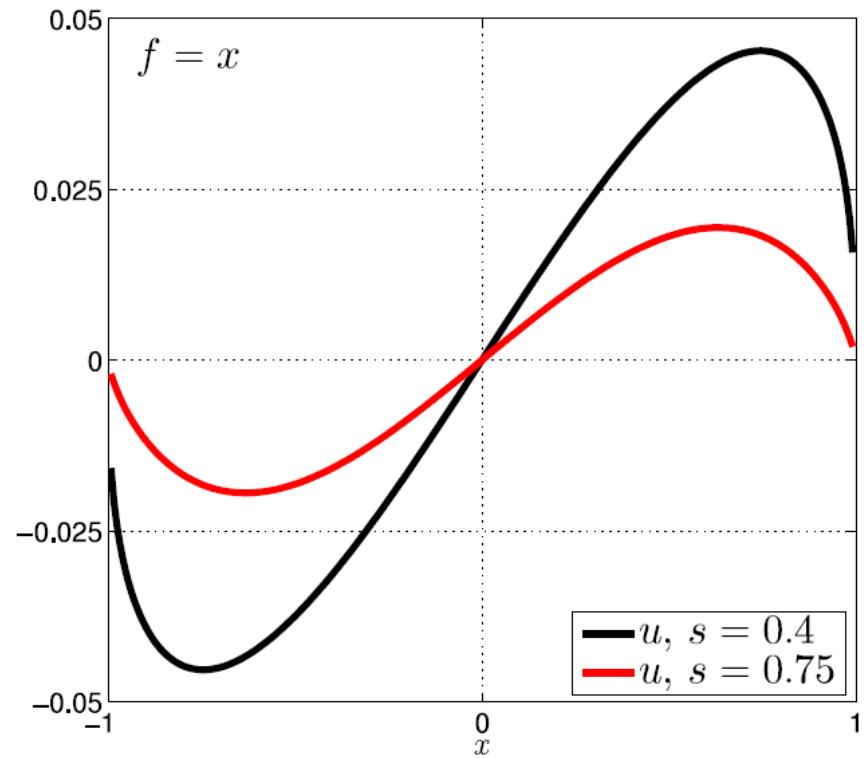
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NUMERICAL APPROXIMATION

convergence: $\tilde{u}_N \rightarrow u$, $s = 0.75$, $\|u - \tilde{u}_N\|_{H^s(\Omega \cup \Omega_{\mathcal{I}})} \cong O(\lambda^{-2s}) = O(\lambda^{-1.5})$

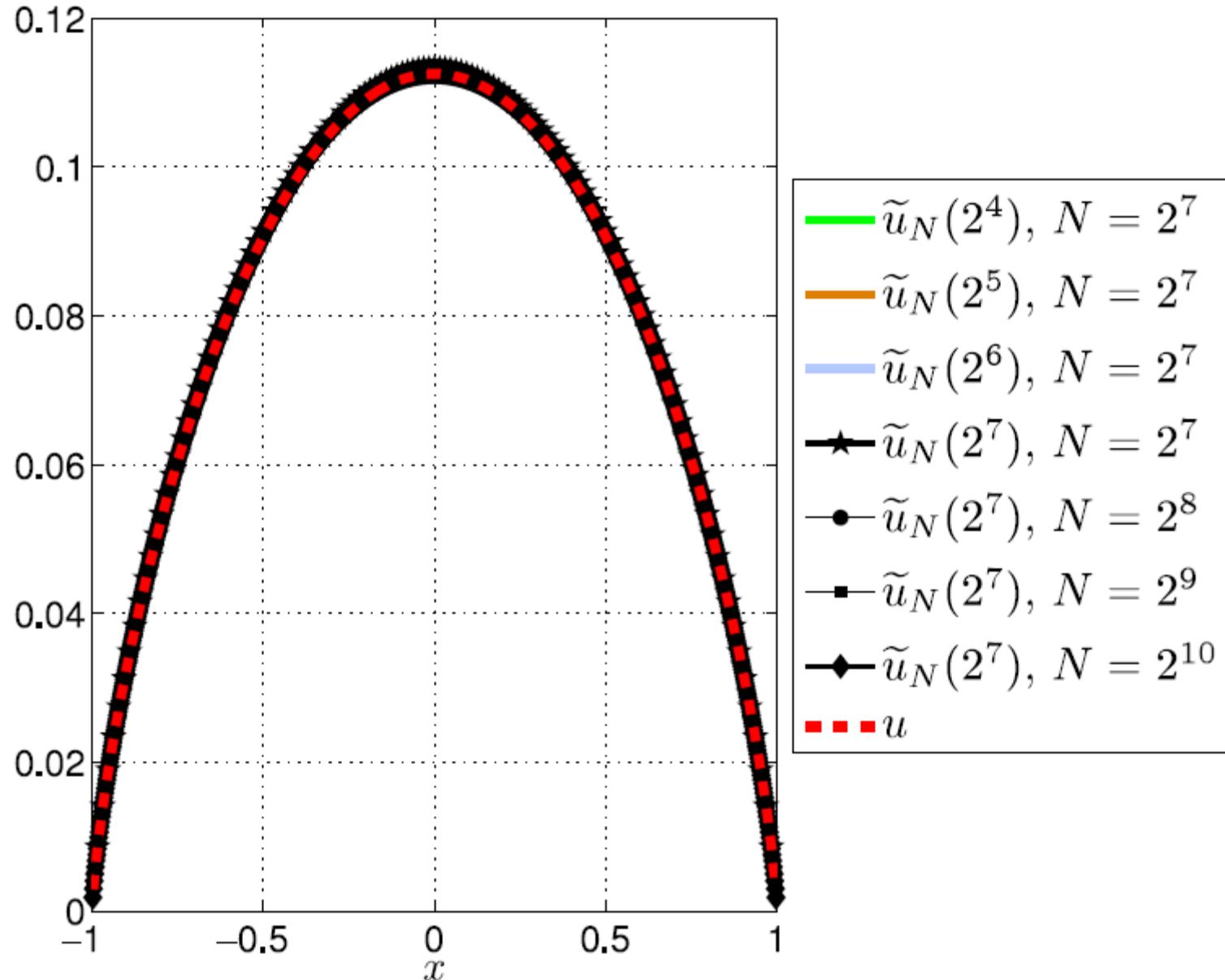
	$f = 1$		$f = x$		$f = 1$		$f = x$	
λ	$\ e\ _{H^s}$	rate	$\ e\ _{H^s}$	rate	$\ e\ _{L^2(\Omega)}$	rate	$\ e\ _{L^2(\Omega)}$	rate
2^3	1.11e-02	-	3.37e-03	-	1.12e-02	-	3.47e-03	-
2^4	3.90e-03	1.51	1.19e-03	1.50	3.92e-03	1.51	1.22e-03	1.50
2^5	1.37e-03	1.51	4.19e-04	1.50	1.38e-03	1.51	4.32e-04	1.50
2^6	4.83e-04	1.51	1.48e-04	1.51	4.87e-04	1.51	1.52e-04	1.51
2^7	1.69e-04	1.52	5.16e-05	1.51	1.70e-04	1.52	5.32e-05	1.51


 H^s

 L^2

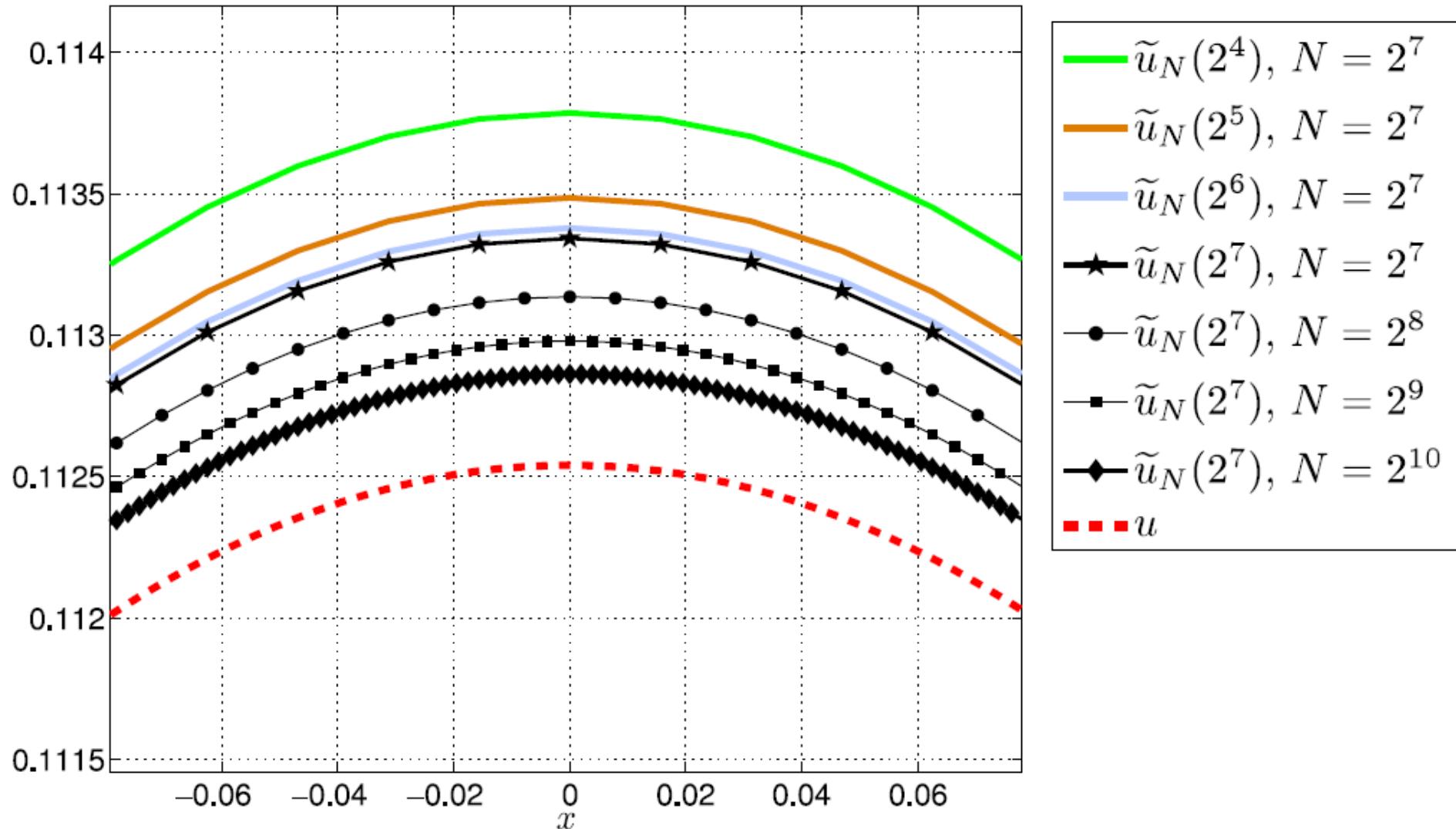
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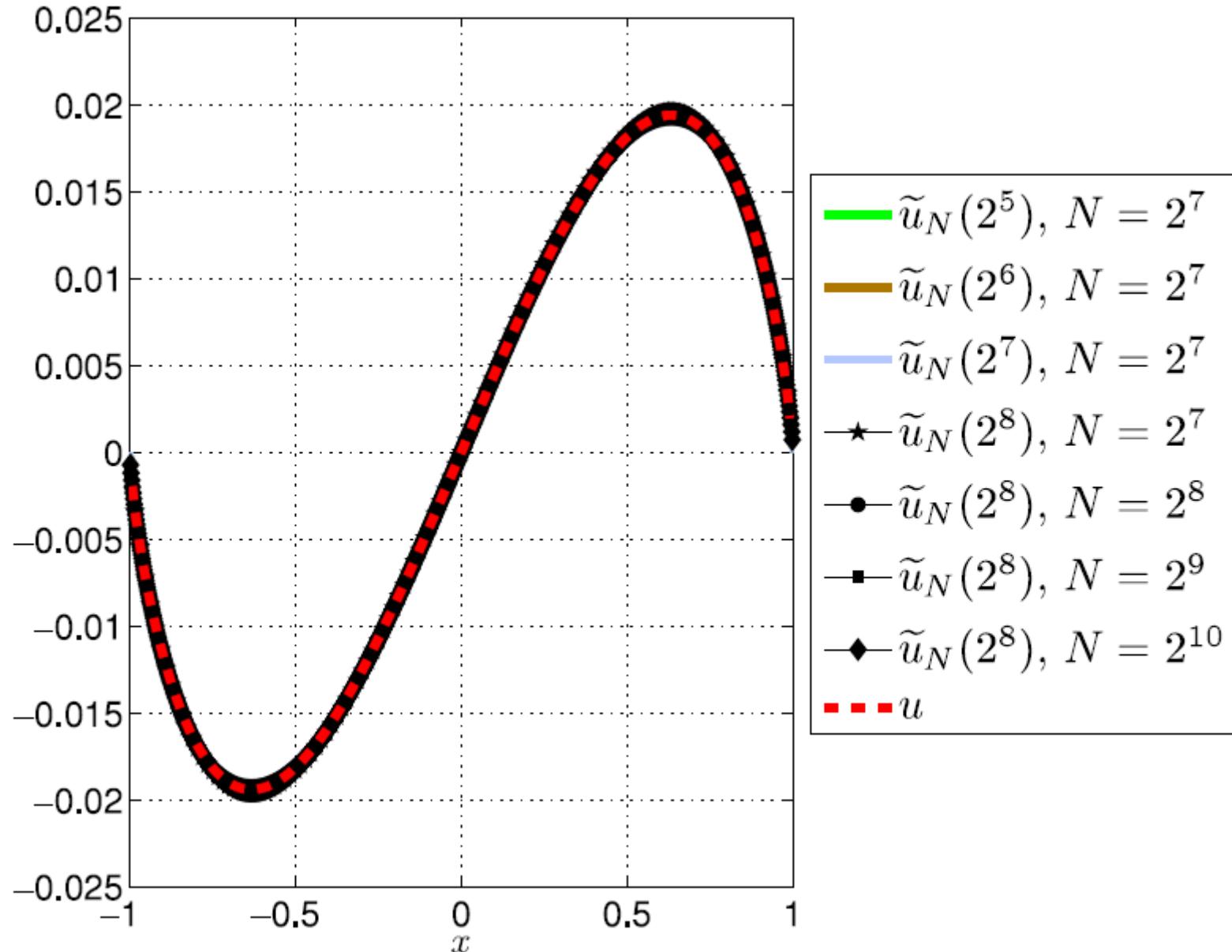
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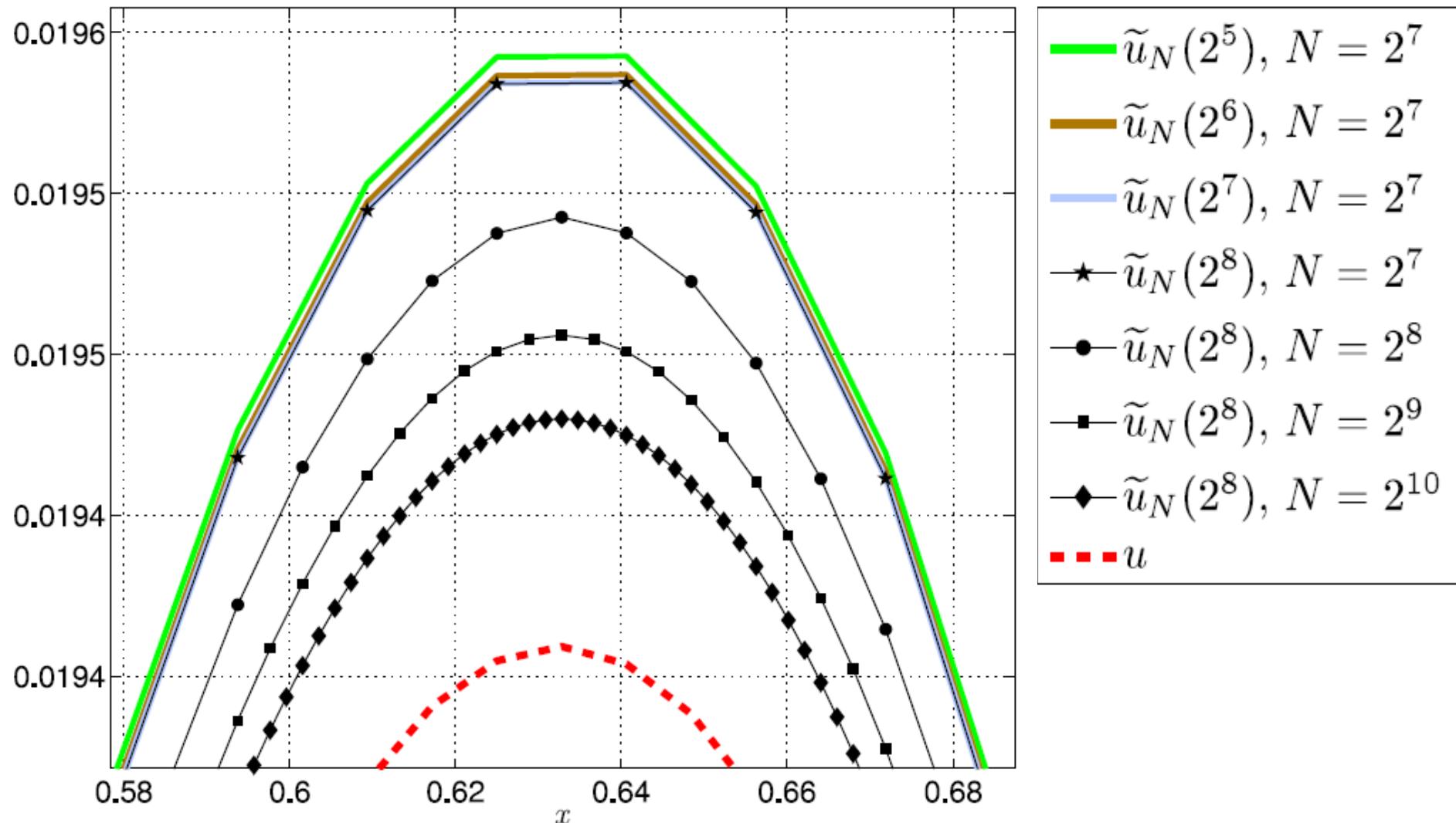
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NONLOCAL CONVECTION-DIFFUSION

– MD, Q. Du, M. Gunzburger, R. Lehoucq, Nonlocal convection-diffusion problems on bounded domains and finite-range jump processes, *Computational Methods in Applied Mathematics*, 29, 2017

question 1: how to obtain this form??

$$\mathcal{L}u(\mathbf{x}) = \int_{\mathbb{R}^n} (u(\mathbf{y})\gamma(\mathbf{y}, \mathbf{x}) - u(\mathbf{x})\gamma(\mathbf{x}, \mathbf{y})) d\mathbf{y}$$

the operator $\mathcal{D}(k\mathcal{D}^*\cdot)$ is not enough

NONLOCAL VECTOR CALCULUS – CONVECTION

- divergence of ν : $\mathcal{D}_i(\nu)(\mathbf{x}) = \int_{\mathbb{R}^n} (\nu(\mathbf{x}, \mathbf{y}) + \nu(\mathbf{y}, \mathbf{x})) \cdot \alpha_i(\mathbf{x}, \mathbf{y}) d\mathbf{y}$
- gradient of u : $-\mathcal{D}_i^*(u)(\mathbf{x}, \mathbf{y}) = (u(\mathbf{y}) - u(\mathbf{x})) \alpha_i(\mathbf{x}, \mathbf{y})$

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- nonlocal convection diffusion of u : $i = d$ (diffusion), $i = c$ (convection)

$$\mathcal{L}u(\mathbf{x}) = -\mathcal{D}_d(\Theta \mathcal{D}_d^* u)(\mathbf{x}) + \mathcal{D}_c(\mu u)(\mathbf{x})$$

$$\mathcal{L}u(\mathbf{x}) = 2 \int_{\mathbb{R}^n} (u(\mathbf{y}) - u(\mathbf{x})) \boldsymbol{\alpha}_d \cdot (\Theta \boldsymbol{\alpha}_d) d\mathbf{y} + \int_{\mathbb{R}^n} (u(\mathbf{y}) + u(\mathbf{x})) \boldsymbol{\mu} \cdot \boldsymbol{\alpha}_c d\mathbf{y}$$

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note: $\mathcal{D}_c(\mu u) = u \mathcal{D}_c \boldsymbol{\mu} - \int_{\mathbb{R}^n} \boldsymbol{\mu} \mathcal{D}_c^* u d\mathbf{y}$

$$\nabla \cdot (\mathbf{v} u) = u \nabla \cdot \mathbf{v} + \mathbf{v} \cdot \nabla u$$

NONLOCAL CONVECTION DIFFUSION PROBLEMS

strong form

$$\begin{cases} -\mathcal{L}u = g & \text{in } \Omega \\ u = 0 & \text{in } \Omega_{\mathcal{I}} \end{cases} \quad \mathcal{L}u = -\mathcal{D}_d(\boldsymbol{\Theta}\mathcal{D}_d^*u) + \mathcal{D}_c(\boldsymbol{\mu}u)$$

weak form

$$\int_{\Omega \cup \Omega_{\mathcal{I}}} \int_{\Omega \cup \Omega_{\mathcal{I}}} \mathcal{D}_d^*(u)(\mathbf{x}, \mathbf{y}) \cdot (\boldsymbol{\Theta}\mathcal{D}_d^*v)(\mathbf{x}, \mathbf{y}) d\mathbf{y} d\mathbf{x} - \int_{\Omega} \mathcal{D}_c(\boldsymbol{\mu}u)(\mathbf{x}) v(\mathbf{x}) d\mathbf{x} = \int_{\Omega} g(\mathbf{x}) v(\mathbf{x}) d\mathbf{x}$$

or, equivalently $a(u, v) = G(v)$

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THEOREM 1 [Lax-Milgram]

IF 1. for θ_i : singular values of Θ , $\exists \underline{\vartheta}, \bar{\vartheta} > 0$ s.t.

$$0 < \underline{\vartheta} \leq \inf_{\mathbf{x} \in \mathbb{R}^n} (\min_i \theta_i) \text{ and } \sup_{\mathbf{x} \in \mathbb{R}^n} (\max_i \theta_i) \leq \bar{\vartheta} < \infty$$

2. μ s.t. $C_p^2 \|\mathcal{D}_c \mu\|_{\infty} \leq 2\underline{\vartheta}$, $\|\mu\|_{\infty} \leq \bar{\mu}$

THEN $a(u, v) = G(v) \quad \forall v \in V_d^0$ is well-posed and its solution u^* is s.t.

$$|||u^*|||_d \leq C \|g\|_{V_d'}$$

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THEOREM 2 [Lax-Milgram]

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2. μ s.t. $\|\mu\|_{\infty} \leq \bar{\mu}$

3. for $\bar{m} = \sup_{\mathbf{x} \in \mathbb{R}^n} (\max_i m_i)$, m_i : eigenvalues of $\mu \mu^T$

$$\underline{\vartheta}/\bar{m} \leq C_p C_{\lambda}$$

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NONLOCAL CONVECTION DIFFUSION PROBLEMS

note!

some non-symmetric fractional differential operators **do satisfy** the assumptions

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NONLOCAL CONVECTION DIFFUSION PROBLEMS

THEOREM 3 [Fredholm alternative]

let $\mu = \bar{\mu} + \hat{C}\hat{\mu}$ s.t. $\hat{C}\hat{\mu}$ is a perturbation that compromises the coercivity of $a(\cdot, \cdot)$

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IF 1. $\left\| \int_{\Omega \cup \Omega_{\mathcal{I}}} \hat{\mu}(\mathbf{x}, \mathbf{y}) \cdot \alpha_c(\mathbf{x}, \mathbf{y}) d\mathbf{y} \right\|_{\infty} < \infty$

2. $\left\| \int_{\Omega \cup \Omega_{\mathcal{I}}} (\hat{\mu}(\mathbf{x}, \mathbf{y}) \cdot \alpha_c(\mathbf{x}, \mathbf{y}))^2 d\mathbf{y} \right\|_{\infty} < \infty$

THEN there exists a countable set $\mathcal{S} = \{1/k_j\}$, with $k_j \neq 0$ such that

$$a(u, v) = G(v) \quad \forall v \in V_c$$

is **well-posed** for all $g \in V'_c$ if and only if $\hat{C} \notin \mathcal{S}$.

TIME-DEPENDENT PROBLEMS

strong form

$$\begin{cases} u_t - \mathcal{L}u = g & \mathbf{x} \in \Omega, t \in (0, T] \\ u(\mathbf{x}, t) = 0 & \mathbf{x} \in \Omega_{\mathcal{I}}, t \in (0, T] \\ u(\mathbf{x}, 0) = u_0(\mathbf{x}) & \mathbf{x} \in \Omega \end{cases}$$

$$u \in L^2(0, T; V_d^0) = \{v(\cdot, t) \in V_d^0 : |||v(\cdot, t)|||_d \in L^2(0, T)\}$$

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weak form

$$\int_{\Omega} u_t v \, d\mathbf{x} + \int_{\Omega \cup \Omega_{\mathcal{I}}} \int_{\Omega \cup \Omega_{\mathcal{I}}} \mathcal{D}_d^* u \cdot (\boldsymbol{\Theta} \mathcal{D}_d^* v) \, d\mathbf{y} \, d\mathbf{x} - \int_{\Omega} \mathcal{D}_c(\boldsymbol{\mu} u) v \, d\mathbf{x} = \int_{\Omega} g v \, d\mathbf{x}.$$

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THEOREM **IF** $\|\mathcal{D}_c \boldsymbol{\mu}\|_{\infty} < \infty$

THEN $(u_t, v)_{\Omega} + a(u, v) = G(v)$ has a unique solution u^*

APPLICATION: MARKOV PROCESSES

master equation of a Markov process

assumptions: X_t : jump process conditioned on $X_0 \in \Omega$

X_t is absorbed at any time t for which $X_t \in \Omega_{\mathcal{I}}$

$g = 0$ and $u_0(\mathbf{x})$: non-negative initial condition s.t. $\int_{\Omega} u_0(\mathbf{x}) d\mathbf{x} = 1$

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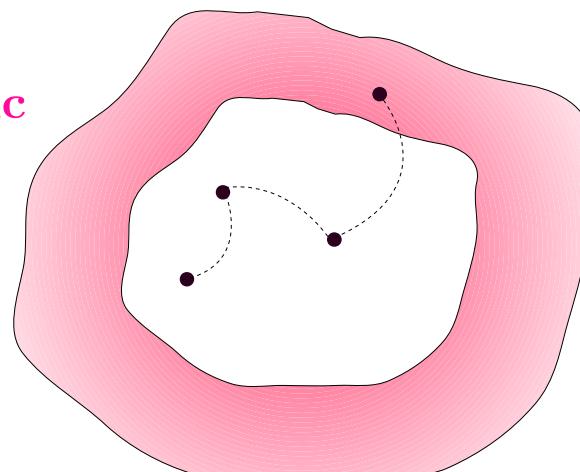
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X_t is a **finite range non-symmetric**
Markov jump process

1. γ is localized
2. γ is non-symmetric



EXPECTED EXIT TIME

Definition: first exit time of X_t from Ω : $\tau := \inf\{t > 0, X_t \in \Omega_{\mathcal{I}} \mid X_0 \in \Omega\}$,

probability distribution $F_{\tau}(t) = 1 - \int_{\Omega} u(\mathbf{x}, t) d\mathbf{x}$.

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Theorem If $u_0(\mathbf{x}) : \Omega \rightarrow [0, \infty)$, $u_0 \in L^2(\Omega)$ and $\int_{\Omega} u_0(\mathbf{x}) d\mathbf{x} = 1$ then

$\mathbb{E}(\tau)$ is **finite**: $\mathbb{E}(\tau) \leq C_{\tau} \|u_0\|_{L^2(\Omega)}^2$,

SPECIAL CASES OF THE NONLOCAL OPERATOR

note: \mathcal{L} is a **generator** of a Lévy or Lévy–type stochastic process

generator of a Lévy process: for a Lévy measure ϕ

$$\mathcal{G}f(\mathbf{x}) = \int_{\mathbb{R}^n} (f(\mathbf{x} - \mathbf{y}) - f(\mathbf{x}) + \mathbf{y} \cdot \nabla f(\mathbf{x}) \mathbf{1}(\|\mathbf{y}\| \leq R)) \phi(d\mathbf{y}), \quad R < \infty, \quad \mathbf{x} \in \mathbb{R}^n.$$

$$\text{if } \phi(d\mathbf{y}) = \phi(\mathbf{y}) d\mathbf{y} \quad \Rightarrow \quad \mathcal{G}f(\mathbf{x}) = \int_{\mathbb{R}^n} (f(\mathbf{x} - \mathbf{y}) - f(\mathbf{x})) \phi(\mathbf{y}) d\mathbf{y} + \mathbf{d} \cdot \nabla f(\mathbf{x}),$$

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SPECIAL CASES OF THE NONLOCAL OPERATOR

note: \mathcal{L} is a **generator** of a Lévy or Lévy–type stochastic process

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CURRENT AND FUTURE WORK

Natural follow-up work

develop an even more general theory that includes a larger class of operators

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Current work even if truncated, the domain is still **huge**

more efficient FEM for nonlocal/fractional operators: a new concept of neighborhoods

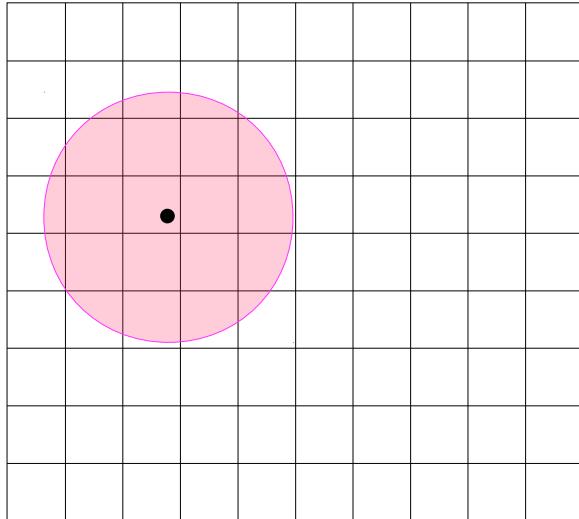
with C. Vollman, V. Schultz (U. Trier, Germany), and M. Gunzburger (FSU)

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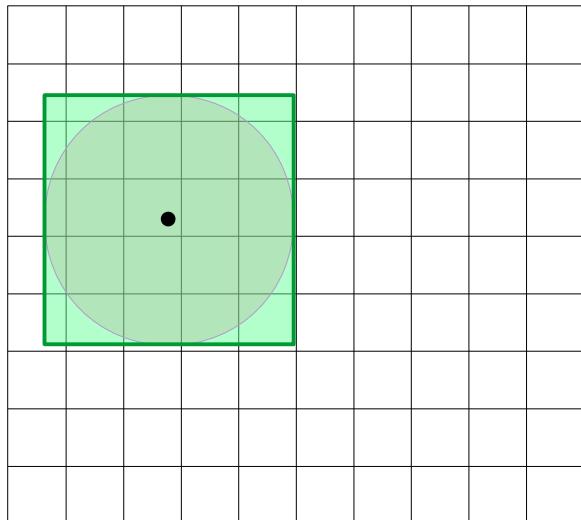


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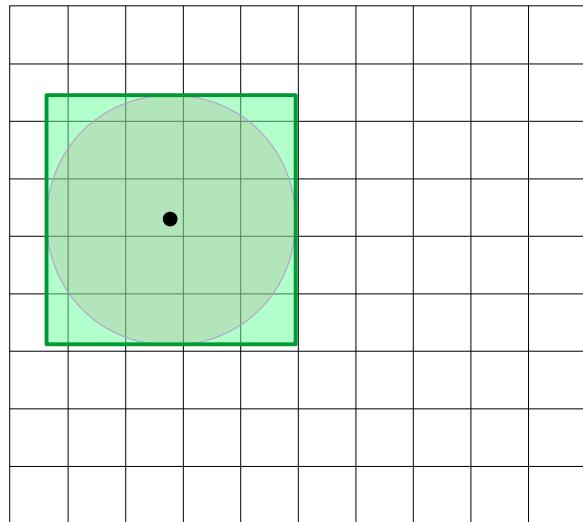
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- ⇒ much easier re-triangulation!

Important questions

0. are the nonlocal problems still well-posed?
1. do we recover local operators as $\varepsilon \rightarrow 0$?
2. do we recover fractional operators as $\varepsilon \rightarrow \infty$?
3. which finite-interaction-radius applications?

DEFINITION

X_t is a **Markov jump process**

1. infinitely divisible
2. $X_0 = 0$
3. has stationary increments: $X_{t+s} - X_t \sim X_s$
4. has independent increments: X_t is independent of $X_{t+s} - X_t$

