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NONLOCAL MODELS with NON-STANDARD INTERACTION DOMAINS

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CCR Center for Computing Research   Sandia National Laboratories

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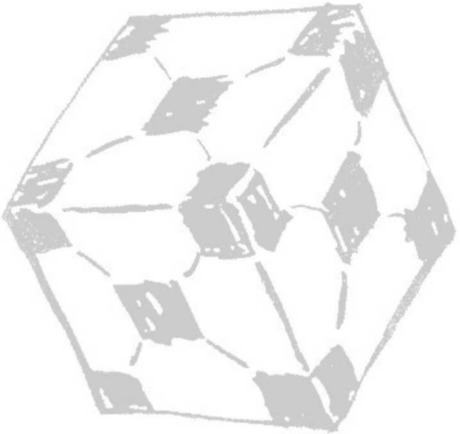

Workshop on Dynamics, Control and Numerics for Fractional PDE's

Isla Verde, Carolina, PR, December 6th 2018

CO-AUTHORS

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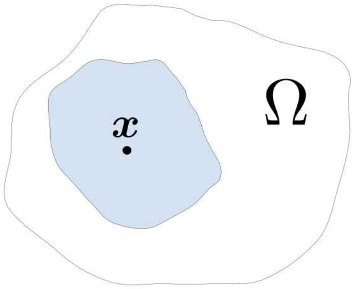
Volker Schulz, University of Trier, Germany

NONLOCAL MODELS AND NON-STANDARD NEIGHBORHOODS

NONLOCAL DIFFUSION MODELS



main feature: interactions can occur at distance, whitout contact

every point $\boldsymbol{x}$ in a domain interacts with a neighborhood

our interest: nonlocal diffusion operators

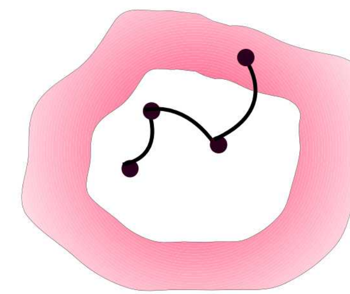
NONLOCAL DIFFUSION MODELS

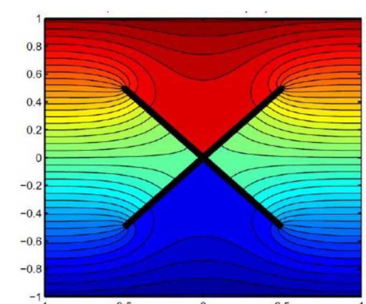
main feature: interactions can occur at distance, whitout contact

every point $\boldsymbol{x}$ in a domain interacts with a neighborhood

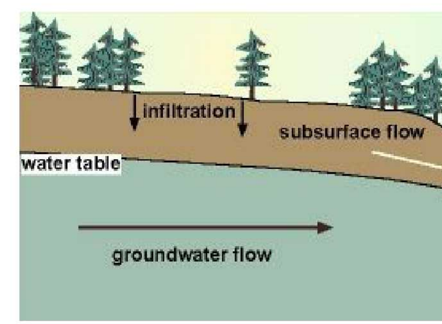
our interest: nonlocal diffusion operators

- nonlocal models for continuum mechanics
- stochastic jump processes
- nonlocal heat conduction
- subsurface flow/porous media
- image processing





Bobaru, 2012

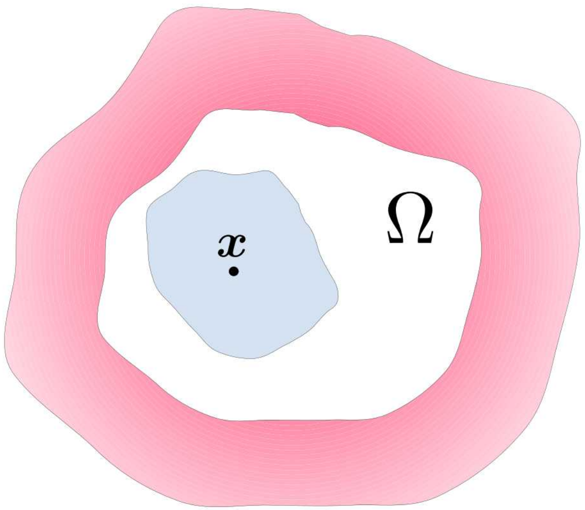


Buades, 2010

NONLOCAL DIFFUSION OPERATORS

how do they look like?

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



what do we want to solve?

$\mathcal{L}u = f$

$+$ volume contraints

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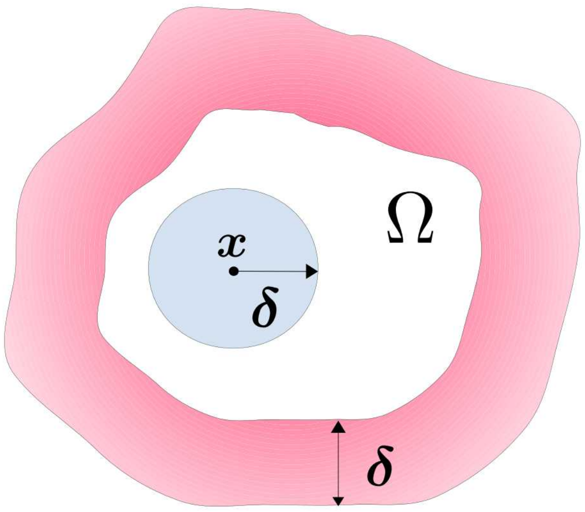
“standard” model



FACTS

facts: • a recently developed theoretical and numerical analysis allows us to study nonlocal problems **similarly** to the local (classical) counterpart

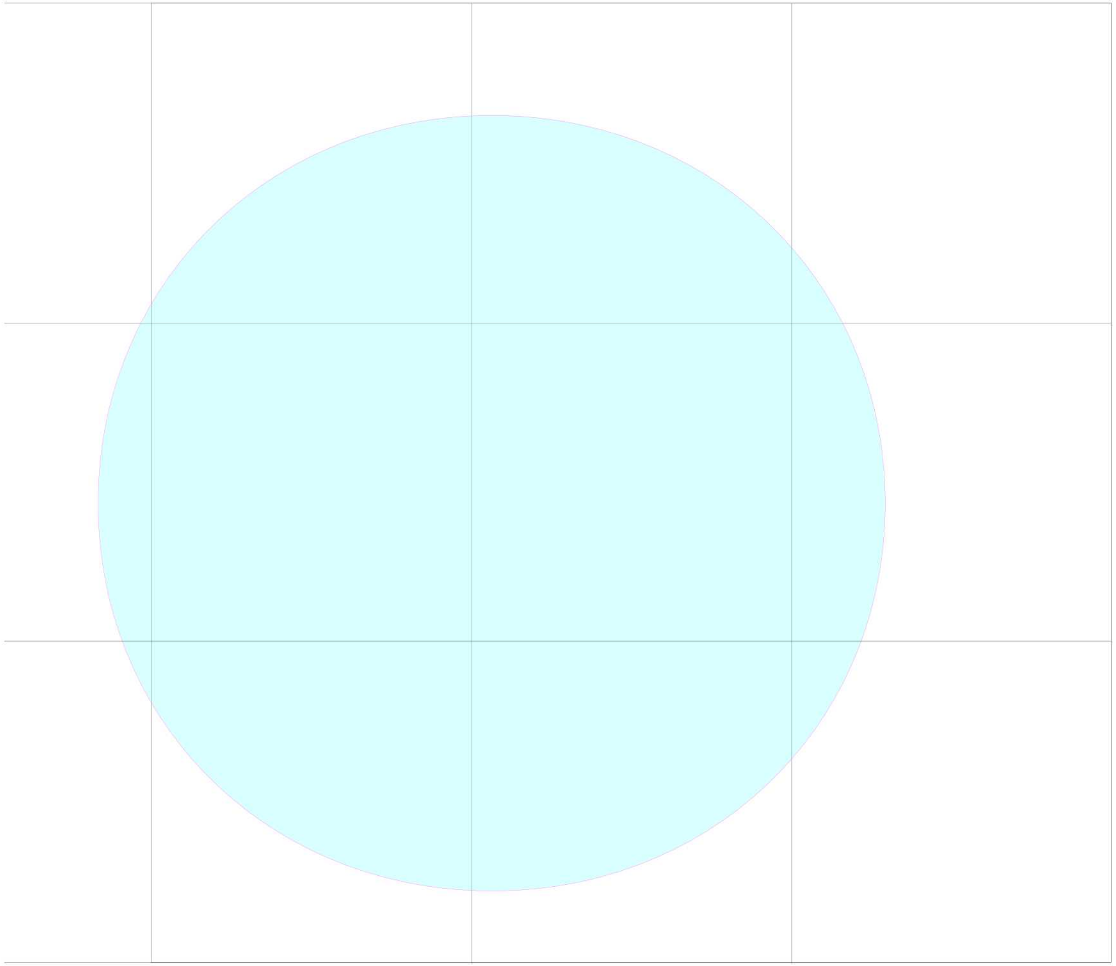
• we have **numerical convergence** results for finite element approximations

challenges: the numerical solution might be **prohibitively expensive**

BALLS AND MESHES

Challenge: matrix assembling using FEM in 2D and 3D simulations

- figure out intersections
- computing integrals of round domains



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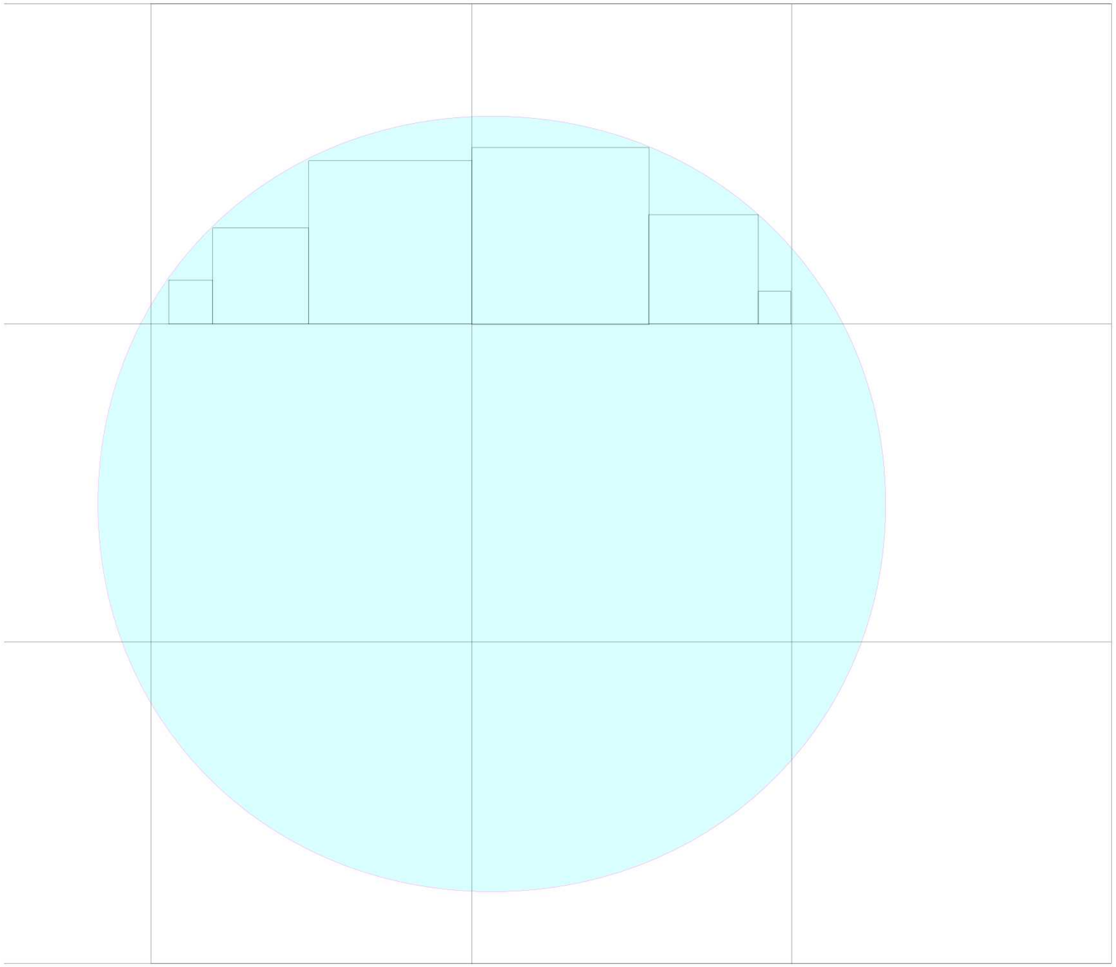

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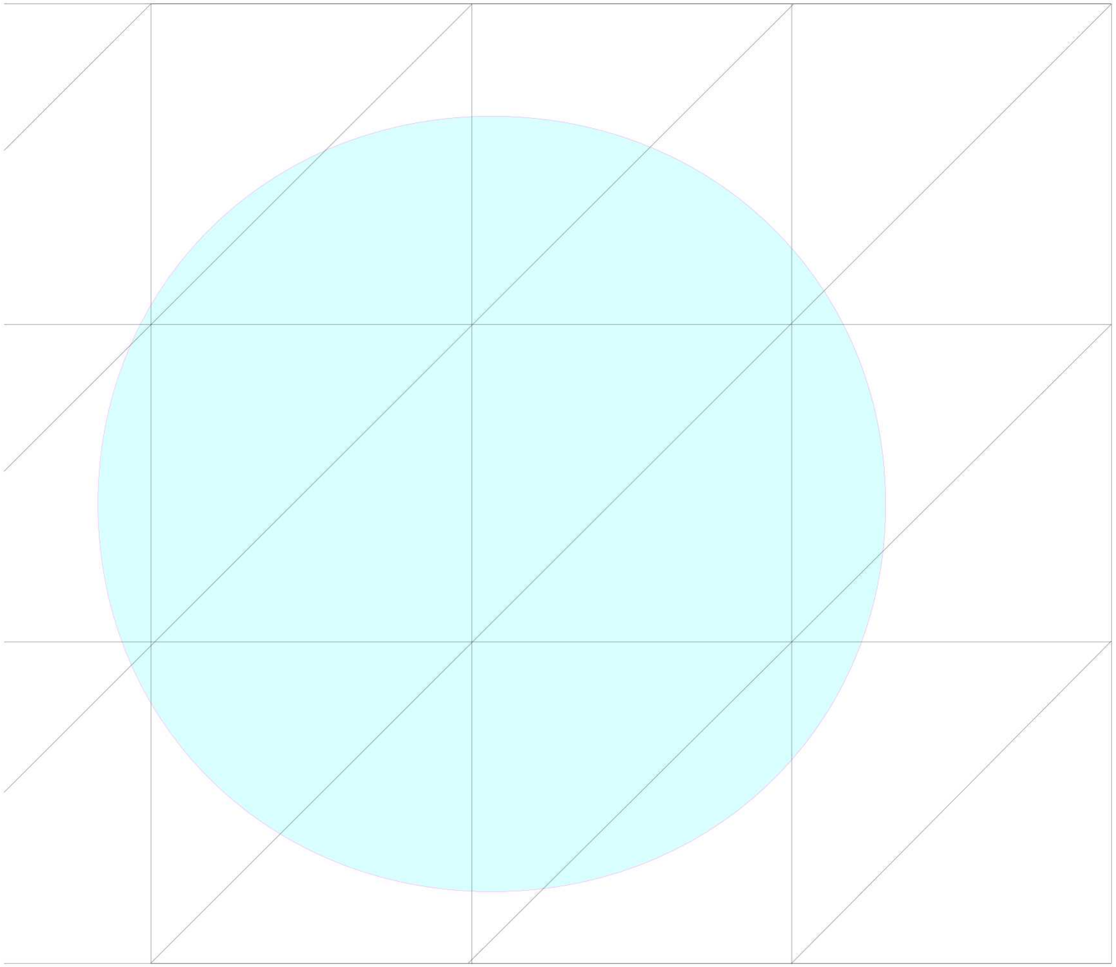

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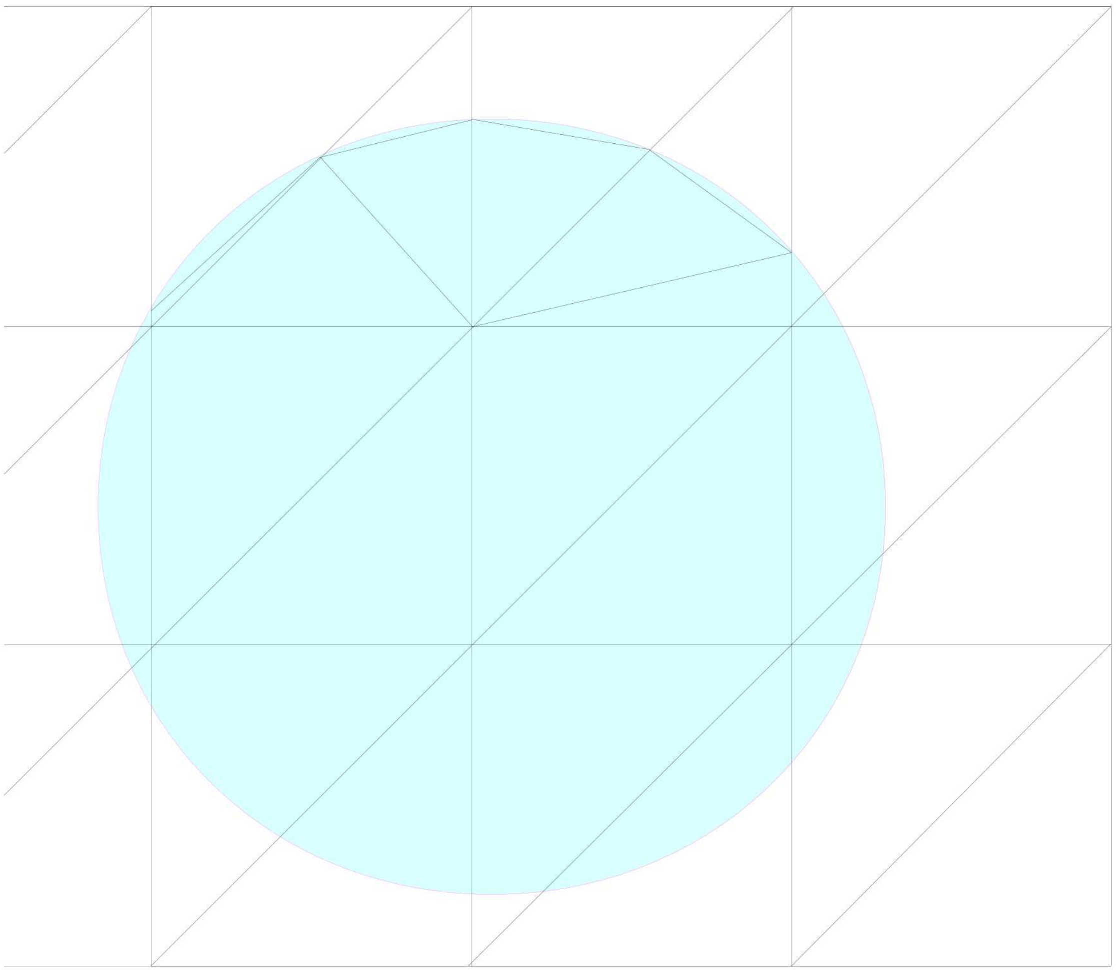

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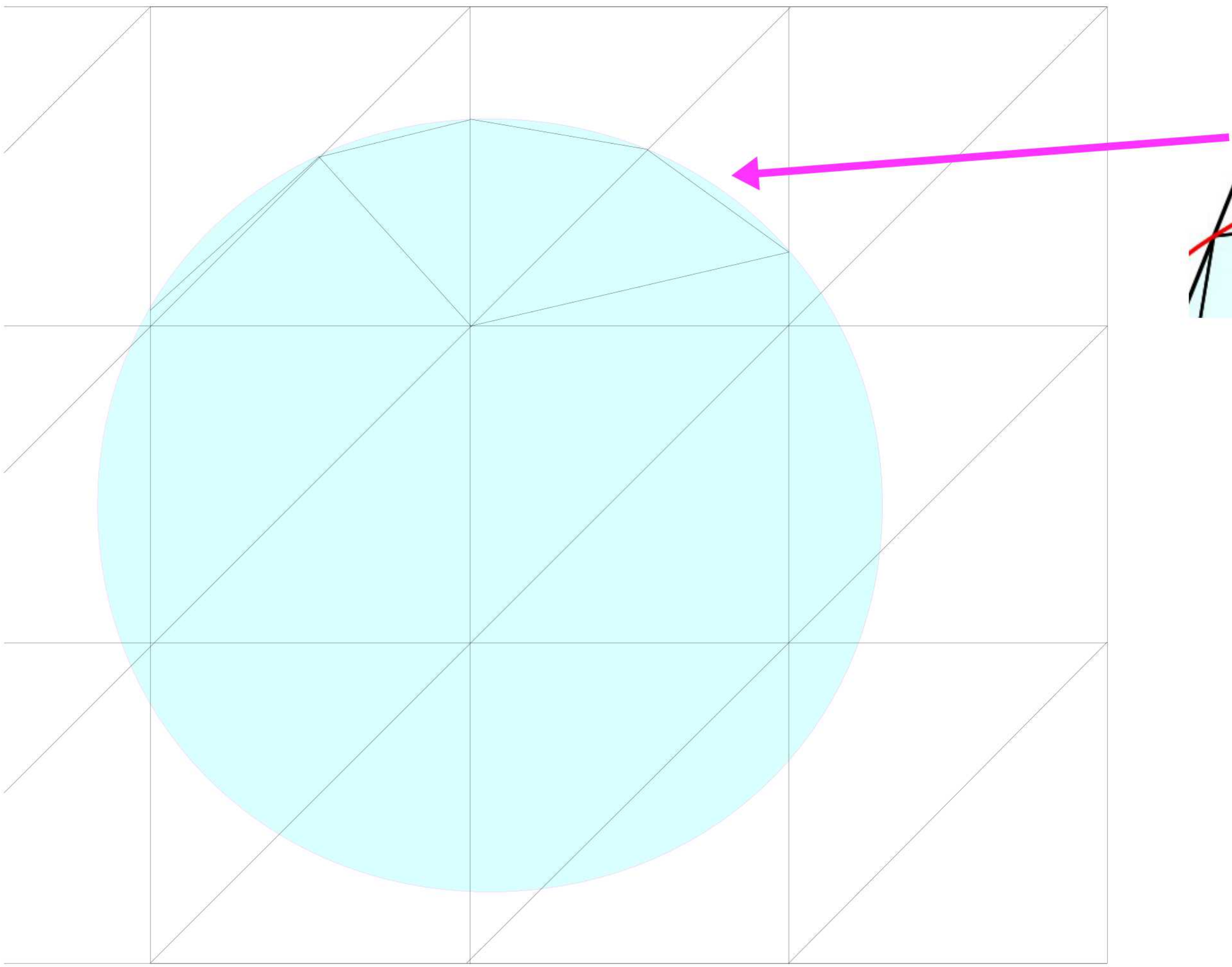

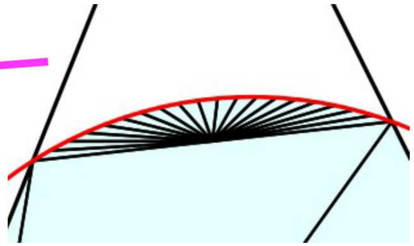

CURRENT STRATEGIES

triangles:

- triangulation of caps (Xu, Google Inc., Stoyanov, ORNL)
- approximation of the ball with a polygon (Bond, SNL)
- inclusion of partial triangles based on barycenters (Borthagaray, U. Maryland)

squares:

- oct-tree mesh refinement at the ball boundaries (Foster, UT Austin)
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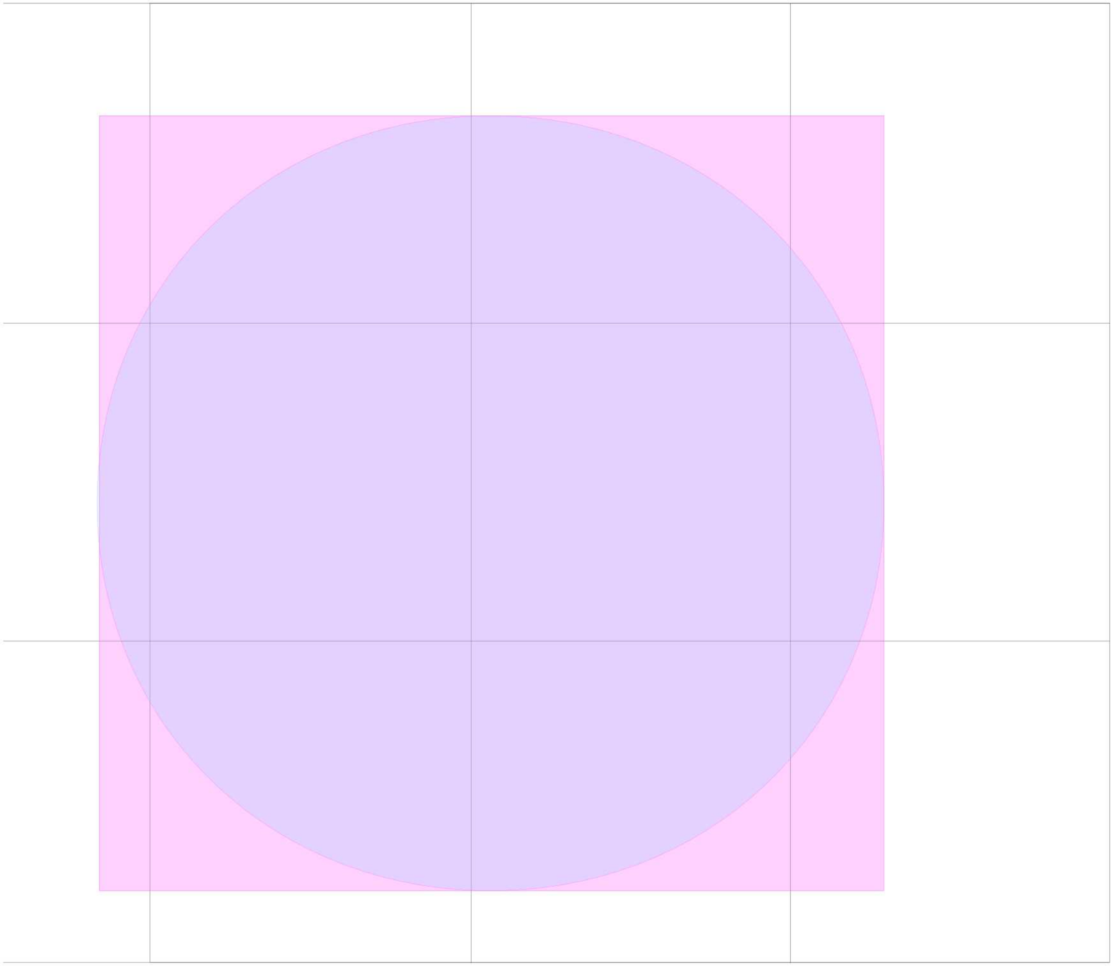
these may be unnecessary, inaccurate or inefficient!

USING DIFFERENT BALLS

what if we consider a different ball?

⇒ triangulation w/o geometry errors

⇒ much easier re-triangulation!



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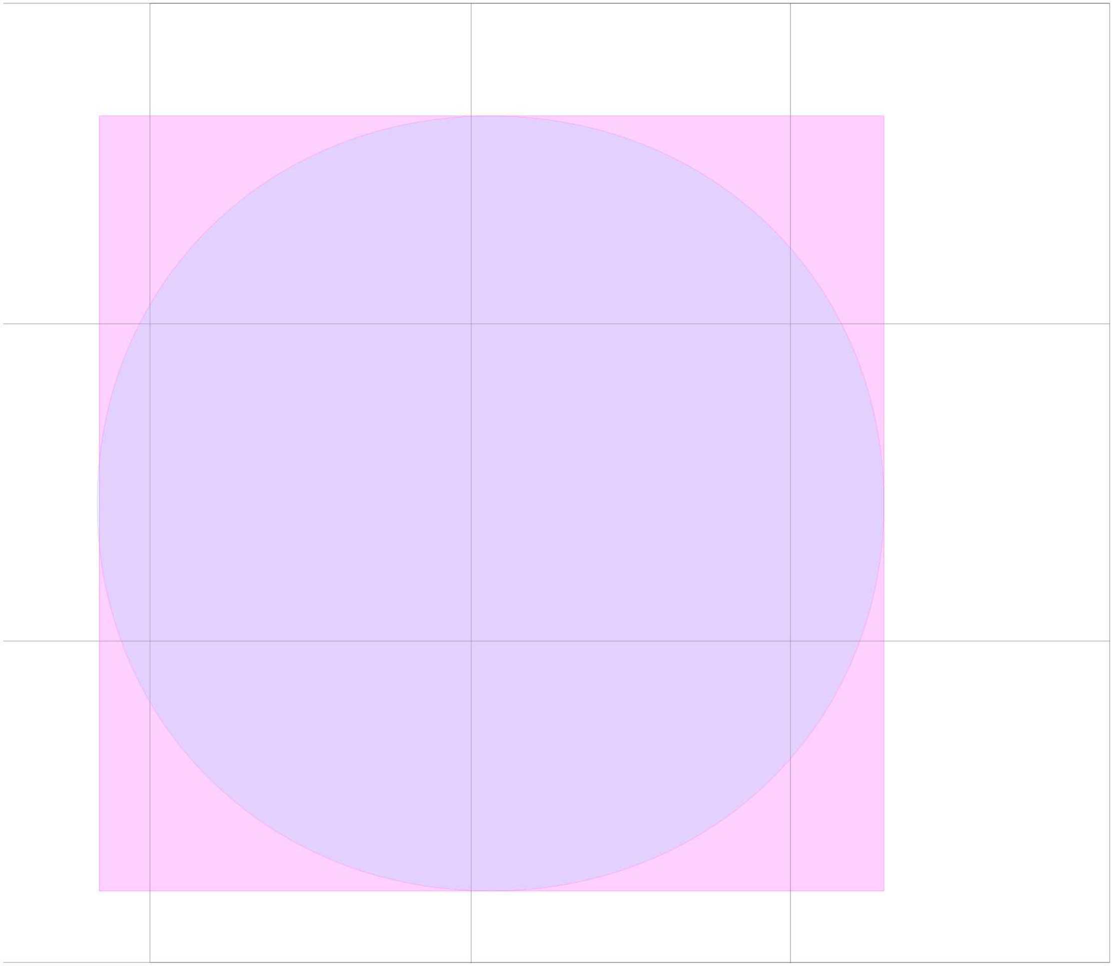

this can be a modeling choice!

- when even round balls are not required by physics
- when the nature of the problem calls for square balls

USING DIFFERENT BALLS

IMPORTANT QUESTIONS

0. does the nonlocal vector calculus still apply?

1. do we recover local operators as $\delta \to 0$?

2. do we recover fractional operators as $\delta \to \infty$?

3. are there applications for which these are *models in their own right*?

OUTLINE

- **Background:** a Nonlocal Vector Calculus

- **Non-standard neighborhoods**

    1. formulation and analysis
    2. numerical tests
    3. applications

A NONLOCAL VECTOR CALCULUS

– M. Gunzburger, R. Lehoucq, A nonlocal vector calculus with application to nonlocal boundary value problems, *Multiscale Modeling & Simulation*, 8, 1581-1598, 2010

– Q. Du, M. Gunzburger, R. Lehoucq, and K. Zhou, Analysis and approximation of nonlocal diffusion problems with volume constraints. *SIAM Review*, 54, 667–696, 2012

– Q. Du, M. Gunzburger, R. Lehoucq, and K. Zhou, A nonlocal vector calculus, nonlocal volume-constrained problems, and nonlocal balance laws. *Math. Model. Meth. Appl. Sci*, 23, 493–540, 2013

NONLOCAL VECTOR CALCULUS

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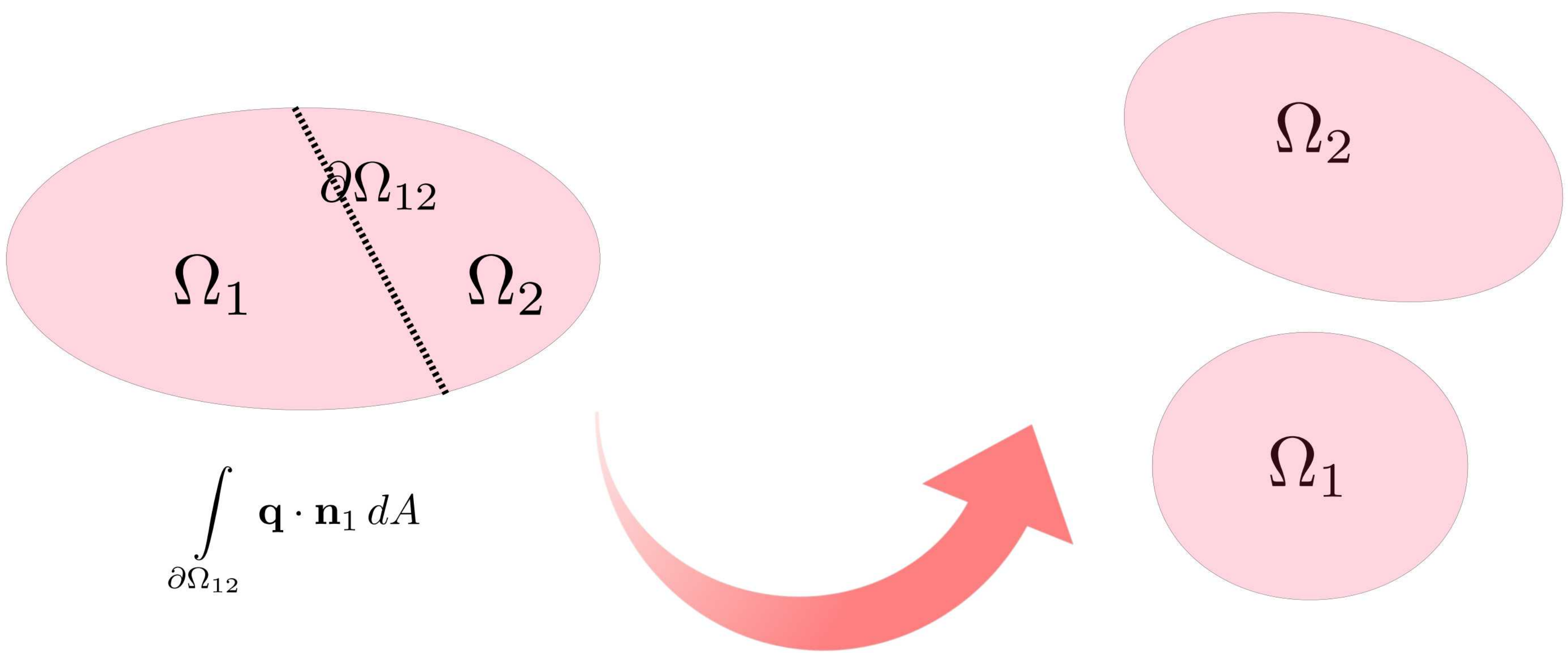

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Nonlocal operators acting on $u(\boldsymbol{x})\colon \mathbb{R}^d \to \mathbb{R}$ and $\boldsymbol{\nu}(\boldsymbol{x},\boldsymbol{y})\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$

- divergence of $\boldsymbol{\nu}$: $\mathcal{D}\big(\boldsymbol{\nu}\big)(\boldsymbol{x}) = \displaystyle\int_{\mathbb{R}^n} \big(\boldsymbol{\nu}(\boldsymbol{x},\boldsymbol{y}) + \boldsymbol{\nu}(\boldsymbol{y},\boldsymbol{x})\big) \cdot \boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y})\, d\boldsymbol{y}$
- gradient of u: $\mathcal{G}\big(u\big)(\boldsymbol{x},\boldsymbol{y}) = \big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y})$
- nonlocal diffusion of u: $\mathcal{L}u(\boldsymbol{x}) = \mathcal{D}(\mathcal{G}u(\boldsymbol{x}))$

$$\mathcal{L}u(\boldsymbol{x}) = 2\int \big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\, \boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y}) \cdot \boldsymbol{\alpha}(\boldsymbol{x},\boldsymbol{y})\, d\boldsymbol{y}$$

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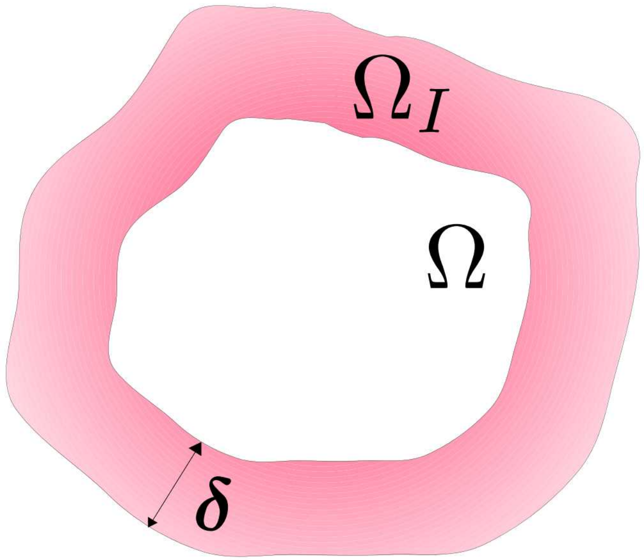
NONLOCAL VECTOR CALCULUS

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

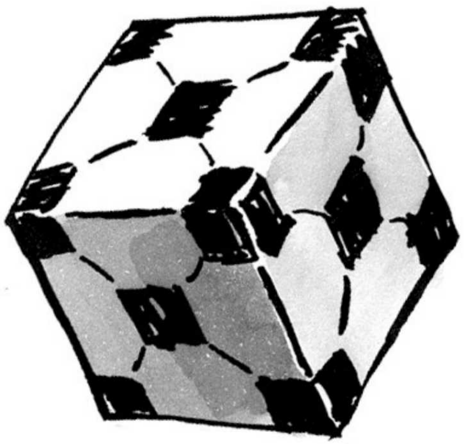
$$\Omega_I = \{\boldsymbol{y} \in \mathbb{R}^d \setminus \Omega : \ \boldsymbol{\alpha}(\boldsymbol{x}, \boldsymbol{y}) \neq 0, \ \boldsymbol{x} \in \Omega\},$$

δ: interaction length, interaction radius



A NEW CONCEPT OF BALLS

– C. Vollman, M. D'Elia, M. Gunzburger, V. Schulz, Formulation and analysis of fast discretization methods for nonlocal FEM by using non-standard nonlocal neighborhoods, *in progress*.

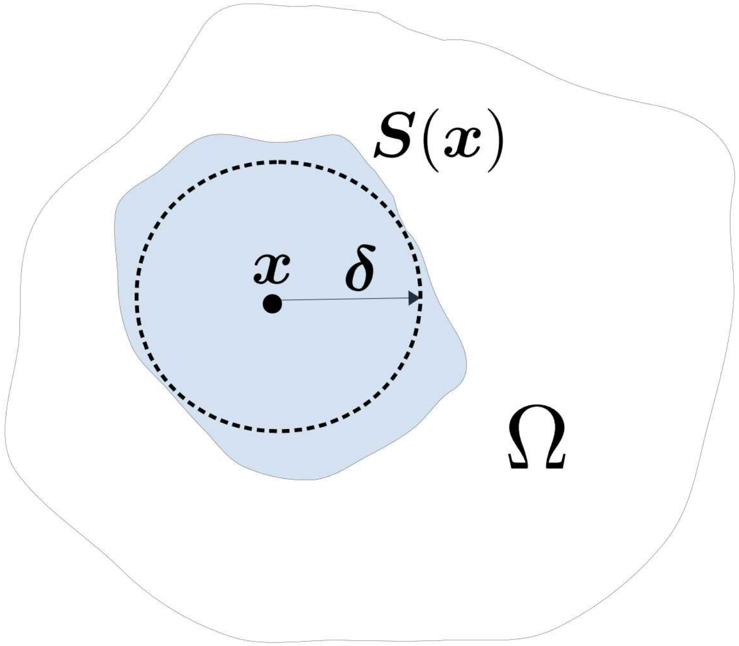


INTERACTION SETS

- **Non-degeneracy:** $\exists\, \delta > 0$ such that

  $\forall \boldsymbol{x} \in (\Omega \cup \Omega_I),\; B_{\delta,2}(\boldsymbol{x}) \subset S(\boldsymbol{x})$

  with $B_{\delta,2}(\boldsymbol{x}) := \{\boldsymbol{y} \in \mathbb{R}^n : \; \|\boldsymbol{x} - \boldsymbol{y}\|_2 < \delta\}$



- **Symmetry:** $\forall\, (\boldsymbol{x}, \boldsymbol{y}) \in (\Omega \cup \Omega_I)$

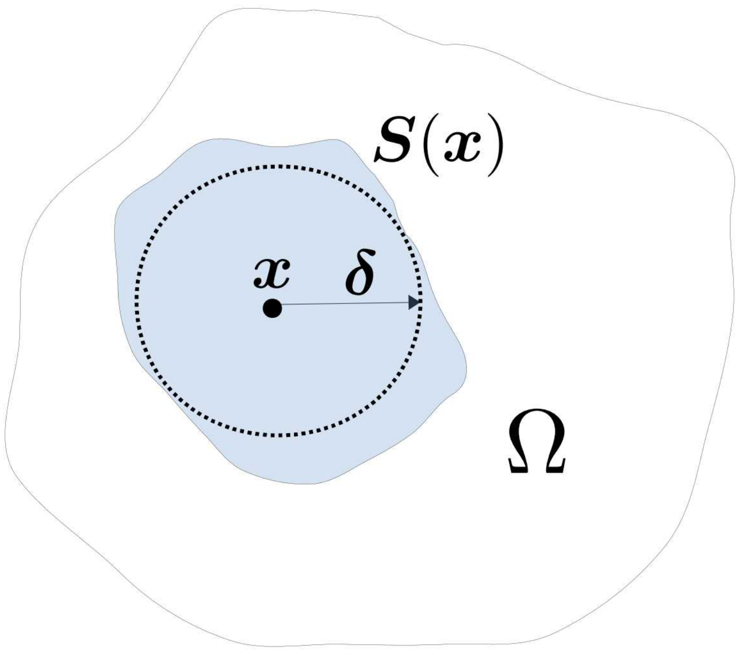
  $\boldsymbol{y} \in S(\boldsymbol{x}) \quad$ if and only if $\quad \boldsymbol{x} \in S(\boldsymbol{y})$

  $\Rightarrow (\boldsymbol{x}, \boldsymbol{y}) \mapsto \mathcal{X}_{S(\boldsymbol{x})}(\boldsymbol{y})$ is symmetric in $(\boldsymbol{x}, \boldsymbol{y})$

KERNELS

assumptions: $\exists\, \gamma_0 > 0$ s.t. $\forall\, \boldsymbol{x} \in (\Omega \cup \Omega_I)$

$$\begin{cases} \gamma(\boldsymbol{x},\boldsymbol{y}) \geq 0 & \forall\; \boldsymbol{y} \in S(\boldsymbol{x}) \\ \gamma(\boldsymbol{x},\boldsymbol{y}) \geq \gamma_0 > 0 & \forall\; \boldsymbol{y} \in B_{\delta,2}(\boldsymbol{x}) \\ \gamma(\boldsymbol{x},\boldsymbol{y}) = 0 & \forall\; \boldsymbol{y} \in \mathbb{R}^n \setminus S(\boldsymbol{x}) \end{cases}$$



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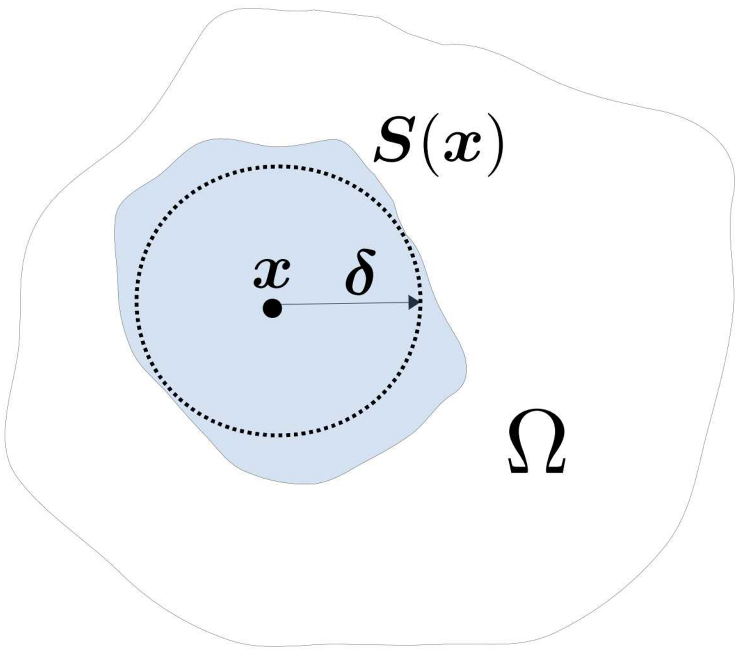
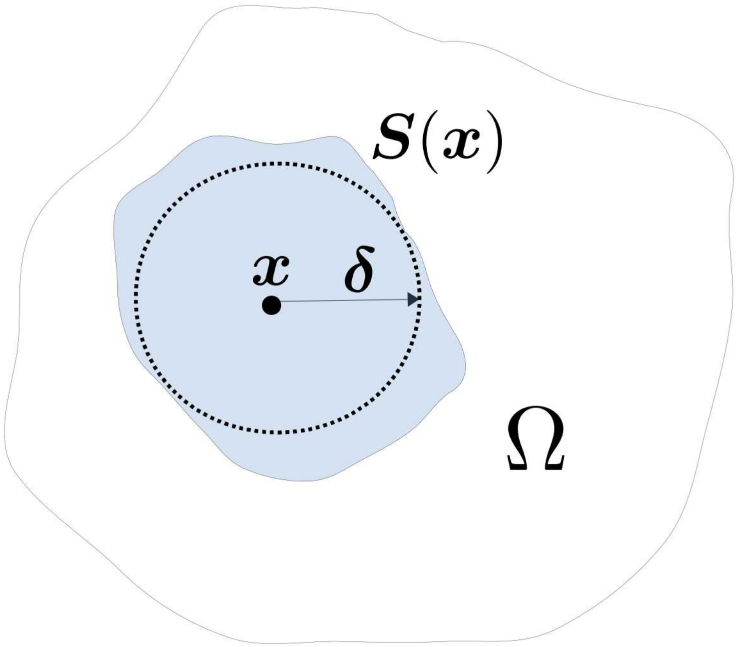


kernel expression:

$$\gamma(\boldsymbol{x},\boldsymbol{y}) = \phi(\boldsymbol{x},\boldsymbol{y})\mathcal{X}_{S(\boldsymbol{x})}(\boldsymbol{y})$$

where $\phi(\boldsymbol{x},\boldsymbol{y})$ is referred to as kernel function

KERNELS



kernel expression:

$$\gamma(\boldsymbol{x},\boldsymbol{y}) = \phi(\boldsymbol{x},\boldsymbol{y})\mathcal{X}_{S(\boldsymbol{x})}(\boldsymbol{y})$$

examples:

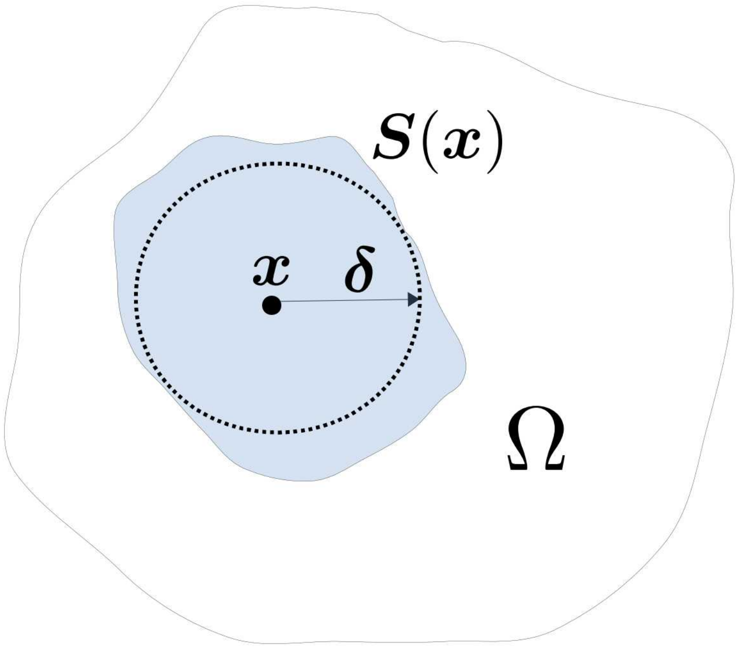
$S(\boldsymbol{x}) := \{\boldsymbol{y} \in \mathbb{R}^n \, : \, \eta(\boldsymbol{x},\boldsymbol{y}) < 0\}$ for a symmetric $\eta(\boldsymbol{x},\boldsymbol{y})$

standard interaction set: $\eta(\boldsymbol{x},\boldsymbol{y}) = \|\boldsymbol{x}-\boldsymbol{y}\|_2 - \delta$

$\Rightarrow S(\boldsymbol{x})$ is the Euclidean ball $B_{\delta,2}(\boldsymbol{x})$

δ: *horizon.*

KERNELS



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general interaction sets: $\eta(\boldsymbol{x},\boldsymbol{y}) = \|\boldsymbol{x}-\boldsymbol{y}\|_\bullet - \delta$, for an arbitrary norm $\|\cdot\|_\bullet$

$\Rightarrow S(\boldsymbol{x})$ are balls $B_{\delta,\bullet}(\boldsymbol{x}) := \{\boldsymbol{y}\in\mathbb{R}^n :\ \|\boldsymbol{x}-\boldsymbol{y}\|_\bullet < \delta\}$.

WEAK FORM AND WELL-POSEDNESS

bilinear form: $A(u,v) = \int_{\Omega\cup\Omega_I}\int_{\Omega\cup\Omega_I} (u(\boldsymbol{y})-u(\boldsymbol{x}))(v(\boldsymbol{y})-v(\boldsymbol{x}))\gamma(\boldsymbol{x},\boldsymbol{y})\,d\boldsymbol{y}d\boldsymbol{x}$

energy seminorm: $|||u||| = \sqrt{A(u,u)}$

unconstrained and constrained energy space:

$$V(\Omega\cup\Omega_I) = \{u \in L^2(\Omega\cup\Omega_I) \,:\, \|u\|_{V(\Omega\cup\Omega_I)} := |||u||| + \|u\|_{L^2(\Omega\cup\Omega_I)} < \infty\}$$

$$V_c(\Omega\cup\Omega_I) = \{u \in V(\Omega\cup\Omega_I) \,:\, u \equiv 0 \text{ a.e. on } \Omega_I\}$$

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weak form:

given $f \in V_c'(\Omega)$ *and* $g \in \widetilde{V}(\Omega_I)$, *find* $u \in V(\Omega\cup\Omega_I)$

such that $u|_{\Omega_I} = g$ *and* $A(u,v) \equiv \int_\Omega f v\,d\boldsymbol{x} \;\; \forall\, v \in V_c(\Omega\cup\Omega_I)$

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norm in V_c

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well-posed by the Riesz representation theorem

KERNELS

KERNEL 1

for $s \in (0,1)$, $\exists\, 0 < c_* \leq c^* < \infty$ s.t. for any $\boldsymbol{x} \in \Omega \subset \mathbb{R}^n$

$$c_* \leq \gamma_1(\boldsymbol{x},\boldsymbol{y}) \|\boldsymbol{y}-\boldsymbol{x}\|_2^{d+2s} \leq c^* \quad \forall\, \boldsymbol{y} \in S(\boldsymbol{x})$$

$S(\boldsymbol{x})$: any set with non-degeneracy and symmetry properties

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- the corresponding energy norm satisfies a Poincaré inequality
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$\Rightarrow \|u\|_{H^s(\Omega\cup\Omega_I)} \leq C\|f\|_{H^{-s}(\Omega\cup\Omega_I)}$

example: $\gamma_1(\boldsymbol{x},\boldsymbol{y}) = \dfrac{\sigma(\boldsymbol{x},\boldsymbol{y})}{\|\boldsymbol{y}-\boldsymbol{x}\|_2^{d+2s}}\, \mathcal{X}_{S(\boldsymbol{x})}(\boldsymbol{y})$

KERNELS

KERNEL 2

$\exists\ 0 < k_* \leq k^* < \infty$ s.t. for any $\boldsymbol{x} \in \Omega \subset \mathbb{R}^n$

$$k_* \leq \inf_{\boldsymbol{x}\in\Omega} \int_{S(\boldsymbol{x})} \gamma_2(\boldsymbol{x},\boldsymbol{y})\, d\boldsymbol{y}$$

$$\sup_{\boldsymbol{x}\in\Omega\cup\Omega_I} \int_{(\Omega\cup\Omega_I)\cap S(\boldsymbol{x})} \gamma_2^2(\boldsymbol{x},\boldsymbol{y})\, d\boldsymbol{y} \leq {k^*}^2$$

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$\exists\, 0 < k_* \leq k^* < \infty$ s.t. for any $\boldsymbol{x} \in \Omega \subset \mathbb{R}^n$

$$k_* \leq \inf_{\boldsymbol{x}\in\Omega} \int_{S(\boldsymbol{x})} \gamma_2(\boldsymbol{x},\boldsymbol{y})\, d\boldsymbol{y}$$

$$\sup_{\boldsymbol{x}\in\Omega\cup\Omega_I} \int_{(\Omega\cup\Omega_I)\cap S(\boldsymbol{x})} \gamma_2^2(\boldsymbol{x},\boldsymbol{y})\, d\boldsymbol{y} \leq k^{*2}$$

$S(\boldsymbol{x})$: any set with non-degeneracy and symmetry properties

properties

- the corresponding energy norm satisfies a Poincaré inequality
- the corresponding unconstrained and constrained energy spaces are **equivalent** to $L^2(\Omega\cup\Omega_I)$ and $L^2_c(\Omega\cup\Omega_I)$

$\Rightarrow \|u\|_{L^2(\Omega\cup\Omega_I)} \leq C\|f\|_{L^2(\Omega\cup\Omega_I)}$

CONVERGENCE TO FRACTIONAL OPERATORS

TRUNCATED FRACTIONAL KERNELS

interaction sets: balls wrt a norm $\|\cdot\|_\bullet \;\;\Rightarrow\;\; S(\boldsymbol{x}) = B_{\delta,\bullet}(\boldsymbol{x})$

assumption: $\delta \geq \text{diam}(\Omega) = \max_{\boldsymbol{x},\boldsymbol{y}\in\Omega} \|\boldsymbol{y}-\boldsymbol{x}\|_\bullet \;\;\Rightarrow\;\; \Omega \subset S(\boldsymbol{x})$ for all $\boldsymbol{x} \in \Omega$

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kernels of type 1: $\gamma(\boldsymbol{x},\boldsymbol{y}) = \dfrac{c_{n,s}}{2\|\boldsymbol{x}-\boldsymbol{y}\|_2^{n+2s}} \mathcal{X}_{B_{\delta,\bullet}(\boldsymbol{x})}(\boldsymbol{y}) \quad \text{for } 0 < s < 1$

truncated fractional Laplacian $\mathcal{L}_\bullet u(\boldsymbol{x}) = c_{n,s} \displaystyle\int_{B_{\delta,\bullet}} \frac{u(\boldsymbol{x}) - u(\boldsymbol{y})}{\|\boldsymbol{x}-\boldsymbol{y}\|_2^{n+2s}}\, d\boldsymbol{y}$

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fractional Laplacian $\mathcal{L}u = (-\Delta)^s u = c_{n,s} \displaystyle\int_{\mathbb{R}^n} \frac{u(\boldsymbol{x})-u(\boldsymbol{y})}{\|\boldsymbol{y}-\boldsymbol{x}\|_2^{n+2s}}\, d\boldsymbol{y}$

TRUNCATED FRACTIONAL KERNELS

want to compare $\begin{cases} -\mathcal{L}u = f & \text{in} \\ u = 0 & \text{in } \mathbb{R}^n\backslash \end{cases}$ and $\begin{cases} -\mathcal{L}_\bullet u_\bullet = f & \text{in} \\ u_\bullet = 0 & \text{in} \end{cases}$

well studied for $S(\boldsymbol{x}) = B_{\delta,2}(\boldsymbol{x})$, see [1]

[1] 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, 12451260, 2013

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result:

$$\|u - u_\bullet\|_{H^s(\Omega\cup\Omega_I)} \leq C_\bullet \|u\|_{L^2(\mathbb{R}^n)} \delta^{-2s}$$

$$\|u - u_\bullet\|_{L^2(\Omega\cup\Omega_I)} \leq C_\bullet C_P \|u\|_{L^2(\mathbb{R}^n)} \delta^{-2s}$$

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TRUNCATED FRACTIONAL KERNELS

numerical test

$S_\bullet(\boldsymbol{x}) = B_{\delta,\infty}(\boldsymbol{x})$ s.t. $\Omega \subset B_{\delta,\infty}(\boldsymbol{x}) \;\; \forall\, \boldsymbol{x} \in \Omega$

$\Omega = [0,1]^2$, uniformly discretized with $h = 2^{-8}$

$s = 0.4$, and $\delta_i = 2^i \delta_0$, $i = 4, 5, \ldots, 8$, with $\delta_0 \cong 1.5$

δ	$\lVert u - u_\bullet \rVert_{L^2}$	rate	$\lVert u - u_\bullet \rVert_{H^s}$	rate
$2^4\,\delta_0$	0.019	0.825	0.027	0.826
$2^5\,\delta_0$	0.011	0.815	0.015	0.814
$2^6\,\delta_0$	0.006	0.809	0.009	0.808
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		$2s$		$2s$

APPLICATIONS

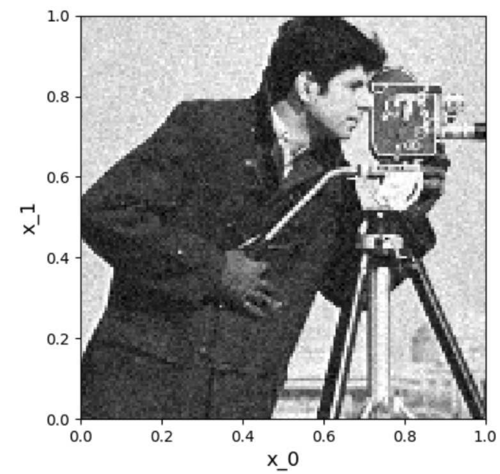
FINITE INTERACTION RADIUS - APPLICATIONS

Mechanics: some thoughts

- ℓ^2 balls make sense only in case of anisotropy $\Rightarrow$ we can use any ball combined with an **influence function** that determines the area of interactions
- ℓ^∞ balls can be used in combination with **mollifiers** when their purpose is to approximate ℓ^2 balls

FINITE INTERACTION RADIUS - APPLICATIONS

Image denoising: the shape of the ball does not matter, the nonlocal model is a tool



f: noisy image
u: denoised image, solution of an **optimization problem**

$$\min_u \frac{1}{2}|||u|||^2 + \frac{\lambda}{2}\|u - f\|_{L^2(\Omega}$$

necessary conditions: $-\mathcal{L}u + \lambda u = \lambda f$ nonlocal diffusion - reaction equation

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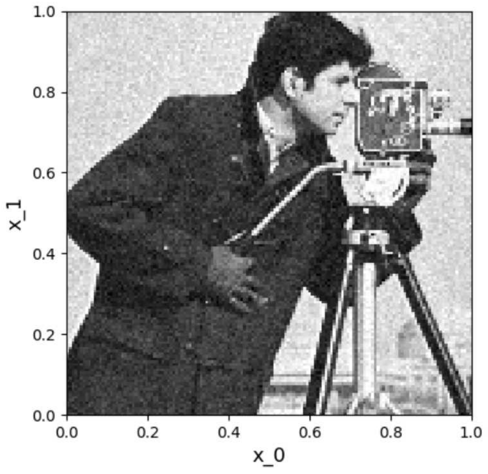

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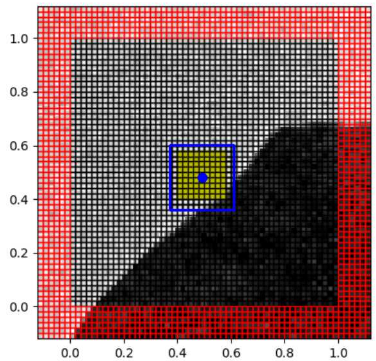
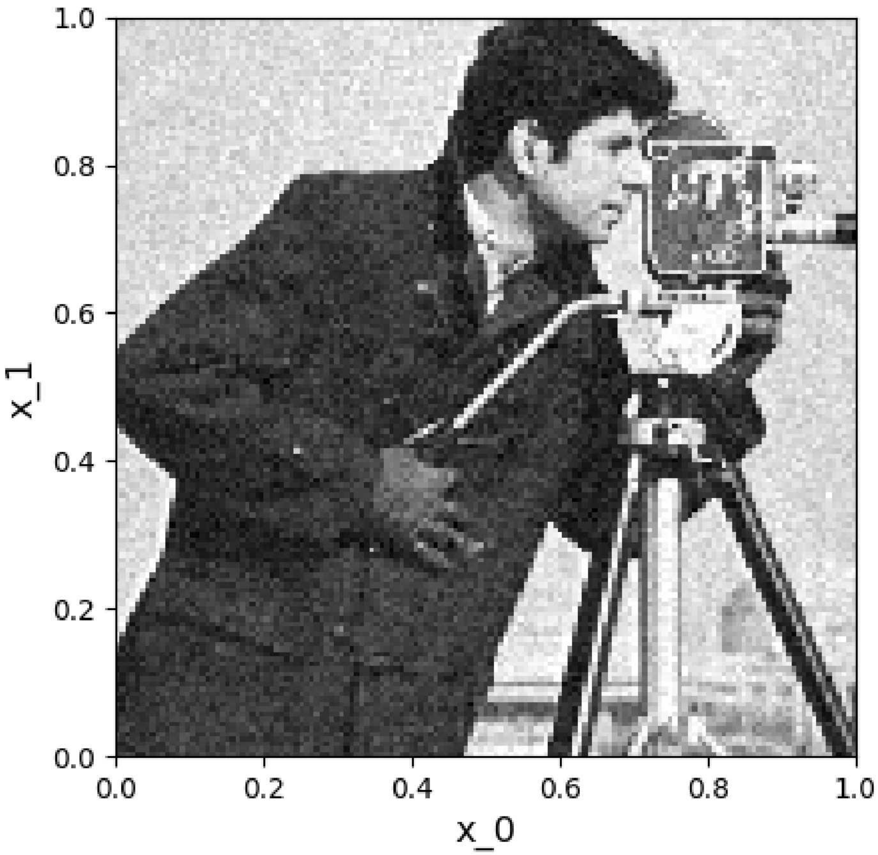
kernel: $\gamma(\boldsymbol{x}, \boldsymbol{y}) = \exp\left\{-\frac{(f(\boldsymbol{x}) - f(\boldsymbol{y}))^2}{\Delta^2}\right\}$ kernel of type 2

NEIGHBORHOODS WITH DIFFERENT NORMS





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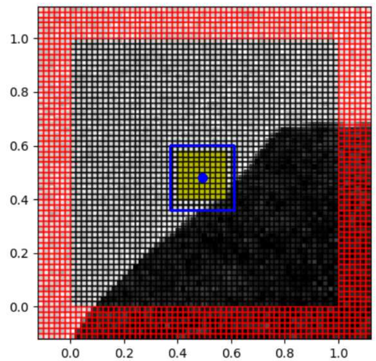

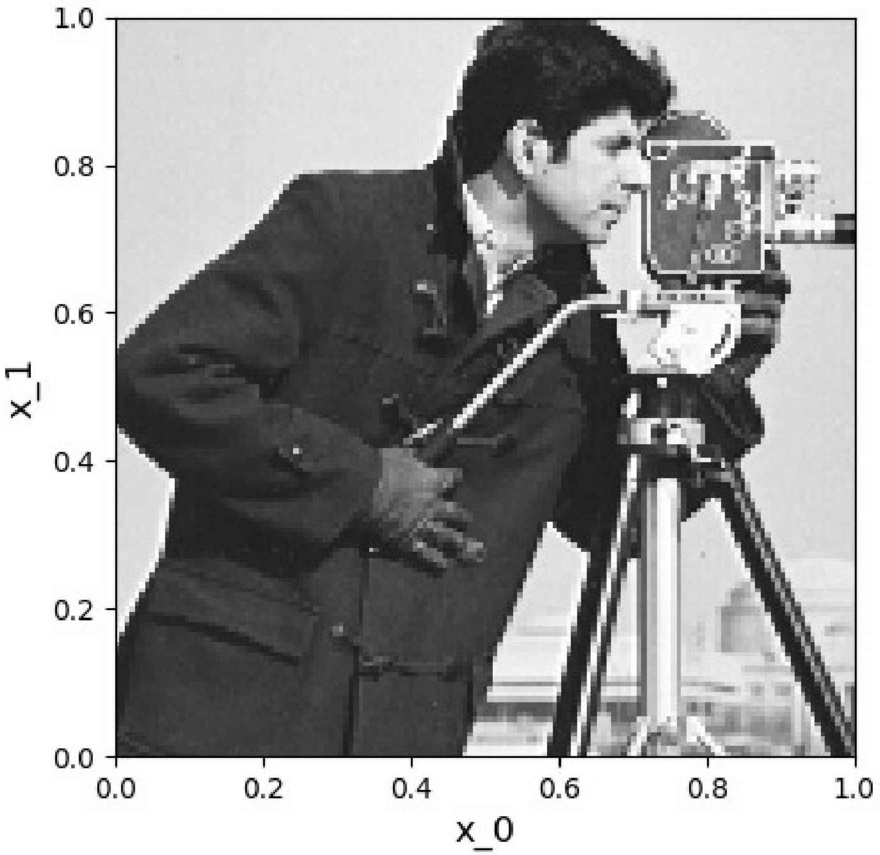

Thank you