NONLOCAL MODELS with NON-STANDARD INTERACTION DOMAINS

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NONLOCAL MODELS AND NON-STANDARD NEIGHBORHOODS
**NONLOCAL DIFFUSION MODELS**

**main feature:** interactions can occur at distance, without contact
  
every point $x$ in a domain interacts with a neighborhood

**our interest:** nonlocal diffusion operators
NONLOCAL DIFFUSION MODELS

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every point $x$ 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
how do they look?

\[ \mathcal{L}u(x) = \int_{\mathbb{R}^n} (u(y) - u(x)) \gamma(x, y) \, dy \]

what do we want to solve?

\[ \mathcal{L}u = f \]

+ volume constraints
how do they look?

\[ \mathcal{L}u(x) = \int_{\mathbb{R}^n} (u(y) - u(x)) \gamma(x, y) \, dy \]

what do we want to solve?

\[ \mathcal{L}u = f \]

+ volume constraints
**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*
**Challenge:** matrix assembling using FEM in 2D and 3D simulations

- determining intersections
- computing integrals of round domains
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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)
  • ??
CURRENT STRATEGIES

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**squares:**  
- oct-tree mesh refinement at the ball boundaries (Foster, UT Austin)

??

these may be unnecessary, inaccurate or inefficient!
what if we consider a different ball?

⇒ triangulation w/o geometry errors

⇒ much easier re-triangulation!
USING DIFFERENT BALLS

what if we consider a different ball?

⇒ triangulation w/o geometry errors

⇒ much easier re-triangulation!

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
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?
• **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


NONLOCAL VECTOR CALCULUS

- generalization of the classical vector calculus to nonlocal operators
- allows us to study nonlocal diffusion similarly to the classical, local, counterpart
- based on the concept of nonlocal fluxes
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\[ \int_{\partial \Omega_{12}} \mathbf{q} \cdot \mathbf{n}_1 \, dA \]
NONLOCAL VECTOR CALCULUS

• generalization of the classical vector calculus to nonlocal operators
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**Nonlocal operators** acting on \( u(x) : \mathbb{R}^d \to \mathbb{R} \) and \( \nu(x, y) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d \)

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

\[
\mathcal{L}u(x) = 2 \int (u(y) - u(x)) \alpha(x, y) \cdot \alpha(x, y) \, dy
\]
NONLOCAL VECTOR CALCULUS

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- gradient of \( u \): \( G(u)(x, y) = (u(y) - u(x)) \alpha(x, y) \)

- nonlocal diffusion of \( u \): \( L u(x) = D(G u(x)) \)
  \[
  L u(x) = 2 \int (u(y) - u(x)) \underline{\alpha(x, y)} \cdot \alpha(x, y) \, dy
  
  L u(x) = 2 \int (u(y) - u(x)) \underline{\gamma(x, y)} \, dy
  \]
**Interaction domain** of an open bounded region $\Omega \in \mathbb{R}^d$

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

$\delta$: interaction length, interaction radius
A NEW CONCEPT OF BALLS

**Non-degeneracy:** \( \exists \delta > 0 \) such that

\[ \forall \mathbf{x} \in (\Omega \cup \Omega_I), \ B_{\delta,2}(\mathbf{x}) \subset S(\mathbf{x}) \]

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

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

\( \mathbf{y} \in S(\mathbf{x}) \) if and only if \( \mathbf{x} \in S(\mathbf{y}) \)

\( \Rightarrow (\mathbf{x}, \mathbf{y}) \mapsto \chi_{S(\mathbf{x})}(\mathbf{y}) \) is symmetric in \((\mathbf{x}, \mathbf{y})\)
assumptions: $\exists \gamma_0 > 0 \text{ s.t. } \forall \ x \in (\Omega \cup \Omega_I)$

\[
\begin{align*}
\gamma(x, y) & \geq 0 \quad \forall \ y \in S(x) \\
\gamma(x, y) & \geq \gamma_0 > 0 \quad \forall \ y \in B_{\delta,2}(x) \\
\gamma(x, y) & = 0 \quad \forall \ y \in \mathbb{R}^n \setminus S(x)
\end{align*}
\]
**KERNELS**

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\end{align*}
\]

**kernel expression:**

\[
\gamma(x, y) = \phi(x, y) \mathcal{X}_{S(x)}(y)
\]

where \( \phi(x, y) \) is referred to as kernel function
KERNELS

kernel expression:
\[ \gamma(x, y) = \phi(x, y) \chi_{S(x)}(y) \]

examples:

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

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

\[ \Rightarrow S(x) \text{ is the Euclidean ball } B_{\delta, 2}(x) \]
\( \delta: \text{ horizon.} \)
KERNELS

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general interaction sets: \[ \eta(x, y) = \|x - y\|_\bullet - \delta, \text{ for an arbitrary norm } \| \cdot \|_\bullet \]
\[ \Rightarrow S(x) \text{ are balls } B_{\delta,\bullet}(x) := \{ y \in \mathbb{R}^n : \|x - y\|_\bullet < \delta \}. \]
WEAK FORM AND WELL-POSEDNESS

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

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 \( g \in \tilde{V}(\Omega_I) \), find \( u \in V(\Omega \cup \Omega_I) \)

such that \( u\big|_{\Omega_I} = g \) and \( A(u, v) \equiv \int_{\Omega} f v \, dx \ \forall v \in V_c(\Omega \cup \Omega_I) \)
WEAK FORM AND WELL-POSEDNESS

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energy seminorm: \[ |||u||| = \sqrt{A(u, u)} \quad \text{norm in } V_c \]

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such that \( u|_{\Omega_I} = g \) and \( A(u, v) = \int_{\Omega} f v \, dx \quad \forall v \in V_c(\Omega \cup \Omega_I) \)

well-posed by the Riesz representation theorem
KERNEL 1

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

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

$S(x)$: any set with non-degeneracy and symmetry properties
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properties

- the corresponding energy norm satisfies a Poincaré inequality
- the corresponding unconstrained and constrained energy spaces are equivalent to \( H^s(\Omega \cup \Omega_I) \) and \( H_c^s(\Omega \cup \Omega_I) \)
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\[\Rightarrow \|u\|_{H^s(\Omega \cup \Omega_I)} \leq C\|f\|_{H^{-s}(\Omega \cup \Omega_I)}\]
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$$\Rightarrow \|u\|_{H^s(\Omega \cup \Omega_I)} \leq C \|f\|_{H^{-s}(\Omega \cup \Omega_I)}$$

example: $\gamma_1(x, y) = \frac{\sigma(x, y)}{\|y - x\|_2^{d+2s}} \chi_{S(x)}(y)$
KERNEL 2

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

\[ k_* \leq \inf_{x \in \Omega} \int_{S(x)} \gamma_2(x, y) \, dy \]

\[ \sup_{x \in \Omega} \int_{(\Omega \cup \Omega) \cap S(x)} \frac{\gamma_2(x, y)}{2} \, dy \leq k_*^2 \]

\( S(x) \): any set with non-degeneracy and symmetry properties
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\[ k_* \leq \inf_{\mathbf{x} \in \Omega} \int_{S(\mathbf{x})} \gamma_2(\mathbf{x}, \mathbf{y}) \, d\mathbf{y} \]

\[ \sup_{\mathbf{x} \in \Omega \cup \Omega_I} \int_{(\Omega \cup \Omega_I) \cap S(\mathbf{x})} \gamma_2^2(\mathbf{x}, \mathbf{y}) \, d\mathbf{y} \leq k_*^2 \]

\[ S(\mathbf{x}): \text{any set with non-degeneracy and symmetry properties} \]

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

assumption: $\delta \geq \text{diam}(\Omega) = \max_{x, y \in \Omega} \| y - x \|_\ast \Rightarrow \Omega \subset S(x)$ for all $x \in \Omega$
TRUNCATED FRACTIONAL KERNELS

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**kernels of type 1:** $\gamma(x, y) = \frac{c_{n,s}}{2\|x - y\|_2^{n+2s}} \chi_{B_{\delta, \bullet}}(x)(y)$ for $0 < s < 1$

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

M. D'Elia – mdelia@sandia.gov
interaction sets: balls wrt a norm $\| \cdot \|_\star \Rightarrow S(x) = B_{\delta, \star}(x)$

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

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

want to compare \[ \begin{aligned} -\mathcal{L} u &= f \quad \text{in } \Omega \\ u &= 0 \quad \text{in } \mathbb{R}^n \setminus \Omega \end{aligned} \quad \text{and} \quad \begin{aligned} -\mathcal{L} u_* &= f \quad \text{in } \Omega \\ u_* &= 0 \quad \text{in } \Omega_I \end{aligned} \]

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

want to compare \[ \begin{cases} -\mathcal{L}u = f & \text{in } \Omega \\ u = 0 & \text{in } \mathbb{R}^n \setminus \Omega \end{cases} \quad \text{and} \quad \begin{cases} -\mathcal{L}_* u_* = f & \text{in } \Omega \\ u_* = 0 & \text{in } \Omega_I \end{cases} \]

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

result:

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

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

numerical test

\[ S(x) = B_{\delta,\infty}(x) \text{ s.t. } \Omega \subset B_{\delta,\infty}(x) \ \forall \ x \in \Omega \]

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

\[ s = 0.4, \text{ and } \delta_i = 2^i \delta_0, \ i = 4, 5, \ldots, 8, \text{ with } \delta_0 \cong 1.5 \]

| \( \delta \) | ||u - u_\ast||_{L^2} | \text{rate} | ||u - u_\ast||_{H^s} | \text{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 |
| \( 2^7 \delta_0 \) | 0.003 | 0.807 | 0.005 | 0.804 |
| \( 2^8 \delta_0 \) | 0.002 | 0.804 | 0.003 | 0.802 |
TRUNCATED FRACTIONAL KERNELS

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<table>
<thead>
<tr>
<th>( \delta )</th>
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\( 2s \quad 2s \)
APPLICATIONS
**Mechanics:** some thoughts

- $\ell^2$ 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.

- $\ell^\infty$ balls can be used in combination with *mollifiers* when their purpose is to approximate $\ell^2$ balls.
**FINITE INTERACTION RADIUS - APPLICATIONS**

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

\[ f: \text{noisy image} \]
\[ u: \text{denoised image, solution of an optimization problem} \]

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

**necessary conditions:** \(-\mathcal{L}u + \lambda u = \lambda f\) nonlocal diffusion - reaction equation
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**necessary conditions:** \[ -\mathcal{L}u + \lambda u = \lambda f \] nonlocal diffusion - reaction equation

**kernel:** \[ \gamma(x, y) = \exp \left\{ -\frac{(f(x) - f(y))^2}{\Delta^2} \right\} \] kernel of type 2
NEIGHBORHOODS WITH DIFFERENT NORMS
Thank you