NONLOCAL MODELS with APPROXIMATE NONLOCAL NEIGHBORHOODS: towards fast FEM

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NONLOCAL MODELS AND RELATED CHALLENGES
Applications

- Nonlocal models for continuum mechanics
- Stochastic jump processes
- Nonlocal heat conduction
- Subsurface flow/porous media
- Image processing

D. Littlewood, Peridigm website

Bobaru, 2012

Martinez, 2018

Buades, 2010
NONLOCAL DIFFUSION OPERATORS

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 contraints
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**Modeling:**  • prescription of volume constraints
  • choice of kernel functions
  • modeling of nonlocal interfaces

**Computations:**  • numerical solution can be prohibitively expensive
  • implementation is troublesome
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  - design of efficient nonlocal solvers
  - design of efficient quadrature rules/approximations
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- design of efficient nonlocal solvers  
- **design of efficient quadrature rules/approximations**

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Meshfree methods: popular means for discretizing nonlocal equations

Variational methods:
- ease in dealing with complicated domains
- higher-order convergence rates
- adaptive meshing methods (for the treatment of, e.g., discontinuities)
- rigorous mathematical treatment of operator and solution properties (convergence, stability, ...)

however... additional challenges
**Challenge:** matrix assembling using FEM in 2D and 3D simulations

- determining intersections
- computing integrals of round domains
- find appropriate quadrature rules
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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)
triangles:  
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these may be unnecessary, inaccurate or inefficient!
CONTRIBUTIONS OF THIS WORK

- introduce **approximate neighborhoods** that facilitate the assembly procedure and mitigate the computational effort

- quantify the **approximation error** and its contribution to the overall accuracy

- provide guidance on the choice of quadrature rules

- introduce a **cheap and easy-to-implement** approximation that
  - preserves **optimal accuracy**
  - **improves** the computational performance
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! making variational methods a preferable alternative?
WEAK FORM AND ITS DISCRETIZATION
FEM FOR NONLOCAL MODELS

\textbf{Weak form:} for \( u = 0 \) in \( \Omega_I \)

\[
0 = \int_{\Omega} (\mathcal{L}u - f) v \, dx = \int_{\Omega} \int_{\Omega \cup \Omega_I} (u(y) - u(x))(v(y) - v(x)) \gamma(x, y) \, dy \, dx - \int_{\Omega} f v \, dx
\]

\( A(u, v) = F(v), \; \forall \; v \in V_c(\Omega \cup \Omega_I) \)

\textbf{Energy norm and spaces:}

- “energy norm”: \( |||w||| = \sqrt{A(w, w)} \) (norm on \( V_c(\Omega \cup \Omega_I) \))

- energy space: \( V(\Omega \cup \Omega_I) = \{ w \in L^2(\Omega \cup \Omega_I) : |||w||| < \infty \} \)

- constrained energy space: \( V_c(\Omega \cup \Omega_I) = \{ w \in V : w = 0 \text{ on } \Omega_I \} \)
Weak form: for $u = 0$ in $\Omega_I$

$$0 = \int_{\Omega} (-L u - f) v \, dx = \int_{\Omega \cup \Omega_I} \int_{\Omega \cup \Omega_I} (u(y) - u(x))(v(y) - v(x)) \gamma(x, y) \, dy \, dx - \int_{\Omega} f v \, dx$$

$A(u, v) = F(v), \; \forall \; v \in V_c(\Omega \cup \Omega_I)$

Energy norm and spaces:

- “energy norm”: $|||w||| = \sqrt{A(w, w)}$ (norm on $V_c(\Omega \cup \Omega_I)$)

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Kernels: $\gamma(x, y) = \psi(x, y) \chi_{B_\delta(x)}(y)$
FEM nodes and basis

- \( \{ \tilde{x}_j \}_{j=1}^J \): set of nodes, with \( \{ \tilde{x}_j \}_{j=1}^{J_\Omega} \subset \Omega \) and \( \{ \tilde{x}_j \}_{j=J_\Omega+1}^J \subset \overline{\Omega}_I \)

- \( \{ \phi_j(x) \}_{j=1}^J \): piecewise-polynomial functions such that \( \phi_j(\tilde{x}_{j'}) = \delta_{jj'} \) for \( j' = 1, \ldots, J \)

- FEM spaces: \( V^h = \text{span}\{ \phi_j(x) \}_{j=1}^J \subset V(\Omega \cup \Omega_I) \) of dimension \( J \)

\[ V^h_c = \text{span}\{ \phi_j(x) \}_{j=1}^{J_\Omega} \subset V_c(\Omega \cup \Omega_I) \) of dimension \( J_\Omega \)
FEM FOR NONLOCAL MODELS

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\[ V_c^h = \text{span}\{ \phi_j(\mathbf{x}) \}_{j=1}^{J_\Omega} \subset V_c(\Omega \cup \Omega_I) \] of dimension \( J_\Omega \)

FEM solution and projection

\[ u_h(\mathbf{x}) = \sum_{j=1}^J U_j \phi_j(\mathbf{x}) \]

discrete weak formulation: projection of the weak form onto \( V^h \), i.e.

find \( u_h(\mathbf{x}) \in V^h \) such that \( A(u_h, \phi_j) = F(\phi_j) \) \( \forall j = 1, \ldots J_\Omega \)
Elements, balls and quadrature rules

\[ \sum_{j=1}^{J} A(\phi_{j'}, \phi_{j}) U_{j} = F(\phi_{j'}) \quad \text{for } j' = 1, \ldots, J, \]

\[ A(\phi_{j'}, \phi_{j}) = \sum_{k=1}^{K} \int \int \left( \phi_{j}(x) - \phi_{j}(y) \right) \left( \phi_{j'}(x) - \phi_{j'}(y) \right) \psi(x, y) \, dy \quad j = 1, \ldots, J, j' = 1, \ldots, J_{\Omega} \]
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\[ A(\phi_{j'}, \phi_j) = \sum_{k=1}^{K} \int_{E_k} \int_{\Omega \cap B_\delta(x)} (\phi_j(x) - \phi_j(y)) (\phi_{j'}(x) - \phi_{j'}(y)) \psi(x, y) dy \quad j = 1, \ldots, J, j' = 1, \ldots, J_\Omega \]
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\[ A_{q}(\phi_{j'}, \phi_{j}) = \sum_{k=1}^{K} \sum_{q=1}^{Q} w_{k,q} \int_{\Omega \cap B_{\delta}(x_{k,q})} (\phi_{j}(x_{k,q}) - \phi_{j}(y))(\phi_{j'}(x_{k,q}) - \phi_{j'}(y)) \psi(x_{k,q}, y) dy \]
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- outer triangle \( \mathcal{E}_k \)
- interaction region of \( \mathcal{E}_k \)
- interaction region of the vertexes
- a triangle intersected by \( B_\delta(\bar{x}) \)

quadrature points for \( \mathcal{E}_k \): integrates cubics exactly and takes care of missing triangles
Elements, balls and quadrature rules

\[ \sum_{j=1}^{J} A(\phi_{j'}, \phi_j) U_j = F(\phi_{j'}) \quad \text{for } j' = 1, \ldots, J, \]

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**Note!** Inner quadrature rules are also needed

(way too messy, not reported)

but **luckily** not as troublesome
APPROXIMATE BALLS

1 Inscribed triangle-based **polygonal approximation** of balls
2 Inscribed cap-based **polygonal approximation** of balls
3 **Whole-triangle** approximation based on barycenter location
4 **Whole-triangle** approximation based on overlap with ball
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2.1 quadrature rules for caps
2.2 re-triangulation of caps
GEOMETRIC APPROXIMATION

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2.1 quadrature rules for caps
2.2 re-triangulation of caps

Are we losing accuracy?
Lemma:

Let $B_{\delta}(\bar{x})$ be the $\ell^2$ ball and $B_{\delta,h}(\bar{x})$ be an approximation, and let $u_h$ and $\tilde{u}_h$ be the corresponding finite element solutions. Then, for exact outer and inner quadrature rules,

$$||| u_h - ||| \leq K \ |\Delta B_{\delta}(\bar{x})| \ |\| L^2(\Omega \cup \Omega_I),$$

where $K$ is a positive constant independent of $\delta$ and $h$, $\bar{x} \in \Omega$ and $\Delta B_{\delta}$ is the “difference ball”:

$$\Delta B_{\delta} = (B_{\delta} \setminus (B_{\delta} \cap B_{\delta,h})) \cup (B_{\delta,h} \setminus (B_{\delta} \cap B_{\delta,h}))$$
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$$\Delta B_\delta = (B_\delta \setminus (B_\delta \cap B_{\delta,h})) \cup (B_{\delta,h} \setminus (B_\delta \cap B_{\delta,h}))$$

the overall accuracy depends on the volume of the difference ball.
**Discretization:** piecewise linear FEM spaces, optimal accuracy \((h^2)\)

<table>
<thead>
<tr>
<th>No caps</th>
<th>Quad rules for caps or retriangulation</th>
<th>Whole triangles based on barycenters</th>
<th>Whole triangles based on overlap</th>
</tr>
</thead>
<tbody>
<tr>
<td>(</td>
<td>\Delta B_{\delta}</td>
<td>= \mathcal{O}(h^2))</td>
<td>(</td>
</tr>
</tbody>
</table>
**Discretization:** piecewise linear FEM spaces, optimal accuracy \( (h^2)\)

<table>
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<tr>
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<tr>
<td>( \Delta B_\delta = \mathcal{O}(h^2) )</td>
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</tr>
<tr>
<td>(</td>
<td></td>
<td>e</td>
<td></td>
</tr>
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</table>
Discretization: piecewise linear FEM spaces, optimal accuracy ($h^2$)

- **no caps**
  - $|\Delta B_\delta| = \mathcal{O}(h^2)$
  - $\|\|e\|| = \mathcal{O}(h^2)$

- **quad rules for caps or retriangulation**
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  - $|\Delta B_\delta| = \mathcal{O}(h^2)$
  - $\|\|e\|| = \mathcal{O}(h)$

- **whole triangles based on overlap**
  - $|\Delta B_\delta| = \mathcal{O}(h)$
  - $\|\|e\|| = \mathcal{O}(h)$
### APPROXIMATION ERROR

1. **No caps**

<table>
<thead>
<tr>
<th>$h$</th>
<th>$L^2$</th>
<th>rate</th>
<th>energy</th>
<th>rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>2.75e-2</td>
<td>-</td>
<td>1.29e-1</td>
<td>-</td>
</tr>
<tr>
<td>0.05</td>
<td>3.86e-3</td>
<td>2.83</td>
<td>1.88e-2</td>
<td>2.77</td>
</tr>
<tr>
<td>0.025</td>
<td>4.00e-4</td>
<td>3.26</td>
<td>3.37e-3</td>
<td>2.48</td>
</tr>
<tr>
<td>0.0125</td>
<td>2.60e-4</td>
<td>0.61</td>
<td>1.20e-3</td>
<td>1.48</td>
</tr>
<tr>
<td>0.00625</td>
<td>7.00e-5</td>
<td>1.86</td>
<td>3.20e-4</td>
<td>1.92</td>
</tr>
</tbody>
</table>

**Note 1:** rate seem erratic, an adaptive quad rule for the outer integral fixes this issue

**Note 2:** CPU(no caps) $\sim 3 \times$ CPU(barycenter)

3. **Barycenter**

<table>
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<th>energy</th>
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<tr>
<td>0.1</td>
<td>1.71e-1</td>
<td>-</td>
<td>7.8e-1</td>
<td>-</td>
</tr>
<tr>
<td>0.05</td>
<td>6.00e-2</td>
<td>1.51</td>
<td>2.64e-1</td>
<td>1.56</td>
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2.09  2.13  2.17  2.15
APPROXIMATION ERROR

- **no caps**
  \[ \|e\| = O(h^2) \]

- **quad rules for caps or retriangulation**
  \[ \|e\| = O(h^2) \]

- **whole triangles based on barycenters**
  \[ \|e\| = O(h^2) \]

- **whole triangles based on overlap**
  \[ \|e\| = O(h) \]
C. Vollman, M. D'Elia, M. Gunzburger, V. Schulz,

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
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Important questions
0. does the nonlocal 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?
USING DIFFERENT BALLS

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Important questions

0. does the nonlocal calculus still apply? ✓
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3. are there applications? ✓
Thank you