NONLOCAL MODELS in COMPUTATIONAL SCIENCE and ENGINEERING: challenges and applications

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WHAT IS A NONLOCAL MODEL?
Note: using nonlocal models to describe natural and social phenomena has been of interest for a long time, but only in recent years the interest has grown.

General definition: model descriptions that, at a point in space and at a instant in time, depend on either or both the state of the system at points at a far distance and at previous time instants appreciably earlier than the given instant.
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**General definition:** model descriptions that, at a point in space and at a instant in time, depend on either or both the state of the system at points at a far distance and at previous time instants appreciably earlier than the given instant.

**Contrast** with local models such as PDEs, described in terms of the state of the system in infinitesimal neighborhoods of the given point and instant.
Types of nonlocal models:

A. Anomalous diffusion $\rightarrow$ fractional differential operators
Types of nonlocal models:

A. Anomalous diffusion $\rightarrow$ fractional differential operators

B. Mechanics with damage/discontinuities $\rightarrow$ nonlocality is restricted to neighborhoods

TWO PERSPECTIVES

M. D'Elia – mdelia@sandia.gov
Let's back up: Classical diffusion

**Molecular definition:** the net movement of molecules or atoms from a region of high concentration to a region of low concentration (deterministic motion of an individual molecule or atom is due to collisions with other molecules or atoms).
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**Molecular definition:** the net movement of molecules or atoms from a region of high concentration to a region of low concentration (deterministic motion of an individual molecule or atom is due to collisions with other molecules or atoms).

**Macroscopic definition:** the particle concentration is governed by the flux equation

\[
\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{q} = 0
\]

and Fick's law \( \mathbf{q} = -D \nabla c \)

leading to the heat equation \( \frac{\partial c}{\partial t} = D \Delta c \)

!!! solutions of these equations are such that particles move from high to low concentration regions
Let's back up: Classical diffusion

**Common feature:** the mean square displacement (MSD) is proportional to $t$.

MSD is a measure of the deviation from a reference point in time, i.e.

\[
\text{MSD}(t) = \langle (x(t) - x_0)^2 \rangle \approx t
\]

\[
\langle f(t) \rangle = \int_{-\infty}^{+\infty} f(x, t) P(x, t) \, dx
\]

\[
P(x, t) = Ce^{-c(x-x_0)^2} \quad \text{(fundamental solution of the diffusion equation )}
\]
ANOMALOUS DIFFUSION

Universal definition: mean square displacement is proportional to $t^\gamma$

$\gamma < 1$ subdiffusion

$\gamma = 1$ classical diffusion

$\gamma > 1$ superdiffusion
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Note: in many settings, the MSD can be observed and it is **NOT** always proportional to \( t \)

→ anomalous diffusion is worth studying

→ many attempts to design and/or validate a model with a desired rate \( \gamma \).
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→ anomalous diffusion is worth studying

→ many attempts to design and/or validate a model with a desired rate $\gamma$.

Examples:

Fractional Laplacian $\partial_t c = -(-\Delta)^s c$, $s \in (0, 1) \Rightarrow$ MSD $\propto t^{1/s}$: superdiffusion

Fractional time derivative $\partial_t^\alpha c = \Delta c$, $\alpha \in (0, 1) \Rightarrow$ MSD $\propto t^\alpha$: subdiffusion
NONLOCAL MODELS

- used to model stochastic jump processes, e.g. Lévy jump processes [1,2]

- example: estimate the first exit time of a particle from a bounded domain [3]

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“It can be said that all physical phenomena are nonlocal. Locality is a fiction invented by idealists.” — A. Cemal Eringen
LOCAL vs NONLOCAL MECHANICS

Classical continuum mechanics assumptions:

1) The medium is continuous
2) Internal forces are contact forces
3) Deformation twice continuously differentiable (relaxed in weak forms)
4) Conservation laws of mechanics apply
LOCAL vs NONLOCAL MECHANICS

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Newton’s Principia:

A) Materials are discontinuous
B) Materials have internal forces across nonzero distances
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Newton’s Principia:
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Challenges for classical continuum mechanics
defects, phase transformations, composites, fracture, dislocations, micro-mechanics, nano-structures, biological materials, colloids, large molecules, complex fluids, etc...

→ common features: discontinuities and long range forces
Objective of peridynamics: unify the mechanics of discrete particles, continuous media, and continuous media with evolving discontinuities.
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**Simplest peridynamic equation:** the displacement \( u \) satisfies

\[
\rho(x, t) \frac{\partial^2 u}{\partial t} = \int_{\Omega \cap B_\varepsilon(x)} \frac{u(x, t) - u(y, t)}{|x - y|} dy + b(x, t)
\]

\( B_\varepsilon(x) \): ball or radius \( \varepsilon \) centered at \( x \)
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**Appealing features of peridynamics**

- No external crack growth law
- Natural complex crack dynamics (natural consequence of the evolution equation)
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**Appealing features of peridynamics**

- No external crack growth law
- Natural complex crack dynamics (natural consequence of the evolution equation)

“In peridynamics, cracks are part of the solution, not part of the problem.”
F. Bobaru, University of Nebraska-Lincoln
MORE APPLICATIONS

- nonlocal models for continuum mechanics

- stochastic jump processes

- nonlocal heat conduction

- subsurface flow/porous media

- image processing

Bobaru, 2012

Buades, 2010
our interest (for now): nonlocal diffusion operators

how do they look like?

\[ \mathcal{L}u(x) = \int (u(y) - u(x)) \gamma(x, y) \, dy \]
SOME FACTS...
**NONLOCAL MODELS**

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

  - we have **well-posedness** results for a large class of nonlocal steady and unsteady-state equations, control problems and parameter identification

  - we have **numerical convergence** results for finite element approximations
facts: • a recently developed theoretical and numerical analysis allows us to study nonlocal problems similarly to the local (classical) counterpart

• we have well-posedness results for a large class of nonlocal steady and unsteady-state equations, control problems and parameter identification

• we have numerical convergence results for finite element approximations

challenges: • the numerical solution might be prohibitively expensive

• prescription of nonlocal “boundary conditions” is not straightforward
**example:** finite element stiffness matrices corresponding to a simple 1D Poisson equation for different radii of interaction

→ increasing interaction radius →
**NONLOCAL vs LOCAL**

**example:** finite element stiffness matrices corresponding to a simple 1D Poisson equation for different radii of interaction

→ increasing interaction radius →

**approaches:**
- coupling
- fast finite element solvers
• **Notation:** a Nonlocal Vector Calculus

• **Approach 1:** local-nonlocal coupling
  1. formulation and analysis
  2. finite dimensional approximation and numerical analysis
  3. numerical tests

• **Approach 2:** fast FEM, a new concept of neighborhood
  1. motivation
  2. formulation and analysis
  3. numerical tests
A 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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**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

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

- 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 \( u \): \( \mathcal{L}u(x) = \mathcal{D}(\mathcal{G}u(x)) \)

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

\[
\mathcal{L}u(x) = 2 \int (u(y) - u(x)) \gamma(x, y) \, dy
\]
**Interaction domain** of an open bounded region $\omega \in \mathbb{R}^d$

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

Define: $\Omega = \omega \cup \eta$
Interaction domain of an open bounded region $\omega \in \mathbb{R}^d$

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

Define: $\Omega = \omega \cup \eta$

Kernel: we assume

$$\begin{cases} 
\gamma(x, y) \geq 0 & \forall y \in B_{\varepsilon}(x) \\
\gamma(x, y) = 0 & \forall y \in \Omega \setminus B_{\varepsilon}(x),
\end{cases}$$

$$B_{\varepsilon}(x) = \{y \in \Omega : |x - y| \leq \varepsilon, \ x \in \omega\}$$
APPROACH 1: COUPLING
Goal: merge two fundamentally different mathematical descriptions of the same physical phenomena: PDEs and nonlocal models.
WHAT ABOUT COUPLING?

**Goal:** merge two fundamentally different mathematical descriptions of the same physical phenomena: PDEs and nonlocal models

**Literature**

(2012) Han and Lubineau: extension of the Arlequin method to continuum mechanics, **energy blending**

(2012) Lubineau et al.: morphing approach, **blending of material properties**

(2013) Seleson et al.: **force blending**

(2015) Silling et al.: **variable horizon**

(2017) Tian and Du.: heterogeneous localization via **nonlocal trace theorems**
WHAT ABOUT COUPLING?

**Our strategy** split the computational domain in a local and a nonlocal domain and *couple* the models at the interfaces or overlapping regions using optimization

**NOTE:** very general, flexible, and applicable to a large variety of mathematical models (e.g. models with different scales)
WHAT ABOUT COUPLING?

**Contribution:** define and analyze a local-to-nonlocal (LtN) coupling method for nonlocal diffusion models that

- passes the patch test
- allows for separate softwares/solvers/meshes for the local and nonlocal problems
WHAT ABOUT COUPLING?

**Contribution:** define and analyze a local-to-nonlocal (LtN) coupling method for nonlocal diffusion models that

- passes the patch test
- allows for separate softwares/solvers/meshes for the local and nonlocal problems

**Novelty:** design a method that differs fundamentally from previous strategies reversing the roles of coupling conditions and models

- coupling conditions = optimization objective
- models = optimization constraints
THE LtN OPTIMIZATION PROBLEM


MODEL PROBLEMS – Dirichlet VC and BC

We start with something **very** simple: Poisson

The nonlocal problem

\[
\begin{cases}
-\mathcal{L}u_n &= f_n \quad x \in \omega \\
 u_n &= \sigma_n \quad x \in \eta,
\end{cases}
\]

where \( \sigma_n \in \widetilde{V}(\eta) \) and \( f_n \in L^2(\omega) \)
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The nonlocal problem

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\]

where $\sigma_n \in \widetilde{V}(\eta)$ and $f_n \in L^2(\omega)$

The local problem: Poisson equation

\[
\begin{cases}
-\Delta u_l &= f_l \quad x \in \Omega \\
 u_l &= \sigma_l \quad x \in \partial\Omega,
\end{cases}
\]

where $\sigma_l \in H^{\frac{1}{2}}(\partial\Omega)$ and $f_l \in L^2(\Omega)$
State equations

$$
\begin{align*}
-\mathcal{L}u_n &= f_n \quad x \in \omega_n \\
u_n &= \theta_n \quad x \in \eta_c \\
u_n &= 0 \quad x \in \eta_D
\end{align*}
\quad
\begin{align*}
-\Delta u_l &= f_l \quad x \in \Omega_l \\
u_l &= \theta_l \quad x \in \Gamma_c \\
u_l &= 0 \quad x \in \Gamma_D
\end{align*}
$$
Optimization problem

\[
\min_{u_n,u_l,\theta_n,\theta_l} J(u_n,u_l) = \min_{u_n,u_l,\theta_n,\theta_l} \frac{1}{2} \|u_n - u_l\|_{0,\Omega_o}^2
\]

s.t. \[
\begin{cases}
-\mathcal{L}u_n = f_n & x \in \omega_n \\
u_n = \theta_n & x \in \eta_c \\
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\]

\[
\begin{cases}
-\Delta u_l = f_l & x \in \Omega_l \\
u_l = \theta_l & x \in \Gamma_c \\
u_l = 0 & x \in \Gamma_D
\end{cases}
\]
LtN solution

- optimal solution: \((\theta_n^*, \theta_l^*) \in \Theta_n \times \Theta_l\)

- LtN solution:
  \[
  u_n^*(\theta_n^*) \quad x \in \Omega_n \\
  u_l^*(\theta_l^*) \quad x \in \Omega_l \setminus \Omega_o
  \]
LtN COUPLING

LtN solution • optimal solution: \((\theta^*_n, \theta^*_l) \in \Theta_n \times \Theta_l\)

• LtN solution: 
\[
\begin{cases} 
  u^*_n(\theta^*_n) & x \in \Omega_n \\
  u^*_l(\theta^*_l) & x \in \Omega_l \setminus \Omega_o 
\end{cases}
\]

Questions: • is it unique?

• what is the “error” wrt the global nonlocal solution \(\hat{u}_n\)?

\[
\left\{ 
  \begin{array}{l}
    -L\hat{u}_n = f \quad x \in \omega \\
    \hat{u}_n = 0 \quad x \in \eta 
  \end{array} \right. 
\]
IS THE SOLUTION UNIQUE?

Reduced form:

\[
\min_{\theta_n, \theta_l} J(\theta_n, \theta_l) = \min_{\theta_n, \theta_l} \frac{1}{2} \| u_n(\theta_n) - u_l(\theta_l) \|^2_{0,\Omega_o}
\]
IS THE SOLUTION UNIQUE?

Reduced form:

$$\min_{\theta_n, \theta_l} J(\theta_n, \theta_l) = \min_{\theta_n, \theta_l} \frac{1}{2} \| u_n(\theta_n) - u_l(\theta_l) \|_{0, \Omega_0}^2$$

split them in a control-dependent and control-independent component

$$u_n(\theta_n) = v_n(\theta_n) + u_n^0$$
$$u_l(\theta_n) = v_l(\theta_n) + u_l^0$$
Reduced form:
\[
\min_{\theta_n, \theta_l} J(\theta_n, \theta_l) = \min_{\theta_n, \theta_l} \frac{1}{2} \| u_n(\theta_n) - u_l(\theta_l) \|_{0, \Omega_o}^2
\]

**split** them in a **control-dependent** and **control-independent** component

\[
u_n(\theta_n) = v_n(\theta_n) + u_n^0 \\
u_l(\theta_n) = v_l(\theta_n) + u_l^0
\]

**harmonic** components and

\[
\begin{cases}
-\mathcal{L} v_n = 0 & x \in \omega_n \\
v_n = \theta_n & x \in \eta_c \\
 + \text{VC}
\end{cases}
\quad \text{and} \quad
\begin{cases}
-\Delta v_l = 0 & x \in \Omega_l \\
v_l = \theta_l & x \in \Gamma_c \\
 + \text{BC}
\end{cases}
\]

**homogeneous** components \(^0\) and \(^0\)

\[
\begin{cases}
-\mathcal{L} u_n^0 = f_n & x \in \omega_n \\
u_n^0 = 0 & x \in \eta_c \\
 + \text{VC}
\end{cases}
\quad \text{and} \quad
\begin{cases}
-\Delta u_l^0 = f_l & x \in \Omega_l \\
u_l^0 = 0 & x \in \Gamma_l \\
 + \text{BC}
\end{cases}
\]
Reduced functional:

\[ J(\theta_n, \theta_i) = \frac{1}{2} \left\| v_n(\theta_n) - v_i(\theta_i) \right\|_{0, \Omega_o}^2 + (u^0 - u^0_i, v_n(\theta_n) - v_i(\theta_i))_{0, \Omega_o} \]
IS THE SOLUTION UNIQUE?

Reduced functional:

\[ J(\theta_n, \theta_l) = \frac{1}{2} \| v_n(\theta_n) - v_l(\theta_l) \|_{0, \Omega_o}^2 + \left( u_n^0 - u_l^0, v_n(\theta_n) - v_l(\theta_l) \right)_{0, \Omega_o} \]

**Lemma:** The reduced space problem has a **unique** solution
IS THE SOLUTION UNIQUE?

Reduced functional:

\[
J(\theta_n, \theta_l) = \frac{1}{2} \| v_n(\theta_n) - v_l(\theta_l) \|_{0, \Omega_o}^2 + (u_n^0 - u_l^0, v_n(\theta_n) - v_l(\theta_l))_{0, \Omega_o}
\]

\[
Q(\theta_n, \theta_l; \theta_n, \theta_l) = \|(\theta_n, \theta_l)\|_*.
\]

**Lemma:** The reduced space problem has a **unique** solution

**Key result:** \[
\int_{\Omega_o} (v_n(\sigma_n) - v_l(\sigma_l)) (v_n(\mu_n) - v_l(\mu_l)) := ((\sigma_n, \sigma_l), (\mu_n, \mu_l))_*
\]

defines an **inner product** in the control variable space

\[
\Rightarrow \| v_n(\theta_n) - v_l(\theta_l) \|_{0, \Omega_o}^2 := \|(\sigma_n, \sigma_l)\|_*
\]

defines a norm in the control variable space
– M. D'Elia, P. Bochev, Formulation, analysis and computation of an optimization-based local-to-nonlocal coupling method, submitted, 2018
Optimization problem

\[
\min_{u_n, u_l, \theta_n, \theta_l} \frac{1}{2} \| u_n - u_l \|_{0, \Omega_o}^2
\]

s.t. \[
\begin{align*}
-\mathcal{L} u_n &= f_n \quad x \in \omega_n \\
u_n &= \theta_n \quad x \in \eta_c \\
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-\Delta u_l &= f_l \quad x \in \Omega_l \\
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\]
Optimization problem

$$\min_{u_n, u_l, \theta_n, \theta_l} \frac{1}{2} \|u_n - u_l\|^2_{0, \Omega_o}$$

s.t. \( -\mathcal{L}u_n = f_n \quad x \in \omega_n \)
\( u_n = \theta_n \quad x \in \gamma_c \)
\( u_n = 0 \quad x \in \gamma_D \)

\( \begin{align*}
-\Delta u_l &= f_l \quad x \in \Omega_l \\
 u_l &= \theta_l \quad x \in \Gamma_c \\
 u_l &= 0 \quad x \in \Gamma_D 
\end{align*} \)

weak form + FEM

$$\int_{\Omega_n} \int_{\Omega_n} \mathcal{G} u_n^h \mathcal{G} z_n^h \, dy \, dx = \int_{\omega_n} f_n z_n^h \, dx$$
$$\int_{\Omega_l} \nabla u_l^h \nabla z_l^h \, dx = \int_{\Omega_l} f_l z_l^h \, dx$$
PRELIMINARY TEST – 1D

\[ \begin{align*}
-\varepsilon & \quad 0 & 0.75 & 1 & 1 + \varepsilon & 1.75 \\
\Omega_n & \quad \Omega_l \\
\text{homogeneous Dirichlet} & \quad \theta_l & \quad \theta_n & \quad \text{homogeneous Dirichlet} \\
\quad u_n = 0 & \quad & \quad \quad \quad u_l = 0
\end{align*} \]
Outcome  • the method is consistent, i.e. passes the patch test

  • for piecewise linear FE (CG and DG) we obtain optimal convergence rates
\begin{align*}
\gamma & \text{ integrable} \\
& u = x^2
\end{align*}

\begin{align*}
\gamma & \text{ integrable} \\
& u = x^3
\end{align*}

\begin{align*}
\gamma & \text{ singular} \\
& u = x^2
\end{align*}

\begin{align*}
\gamma & \text{ singular} \\
& u = x^3
\end{align*}
## Accuracy tests

<table>
<thead>
<tr>
<th>ε</th>
<th>h</th>
<th>$e(u_n)$</th>
<th>rate</th>
<th>$e(u_l)$</th>
<th>rate</th>
<th>$e(\theta_n)$</th>
<th>rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^{-3}$</td>
<td>2.36e-03</td>
<td>-</td>
<td>2.62e-03</td>
<td>-</td>
<td>6.52e-04</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>$2^{-4}$</td>
<td>7.54e-04</td>
<td>1.65</td>
<td>7.12e-04</td>
<td>1.88</td>
<td>1.78e-04</td>
<td>1.87</td>
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</tr>
<tr>
<td>$2^{-5}$</td>
<td>1.88e-04</td>
<td>2.00</td>
<td>1.78e-04</td>
<td>2.00</td>
<td>4.45e-05</td>
<td>2.00</td>
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</tr>
<tr>
<td>$2^{-6}$</td>
<td>4.67e-05</td>
<td>2.01</td>
<td>4.44e-05</td>
<td>2.00</td>
<td>1.11e-05</td>
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<td></td>
</tr>
<tr>
<td>$2^{-7}$</td>
<td>1.14e-05</td>
<td>2.04</td>
<td>1.10e-05</td>
<td>2.01</td>
<td>2.76e-06</td>
<td>2.01</td>
<td></td>
</tr>
</tbody>
</table>

**quadratic**

$u_n = u_l = x^2$

0.065

<table>
<thead>
<tr>
<th>ε</th>
<th>h</th>
<th>$e(u_n)$</th>
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<th>rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^{-3}$</td>
<td>9.70e-03</td>
<td>-</td>
<td>2.95e-02</td>
<td>-</td>
<td>4.86e-03</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>$2^{-4}$</td>
<td>2.68e-03</td>
<td>1.86</td>
<td>7.54e-03</td>
<td>1.97</td>
<td>1.20e-03</td>
<td>2.01</td>
<td></td>
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<tr>
<td>$2^{-5}$</td>
<td>7.02e-04</td>
<td>1.93</td>
<td>1.90e-03</td>
<td>1.99</td>
<td>3.11e-04</td>
<td>1.95</td>
<td></td>
</tr>
<tr>
<td>$2^{-6}$</td>
<td>1.78e-04</td>
<td>1.98</td>
<td>4.76e-04</td>
<td>2.00</td>
<td>7.89e-05</td>
<td>1.98</td>
<td></td>
</tr>
<tr>
<td>$2^{-7}$</td>
<td>4.48e-05</td>
<td>1.99</td>
<td>1.19e-04</td>
<td>2.00</td>
<td>1.99e-05</td>
<td>1.98</td>
<td></td>
</tr>
</tbody>
</table>

**cubic**

$u_n = u_l = x^3$

0.065
STATIC NONLOCAL ELASTICITY

**THE PERIDYNAMIC MODEL**

Peridynamic (PD) equilibrium equation:

\[-\mathcal{L}[\mathbf{u}](\mathbf{x}) := - \int_{\Omega^+} \{ \mathbf{T}[\mathbf{x}]\langle \mathbf{x}' - \mathbf{x} \rangle - \mathbf{T}[\mathbf{x}']\langle \mathbf{x} - \mathbf{x}' \rangle \} \, dV_{\mathbf{x}'} = \mathbf{b}(\mathbf{x})\]

\(\mathbf{u}\): displacement field, \(\mathbf{b}\): given body force, \(\mathbf{T}\): force state field
THE PERIDYNAMIC MODEL

Peridynamic (PD) equilibrium equation:

\[-\mathcal{L}[u](x) := -\int_{\Omega^+} \{ T[x](x' - x) - T[x'](x - x') \} \, dV_{x'} = b(x)\]

\(u\): displacement field, \(b\): given body force, \(T\): force state field

PD model: linearized linear peridynamic solid (LPS) model

\[T[x]\xi = \frac{\omega(|\xi|)}{m} \left\{ (3K - 5G) \theta(x)\xi + 15G \frac{\xi \otimes \xi}{|\xi|^2} (u(x + \xi) - u(x)) \right\}\]

\(K\): bulk modulus, \(G\): shear modulus, \(\theta\): linearized nonlocal dilatation

LPS equation: \(-\mathcal{L}_{LPS}[u](x) = b(x) \quad x \in \omega_n, \quad u(x) = g(x) \quad x \in \eta_D,\)
Local equation: \(-\mathcal{L}_{NC}[u](x) = b(x)\), where \(\mathcal{L}_{NC}\) is Navier-Cauchy model

\[
\mathcal{L}_{NC}[u](x) := \left[ (K + \frac{1}{3}G) \nabla(\nabla \cdot u)(x) + G \nabla^2 u(x) \right]
\]

Note:  
- for a quadratic displacement field LPS reduces to NC  
- for \(\varepsilon \to 0\), LPS \(\to\) NC
THE COUPLING STRATEGY

Optimization-based coupling

$$\min_{u_n, u_l, \nu_n, \nu_l} J(u_n, u_l) = \frac{1}{2} \int_{\Omega_o} |u_n - u_l|^2 \, dx$$

\[
\begin{align*}
-\mathcal{L}_{\text{LPS}}[u_n] &= b \quad x \in \omega_n & -\mathcal{L}_{\text{NC}}[u_l] &= b \quad x \in \Omega_l \\
\text{s.t.} \quad u_n &= 0 \quad x \in \eta_D & u_l &= 0 \quad x \in \Gamma_D \\
\quad u_n &= \nu_n \quad x \in \eta_c & \quad u_l &= \nu_l \quad x \in \Gamma_c
\end{align*}
\]

Discretization:

**local problem:** variational form with FEM

**nonlocal problem:** strong form with mesh free method \(\Rightarrow\) modified operator

$$L[x_i] := \sum_{j \in \mathcal{N}_i} \{T[x_i] \langle x_j - x_i \rangle - T[x_j] \langle x_i - x_j \rangle\} \ V_j^{(i)}$$

$$V_j^{(i)} = |B_\varepsilon(x_i) \cap B_\varepsilon(x_j)|$$
Coupling Peridigm and Albany

peridigm.sandia.gov  software.sandia.gov/albany/  trilinos.org/packages/rol
THE GEOMETRY

\[ \Omega_n \quad \Omega_o \quad \Omega_l \]
Analytic solution: \( u = 10^{-3}(x, 0, 0) \), linear patch test, \( b(x) = 0 \)

\[ \Omega = [0, 100] \times [-12.5, 12.5] \times [-12.5, 12.5] \text{ mm}^3 \]
**THE PATCH TEST**

Analytic solution: $\mathbf{u} = 10^{-3}(x, 0, 0)$, linear patch test, $\mathbf{b}(\mathbf{x}) = 0$

$$\Omega = [0, 100] \times [-12.5, 12.5] \times [-12.5, 12.5] \text{ mm}^3$$
**Analytic solution:** $\mathbf{u} = 10^{-5}(x^2, 0, 0)$, **quadratic** patch test

$K = 150\text{GPa}$, $G = 81.496\text{GPa}$ (stainless steel), $\varepsilon = 4.270\text{mm}$

$b = 10^{-5}\left(\frac{8G}{3} + 2K\right) = 5.173\text{Nmm}^{-3}$

$\Omega = [0, 100] \times [-12.5, 12.5] \times [-12.5, 12.5] \text{mm}^3$
Analytic solution: \( u = 10^{-5}(x^2, 0, 0) \), **quadratic** patch test
**Boundary conditions:** opposite displacement (left and right) along the $x$ direction.

**Parameters:**

$\Omega := [-50, 50] \times [-12.5, 12.5] \times [-12.5, 12.5]$ mm$^3$

$K = 150$GPa, $G = 81.496$GPa (stainless steel), $\varepsilon = 2.707$mm
Boundary conditions: opposite displacement (left and right) along the $x$ direction.
TENSILE BAR

Dimensions: height = 100mm, width at mid point = 6.25mm

Parameters: $K = 160\text{GPa}$, $G = 81.496\text{GPa}$, $\varepsilon = 0.54\text{mm}$
**TENSILE BAR – WITH CRACK**

**Dimensions:** height=100mm, width at mid point=6.25mm

**Parameters:** $K = 160\text{GPa}$, $G = 81.496\text{GPa}$, $\varepsilon = 0.54\text{mm}$
Boundary conditions: Neumann on the left, Dirichlet on the right along the $x$ direction.

how can we guess nonlocal Neumann conditions???

pressure conditions can only be obtained on a surface
Boundary conditions: Neumann on the left, Dirichlet on the right along the $x$ direction.

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*how can we guess nonlocal Neumann conditions???

pressure conditions can only be obtained on a surface, i.e. locally!*
APPORACH 2: A NEW CONCEPT OF BALLS
(\ell^\infty NEIGHBORHOODS)

– C. Vollman, M. D'Elia, M. Gunzburger, V. Schulz, Formulation and analysis
of fast discretization methods for nonlocal FEM by using \ell^\infty nonlocal
neighborhoods, in progress.
APPROACH 2: A NEW CONCEPT OF BALLS
($\ell^\infty$ NEIGHBORHOODS)

*Christian Vollman, University of Trier, Germany
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NEIGHBORHOODS WITH DIFFERENT NORMS

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

- figure out intersections
- computing integrals of round domains
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- figure out intersections
- computing integrals of round domains

what if we consider a “square” ball?
⇒ retriangulation w/o geometry errors
⇒ much easier re-triangulation!
How do the new kernels look like?

\[ \gamma(x, y) = \phi(x, y) \chi_{B_{\varepsilon,*}}(x) \]

\[ B_{\varepsilon,*} = \{ y \in \mathbb{R}^n : \|x - y\|_* \leq \varepsilon \}, \text{ with } * = 1, 2, \infty \]
How do the new kernels look like?

$$\gamma(x, y) = \phi(x, y) \chi_{B_{\varepsilon,*}}(x)$$

$$B_{\varepsilon,*} = \{ y \in \mathbb{R}^n : \| x - y \|_* \leq \varepsilon \}, \text{ with } * = 1, 2, \infty$$

**IMPORTANT QUESTIONS**

0. are the nonlocal problems still well-posed?
1. do we recover local operators as $\varepsilon \to 0$?
2. do we recover fractional operators as $\varepsilon \to \infty$?
3. can we apply this technique to finite-interaction-radius applications?
NEIGHBORHOODS WITH DIFFERENT NORMS

How do the new kernels look like?

$$\gamma(x, y) = \phi(x, y) \chi_{B_{\varepsilon, \ast}}(x)$$

$$B_{\varepsilon, \ast} = \{y \in \mathbb{R}^n : \|x - y\|_{\ast} \leq \varepsilon\}, \text{ with } \ast = 1, 2, \infty$$

IMPORTANT QUESTIONS

0. are the nonlocal problems still well-posed? 
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2. do we recover fractional operators as $\varepsilon \to \infty$?
3. can we apply this technique to finite-interaction-radius applications?
NEIGHBORHOODS WITH DIFFERENT NORMS

1. Do we recover the local limit?

\[ \mathcal{L}_\varepsilon u(x) = \Delta u(x) + \mathcal{O}(\varepsilon^2) \]

\[ |a_\varepsilon(u,v) - a_0(u,v)| \to 0, \text{ as } \varepsilon \to 0 \]

\[ \|u_\varepsilon - u_0\|_{L^2(\Omega)} \to 0, \text{ as } \varepsilon \to 0 \]
1. Do we recover the local limit? ✓

\[ \mathcal{L}_\varepsilon u(x) = \Delta u(x) + O(\varepsilon^2) \]

\[ |a_\varepsilon(u, v) - a_0(u, v)| \rightarrow 0, \text{ as } \varepsilon \rightarrow 0 \]

\[ \|u_\varepsilon - u_0\|_{L^2(\Omega)} \rightarrow 0, \text{ as } \varepsilon \rightarrow 0 \text{ tested!} \]
2. Do we recover the fractional limit?

\[ \gamma_0(x, y) = C_s \int_{\mathbb{R}^n} \frac{1}{\|x - y\|^{n+2s}} \, dy \]

\[ \gamma_s(x, y) = C_{\varepsilon,s} \int_{B_{\varepsilon,s}(x)} \frac{1}{\|x - y\|^{n+2s}} \, dy \]

\[ a_s(u, v) = a_0(u, v) + K_s \frac{1}{\varepsilon^{2s}} \]

\[ \|u_s - u_0\|_{H^s(\Omega)} \leq \tilde{C}_s \|u_0\|_{L^2(\mathbb{R}^n)} \frac{1}{\varepsilon^{2s}} \]

\[ \|u_s - u_0\|_{L^2(\Omega)} \leq \hat{C}_s \|u_0\|_{L^2(\mathbb{R}^n)} \frac{1}{\varepsilon^{2s}} \]
2. Do we recover the fractional limit? ✓

\[
\gamma_0(x, y) = C_s \int_{\mathbb{R}^n} \frac{1}{\|x - y\|^{n+2s}} \, dy
\]

\[
\gamma_s(x, y) = C_{\varepsilon,s} \int_{B_{\varepsilon,s}(x)} \frac{1}{\|x - y\|^{n+2s}} \, dy
\]

\[
a_s(u, v) = a_0(u, v) + K_s \frac{1}{\varepsilon^{2s}}
\]

\[
\|u_s - u_0\|_{H^s(\Omega)} \leq \tilde{C}_s \|u_0\|_{L^2(\mathbb{R}^n)} \frac{1}{\varepsilon^{2s}} \quad \text{tested!}
\]

\[
\|u_s - u_0\|_{L^2(\Omega)} \leq \hat{C}_s \|u_0\|_{L^2(\mathbb{R}^n)} \frac{1}{\varepsilon^{2s}} \quad \text{tested!}
\]
3. Applications with finite interaction radius?

Mechanics??

Image denoising: the shape of the ball does not matter, the nonlocal model is a tool
3. Applications with finite interaction radius?

Mechanics??

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

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

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

nonlocal energy norm \( \sim \|\nabla u\|_{L^2(\Omega)}^2 \)

**necessary conditions:** \(-Lu + \lambda u = \lambda f\)

nonlocal diffusion - reaction equation
3. Applications with finite interaction radius?

Mechanics??

**Image denoising:** the shape of the ball does not matter, the nonlocal model is a tool
3. Applications with finite interaction radius?

Mechanics??

**Image denoising:** the shape of the ball does not matter, the nonlocal model is a tool
Thank you
ADDITIONAL STUFF
Optimization problem:

\[
\min_{u_n, u_l, \theta_n, \theta_l} J(u_n, u_l) = \frac{1}{2} \int_{\Omega_b} (u_n - u_l)^2 \, dx = \frac{1}{2} \|u_n - u_l\|^2_{0, \Omega_b}
\]

\[
\left\{ \begin{array}{ll}
-\mathcal{L} u_n &= f_n \quad x \in \Omega_n \\
u_n &= \theta_n \quad x \in \bar{\Omega}_c \\
u_n &= 0 \quad x \in \Omega_n^D \\
-\mathcal{N}(\mathcal{G} u_n) &= 0 \quad x \in \bar{\Omega}_n^N
\end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{ll}
-\Delta u_l &= f_l \quad x \in \Omega_l \\
u_l &= \theta_l \quad x \in \Gamma_c \\
u_l &= 0 \quad x \in \Gamma_l^D \\
\nabla u_l \cdot \mathbf{n} &= 0 \quad x \in \Gamma_l^N,
\end{array} \right.
\]
IS THE SOLUTION UNIQUE?

Reduced form:

$$\min_{\theta_n, \theta_l} J(\theta_n, \theta_l) = \frac{1}{2} \int_{\Omega_b} (u_n(\theta_n) - u_l(\theta_l))^2 \, dx = \frac{1}{2} \|u_n(\theta_n) - u_l(\theta_l)\|_{0, \Omega_b}^2$$

Solution splitting:

$$u_n = v_n(\theta_n) + u_n^0 \quad \text{and} \quad u_l = v_l(\theta_l) + u_l^0$$

Reduced functional:

$$J(\theta_n, \theta_l) = \frac{1}{2} \|v_n(\theta_n) - v_l(\theta_l)\|_{0, \Omega_b}^2 + (u_n^0 - u_l^0, v_n(\theta_n) - v_l(\theta_l))_{0, \Omega_b} + \frac{1}{2} \|u_n^0 - u_l^0\|_{0, \Omega_b}^2$$

*norm in the control space*

**Lemma:** The reduced space problem has a **unique** solution

**(Lemma):** Nonlocal max principle
**Goal:** exploit the flexibility of the method and use two fundamentally different discretization schemes for the local and the nonlocal models

\[
\begin{aligned}
-\mathcal{L}u_n &= f_n \quad x \in \Omega_n \\
\theta_n &= \theta_n \quad x \in \tilde{\Omega}_c \\
+VC &
\end{aligned}
\quad 
\begin{aligned}
-\Delta u_l &= f_l \quad x \in \Omega_l \\
u_l &= \theta_l \quad x \in \Gamma_c \\
+BC &
\end{aligned}
\]

Strong form + particle method \quad Weak form + finite element method

\[
\mathcal{L}[x_i] \approx 2 \sum_{j \in \mathcal{N}_i} (u(x_j) - u(x_i)) \gamma(x_i, x_j) V_j
\]

\[
J_d(U_n, U_l) = \frac{1}{2} \sum_{i \in \mathcal{N}_b} |(U_n)_i - (U_l)_i|^2 \tilde{V}_i
\]
SOLUTION WITH A CRACK

\[ \Omega_l \quad \Omega_b \quad \Omega_n \quad \Omega_b \quad \Omega_l \]
SOLUTION WITH A CRACK

\[\Omega_l \quad \Omega_b \quad \Omega_n \quad \Omega_b \quad \Omega_l\]
SOLUTION WITH A CRACK

Nonlocal solution (top)

points along length of the bar
THE PERIDYNAMIC MODEL

Time-dependent problem:

\[ \rho(x, t) \frac{\partial^2 u(x, t)}{\partial t^2} = \int_{\Omega} \left\{ T[x, t] \langle x' - x \rangle - T[x', t] \langle x - x' \rangle \right\} dV_{x'} + b(x, t) \]

- \( \rho: \Omega \times \mathbb{R}^+ \rightarrow \mathbb{R}^+ \): mass density
- \( u: \Omega \times \mathbb{R}^+ \rightarrow \mathbb{R}^3 \): displacement field
- \( b: \Omega \times \mathbb{R}^+ \rightarrow \mathbb{R}^3 \): given body force density
- \( T: \Omega \times \mathbb{R}^+ \rightarrow \mathbb{R}^{(3, 3)} \): force state field

Static:

\[ -\mathcal{L}[u](x) := -\int_{\Omega} \left\{ T[x] \langle x' - x \rangle - T[x'] \langle x - x' \rangle \right\} dV_{x'} = b(x) \]
THE PERIDYNAMIC MODEL

\[ T[x](x' - x) = 0, \quad \forall x' \notin B_\delta(x) \]

**averaging bond elongation**

\[ T[x] \langle \xi \rangle = \frac{w(|\xi|)}{m} \left\{ (3K - 5G) \theta(x) \xi + 15G \frac{\xi \otimes \xi}{|\xi|^2} (u(x + \xi) - u(x)) \right\} \quad \forall x \in \Omega, \quad \xi = x' - x \]

**volume change, deviation, shear dilatation**

\[ K: \text{bulk modulus}, \quad G: \text{shear modulus} \]

\[ \theta: \Omega \rightarrow \mathbb{R}, \text{linearized nonlocal dilatation} \]

\[ \theta(x) = \frac{3}{m} \int_{B_\delta(0)} w(|\zeta|) \zeta \cdot (u(x + \zeta) - u(x)) dV_\zeta \]

\[ m = \int_{B_\delta(0)} w(|\zeta|) |\zeta|^2 dV_\zeta \]

\[ w: \text{spherical influence function, scalar valued function that determines the support of force states and modulates the bond strength} \]
ANOMALOUS DIFFUSION

Subsurface flow

\((-\Delta)^s c = k_{n,s} \int_{\mathbb{R}^n} \frac{c(x) - c(y)}{|x - y|^{n+2s}} \, dy\)

\(s \in (0, 1)\): rate of the mean square displacement of the diffusing quantity

Generalized model:

\(L^s u(x) = C \int \frac{u(y) - u(x)}{|x - y|^{n+2s(x,y)}} \, dy\)

\(s\): space dependent function

the diffusion rate changes partially due to changes in the size of unresolved voids in the medium
ANOMALOUS DIFFUSION

Nonlocal Darcy flow

- flow in natural porous media: the flux at a given point depends on a neighborhood that includes multiscale pathways of varying length and conductivity

- the total flow at a given location is composed of contributions from multiple pathways → nonlocality

- **volumetric flow rate** = integral of the pressure difference between a given point and any other point in the domain (or neighborhood)

Nonlocal Darcy’s equation: [Sen and Ramos 2012]

\[-\mathcal{L}p(x) = \int_D T(x, y)(p(x) - p(y)) \, dy = q\]

\(T\): conductivity kernel – aggregate strength of all the connections
\(q\): net flux
IS THE SOLUTION UNIQUE?

Discrete reduced functional:

\[ J_h(\theta_n^h, \theta_l^h) = \frac{1}{2} \| v_n^h(\theta_n^h) - v_l^h(\theta_l^h) \|_{0, \Omega_o}^2 + (u_n^{h_0} - u_l^{h_0}, v_n^h(\theta_n^h) - v_l^h(\theta_l^h))_{0, \Omega_o} \]
IS THE SOLUTION UNIQUE?

Discrete reduced functional:

\[ J_h(\theta_n^h, \theta_i^h) = \frac{1}{2} \left\| v_n^h(\theta_n^h) - v_i^h(\theta_i^h) \right\|_{0, \Omega_o}^2 + (u_n^{h0} - u_i^{h0}, v_n^h(\theta_n^h) - v_i^h(\theta_i^h))_{0, \Omega_o} \]

\[ Q_h(\theta_n^h, \theta_i^h; \theta_n^h, \theta_i^h) = \|(\theta_n^h, \theta_i^h)\|_{h^*} \]

Lemma: The discrete reduced space problem has a unique solution in the discrete control space
IS THE SOLUTION UNIQUE?

Discrete reduced functional:

\[ J_h(\theta_n^h, \theta_l^h) = \frac{1}{2} \left\| v_n^h(\theta_n^h) - v_l^h(\theta_l^h) \right\|_{0,\Omega_o}^2 + (u_n^{h0} - u_l^{h0}, v_n^h(\theta_n^h) - v_l^h(\theta_l^h))_{0,\Omega_o} \]

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Lemma: The discrete reduced space problem has a unique solution in the discrete control space

Key results: • strong discrete Cauchy-Schwarz inequality

\[ |(v_n^h(\sigma_n^h), v_l^h(\sigma_l^h))_{0,\Omega_o}| < \delta \| v_n^h(\sigma_n^h)\|_{0,\Omega_o} \| v_l^h(\sigma_l^h)\|_{0,\Omega_o}, \quad \delta < 1 \]

• inner product in the discrete control space

\[ \int_{\Omega_o} (v_n^h(\sigma_n^h) - v_l^h(\sigma_l^h)) (v_n^h(\mu_n^h) - v_l^h(\mu_l^h)) := ((\sigma_n^h, \sigma_l^h), (\mu_n^h, \mu_l^h))_{h^*} \]
IS THE SOLUTION UNIQUE?

Discrete reduced functional:

\[ J_h(\theta^h_n, \theta^h_l) = \frac{1}{2} \left\| v_n^h(\theta^h_n) - v_l^h(\theta^h_l) \right\|_{0,\Omega_o}^2 + (u^h_{n0} - u^h_{l0}, v_n^h(\theta^h_n) - v_l^h(\theta^h_l))_{0,\Omega_o} \]

\[ Q_h(\theta^h_n, \theta^h_l; \theta^h_n, \theta^h_l) = \| (\theta^h_n, \theta^h_l) \|_{h_*} \]

**Lemma:** The discrete reduced space problem has a **unique** solution in the discrete control space

**Key results:**

- **strong discrete Cauchy-Schwarz inequality**

\[ |(v_n^h(\sigma^h_n), v_l^h(\sigma^h_l))_{0,\Omega_o}| < \delta \| v_n^h(\sigma^h_n)\|_{0,\Omega_o} \| v_l^h(\sigma^h_l)\|_{0,\Omega_o}, \ \delta < 1 \]

- **inner product** in the discrete control space

\[ \int_{\Omega_o} (v_n^h(\sigma^h_n) - v_l^h(\sigma^h_l)) (v_n^h(\mu^h_n) - v_l^h(\mu^h_l)) := ((\sigma^h_n, \sigma^h_l), (\mu^h_n, \mu^h_l))_{h_*} \]
Approximation error (from 2nd Strang’s lemma)

$$\|(\theta_{n}^* - \theta_{n}^{h*}, \theta_{l}^* - \theta_{l}^{h*})\|_{h^*} \leq C_n h_n^{p_n+t} + C_l h_l^{p_l+1}$$

by using equivalence of norms

$$\|(\theta_{n}^* - \theta_{n}^{h*}, \theta_{l}^* - \theta_{l}^{h*})\|_{L^2 \times H^\frac{1}{2}}^2 \leq K_n h_n^{2(p_n+t)} + K_l h_l^{2p_l+1}$$
Approximation error (from 2nd Strang’s lemma)

\[ \| (\theta_n^* - \theta_h^*, \theta_i^* - \theta_l^h) \|_{h^*} \leq C_n h_n^{p_n+t} + C_l h_l^{p_l+1} \]

by using equivalence of norms

\[ \| (\theta_n^* - \theta_h^*, \theta_i^* - \theta_l^h) \|^2_{L^2 \times H^{1/2}} \leq K_n h_n^{2(p_n+t)} + K_l h_l^{2p_l+1} \]  \rightarrow \text{we lose } \frac{1}{2} \text{ order}