



A VECTOR CALCULUS AND FINITE ELEMENT METHODS FOR NONLOCAL DIFFUSION EQUATIONS

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LOCAL AND NONLOCAL DIFFUSION

- The elliptic equation

$$-\nabla \cdot (\mathbb{D}(\mathbf{x}) \cdot \nabla w(\mathbf{x})) = b(\mathbf{x}) \quad \text{in } \Omega \subset \mathbb{R}^d$$

models (steady state) diffusion

- The “nonlocal” equation

$$2 \int_{\Omega} (u(\mathbf{x}') - u(\mathbf{x})) \mu(\mathbf{x}, \mathbf{x}') d\mathbf{x}' = b(\mathbf{x}) \quad \text{in } \Omega \subset \mathbb{R}^d$$

with

$$\mu(\mathbf{x}, \mathbf{x}') = \mu(\mathbf{x}', \mathbf{x}) \geq 0$$

models (steady state) **nonlocal** diffusion

- to see this, consider the nonlocal diffusion equation

$$u_t = \int_{\Omega} (u(\mathbf{x}') - u(\mathbf{x})) \mu(\mathbf{x}, \mathbf{x}') d\mathbf{x}'$$

- suppose that

$$\int_{\Omega} \int_{\Omega} \mu(\mathbf{x}, \mathbf{x}') d\mathbf{x}' d\mathbf{x} = 1$$

and

$$\mu(\mathbf{x}, \mathbf{x}') = \mu(\mathbf{x}', \mathbf{x}) \geq 0$$

so that $\mu(\mathbf{x}, \mathbf{x}')$ can be interpreted as the joint probability density of moving between \mathbf{x} and \mathbf{x}'

- then

$$\begin{aligned} \int_{\Omega} (u(\mathbf{x}') - u(\mathbf{x})) \mu(\mathbf{x}, \mathbf{x}') d\mathbf{x}' \\ = \int_{\Omega} u(\mathbf{x}') \mu(\mathbf{x}, \mathbf{x}') d\mathbf{x}' - u(\mathbf{x}) \int_{\Omega} \mu(\mathbf{x}, \mathbf{x}') d\mathbf{x}' \end{aligned}$$

is the rate at which u “enters” \mathbf{x} less the rate at which u “departs” \mathbf{x}

- the nonlocal diffusion equation can be derived from a “nonlocal” random walk
- $\mu(\mathbf{x}, \mathbf{x}') = -\mu(\mathbf{x}', \mathbf{x})$ results in drift
- the nonlocal diffusion equation is an example of a differential Chapman-Kolmogorov equation

Motivations and goals

$$\int_{\Omega} (u(\mathbf{x}') - u(\mathbf{x})) \mu(\mathbf{x}, \mathbf{x}') d\mathbf{x}' \quad \text{vs.} \quad \nabla \cdot (\mathbb{D}(\mathbf{x}) \cdot \nabla w(\mathbf{x}))$$

- The nonlocal operator contains length scales
it is a multiscale operator
 - the local operator contains length scales only when the diffusion tensor \mathbb{D} does
- The nonlocal operator has lower regularity requirements
 u may be discontinuous
- The nonlocal diffusion equation does not necessarily smooth discontinuous initial conditions

- Extension to the vector case is (formally) straightforward
 - our ultimate goal – the analysis and numerical analysis of Silling's nonlocal, continuum peridynamic model for materials – then follows
 - note that the peridynamic model is a mechanical model so that we have u_{tt} and not u_t
- Here we consider the steady-state case
 - which we can view as either steady-state diffusion problem or as a mechanical equilibrium problem
- Nonlocal models are able to model phenomena at smaller length and time scales at which the underlying assumption of locality associated with the classical diffusion equation or the classical balance of linear momentum lead to less accurate modeling

A NONLOCAL GAUSS'S THEOREM

- For any mapping $r(\mathbf{x}, \mathbf{x}') : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$, it is easily seen that

$$\int_{\widehat{\Omega}} \int_{\widehat{\Omega}} r(\mathbf{x}, \mathbf{x}') d\mathbf{x}' d\mathbf{x} = \int_{\widehat{\Omega}} \int_{\widehat{\Omega}} r(\mathbf{x}', \mathbf{x}) d\mathbf{x}' d\mathbf{x} \quad \forall \widehat{\Omega} \subseteq \mathbb{R}^d$$

- If $p(\mathbf{x}', \mathbf{x})$ denotes an **anti-symmetric** mapping, i.e.,

$$p(\mathbf{x}', \mathbf{x}) = -p(\mathbf{x}, \mathbf{x}') \text{ for all } \mathbf{x}, \mathbf{x}' \in \mathbb{R}^d$$

then

$$\int_{\widehat{\Omega}} \int_{\widehat{\Omega}} p(\mathbf{x}, \mathbf{x}') d\mathbf{x}' d\mathbf{x} = 0 \quad \forall \widehat{\Omega} \subseteq \mathbb{R}^d$$

- Let Ω denote an open bounded subset of \mathbb{R}^d . Obviously, if $\Gamma \subseteq \mathbb{R}^d \setminus \Omega$ and $p(\mathbf{x}', \mathbf{x})$ is **anti-symmetric**, by setting $\widehat{\Omega} = \Omega \cup \Gamma$, we have

$$\int_{\Omega} \int_{\Omega \cup \Gamma} p(\mathbf{x}, \mathbf{x}') d\mathbf{x}' d\mathbf{x} = - \int_{\Gamma} \int_{\Omega \cup \Gamma} p(\mathbf{x}, \mathbf{x}') d\mathbf{x}' d\mathbf{x}$$

- Let $\boldsymbol{\alpha}(\mathbf{x}, \mathbf{x}') : \Omega \cup \Gamma \times \Omega \cup \Gamma \rightarrow \mathbb{R}^d$ and $\mathbf{f}(\mathbf{x}, \mathbf{x}') : \Omega \cup \Gamma \times \Omega \cup \Gamma \rightarrow \mathbb{R}^d$ denote vector-valued mappings

- Let \mathcal{D} denote the linear operator mapping vector-valued functions \mathbf{f} into scalar-valued functions defined over Ω given by

$$\mathcal{D}(\mathbf{f})(\mathbf{x}) := \int_{\Omega \cup \Gamma} (\mathbf{f}(\mathbf{x}, \mathbf{x}') \cdot \boldsymbol{\alpha}(\mathbf{x}, \mathbf{x}') - \mathbf{f}(\mathbf{x}', \mathbf{x}) \cdot \boldsymbol{\alpha}(\mathbf{x}', \mathbf{x})) d\mathbf{x}' \quad \text{for } \mathbf{x} \in \Omega$$

- \mathcal{D} is a nonlocal “divergence” operator

- Similarly, let \mathcal{N} denote the linear operator mapping vector-valued functions \mathbf{f} into scalar-valued functions defined over Γ given by

$$\mathcal{N}(\mathbf{f})(\mathbf{x}) := - \int_{\Omega \cup \Gamma} (\mathbf{f}(\mathbf{x}, \mathbf{x}') \cdot \boldsymbol{\alpha}(\mathbf{x}, \mathbf{x}') - \mathbf{f}(\mathbf{x}', \mathbf{x}) \cdot \boldsymbol{\alpha}(\mathbf{x}', \mathbf{x})) d\mathbf{x}' \quad \text{for } \mathbf{x} \in \Gamma$$

- \mathcal{N} is a nonlocal “normal flux” operator

- Note that the operators \mathcal{D} and \mathcal{N} differ only in their domains and in their signs

- Then,

$$\text{setting } p(\mathbf{x}, \mathbf{x}') = \mathbf{f}(\mathbf{x}, \mathbf{x}') \cdot \boldsymbol{\alpha}(\mathbf{x}, \mathbf{x}') - \mathbf{f}(\mathbf{x}', \mathbf{x}) \cdot \boldsymbol{\alpha}(\mathbf{x}', \mathbf{x})$$

results in the **nonlocal Gauss's theorem**

$$\int_{\Omega} \mathcal{D}(\mathbf{f}) d\mathbf{x} = \int_{\Gamma} \mathcal{N}(\mathbf{f}) d\mathbf{x}$$

Relation to the classical Gauss's theorem

- We apply two remarkable lemmas due to Walter Noll

W. NOLL, Die Herleitung der Grundgleichungen der Thermomechanik der Kontinua aus der statistischen Mechanik; *Indiana Univ. Math. J.* **4** 1955, 627–646. Originally published in *J. Rational Mech. Anal.*

See also W. NOLL, Derivation of the fundamental equations of continuum thermodynamics from statistical mechanics; Translation with corrections by R. Lehoucq and O. von Lilienfeld, to appear in *J. Elasticity*, 2009

- Given a mapping $\mathbf{f}(\mathbf{x}, \mathbf{x}')$, let

$$\textcolor{red}{p}(\mathbf{x}, \mathbf{x}') = p(\mathbf{x}, \mathbf{x}') = \mathbf{f}(\mathbf{x}, \mathbf{x}') \cdot \boldsymbol{\alpha}(\mathbf{x}, \mathbf{x}') - \mathbf{f}(\mathbf{x}', \mathbf{x}) \cdot \boldsymbol{\alpha}(\mathbf{x}', \mathbf{x})$$

and, with $\mathbf{z} = \mathbf{x}' - \mathbf{x}$

$$\textcolor{red}{\varphi}(\mathbf{x}, \mathbf{z}) = \int_0^1 \textcolor{blue}{p}(\mathbf{x} + \lambda \mathbf{z}, \mathbf{x} - (1 - \lambda) \mathbf{z}) d\lambda$$

$$\textcolor{red}{\mathbf{q}}(\mathbf{x}) = - \int_{\mathbb{R}^d} (\mathbf{x}' - \mathbf{x}) \textcolor{blue}{\varphi}(\mathbf{x}, \mathbf{x}' - \mathbf{x}) d\mathbf{x}'$$

- Then, a formal application of Lemma I of Noll implies

$$\nabla \cdot \mathbf{q} = \int_{\mathbb{R}^d} (\mathbf{f}(\mathbf{x}, \mathbf{x}') \cdot \boldsymbol{\alpha}(\mathbf{x}, \mathbf{x}') - \mathbf{f}(\mathbf{x}', \mathbf{x}) \cdot \boldsymbol{\alpha}(\mathbf{x}', \mathbf{x})) d\mathbf{x}' \quad \text{for } \mathbf{x} \in \Omega$$

- using the definition of the operator $\mathcal{D}(\cdot)$, we then have

$$\nabla \cdot \mathbf{q} = \mathcal{D}(\mathbf{f}) \quad \text{for } \mathbf{x} \in \Omega$$

- Lemma II of Noll implies

$$\int_{\partial\Omega} \mathbf{q}(\mathbf{x}) \cdot \mathbf{n} dA = \int_{\Omega} \int_{\Gamma} (\mathbf{f}(\mathbf{x}, \mathbf{x}') \cdot \boldsymbol{\alpha}(\mathbf{x}, \mathbf{x}') - \mathbf{f}(\mathbf{x}', \mathbf{x}) \cdot \boldsymbol{\alpha}(\mathbf{x}', \mathbf{x})) d\mathbf{x}' d\mathbf{x}$$

where

$\partial\Omega$ = boundary of Ω

dA = surface element on $\partial\Omega$

\mathbf{n} = outward pointing unit normal vector along $\partial\Omega$

- using the definition of the operator $\mathcal{N}(\cdot)$, we then have

$$\int_{\partial\Omega} \mathbf{q}(\mathbf{x}) \cdot \mathbf{n} dA = \int_{\Gamma} \mathcal{N}(\mathbf{f}) d\mathbf{x}$$

- Summarizing, given a function $\mathbf{f}(\cdot, \cdot)$, if $\mathbf{q}(\cdot)$ is determined from $\mathbf{f}(\cdot, \cdot)$ according to

$$p(\mathbf{x}, \mathbf{x}') = p(\mathbf{x}, \mathbf{x}') = \mathbf{f}(\mathbf{x}, \mathbf{x}') \cdot \boldsymbol{\alpha}(\mathbf{x}, \mathbf{x}') - \mathbf{f}(\mathbf{x}', \mathbf{x}) \cdot \boldsymbol{\alpha}(\mathbf{x}', \mathbf{x})$$

$$\varphi(\mathbf{x}, \mathbf{z}) = \int_0^1 p(\mathbf{x} + \lambda \mathbf{z}, \mathbf{x} - (1 - \lambda)\mathbf{z}) d\lambda \quad \text{with } \mathbf{z} = \mathbf{x}' - \mathbf{x}$$

$$\mathbf{q}(\mathbf{x}) = - \int_{\mathbb{R}^d} (\mathbf{x}' - \mathbf{x}) \varphi(\mathbf{x}, \mathbf{x}' - \mathbf{x}) d\mathbf{x}'$$

then, **the nlocal Gauss's theorem for \mathbf{f}**

$$\int_{\Omega} \mathcal{D}(\mathbf{f}) d\mathbf{x} = \int_{\Gamma} \mathcal{N}(\mathbf{f}) d\mathbf{x}$$

implies the classical Gauss's theorem for \mathbf{q}

$$\int_{\Omega} \nabla \cdot \mathbf{q} d\mathbf{x} = \int_{\partial\Omega} \mathbf{q} \cdot \mathbf{n} d\mathbf{x}$$

- In the paper

G. GILBOA AND S. OSHER, Nonlocal operators with applications to image processing; *Multiscale Model. Simul.* **7** 2008, 1005-1028.

the nonlocal “divergence theorem”

$$\int_{\Omega} (\mathcal{D}f)(\mathbf{x}) \, d\mathbf{x} = 0$$

is given

- this is a the special case of our nonlocal Gauss’s theorem for $\Gamma = \emptyset$ and for scalar-valued f
- Gilboa and Osher also provide the germs of a nonlocal calculus but do not provide Green’s identities or consider nonlocal BVPs

- Important related papers by Rossi and co-workers that deal with nonlocal diffusion problems

F. ANDREU, J. MAZON, J. ROSSI, AND J. TOLEDO, A nonlocal p -Laplacian evolution equation with Neumann boundary conditions; *J. Math. Pures Appl.* **40** 2008, 201–227.

F. ANDREU, J. MAZON, J. ROSSI, AND J. TOLEDO, A nonlocal p -Laplacian evolution equation with nonhomogeneous Dirichlet boundary conditions; *SIAM J. Math. Anal.* **40** 2009, 1815–1851.

+ several others

Notational simplification

- In the sequel, we frequently let

$$u = u(\mathbf{x}) \qquad u' = u(\mathbf{x}')$$

$$v = v(\mathbf{x}) \qquad v' = v(\mathbf{x}')$$

$$\mathbf{f} = \mathbf{f}(\mathbf{x}, \mathbf{x}') \qquad \mathbf{f}' = \mathbf{f}(\mathbf{x}', \mathbf{x})$$

$$\boldsymbol{\alpha} = \boldsymbol{\alpha}(\mathbf{x}, \mathbf{x}') \qquad \boldsymbol{\alpha}' = \boldsymbol{\alpha}(\mathbf{x}', \mathbf{x})$$

and similarly for functions still to be introduced

- Also,
 - scalar-valued functions are denoted in plain face – u, β
 - vector-valued functions are denoted in bold face – $\mathbf{x}, \boldsymbol{\alpha}$
 - tensor-valued functions are denoted in blackboard face – \mathbb{K}, \mathbb{D}

An application of the nonlocal Gauss's theorem

- For functions $v(\mathbf{x})$ and $\mathbf{s}(\mathbf{x}, \mathbf{x}')$, set $\mathbf{f} = v\mathbf{s}$ so that

$$\mathbf{f}\boldsymbol{\alpha} - \mathbf{f}'\boldsymbol{\alpha}' = v\mathbf{s} \cdot \boldsymbol{\alpha} - v'\mathbf{s}' \cdot \boldsymbol{\alpha}' = v(\mathbf{s} \cdot \boldsymbol{\alpha} - \mathbf{s}' \cdot \boldsymbol{\alpha}') + (v - v')\mathbf{s}' \cdot \boldsymbol{\alpha}'$$

- Using the definitions of the operators \mathcal{D} and \mathcal{N} , one obtains from the nonlocal Gauss's theorem

$$\int_{\Omega} v\mathcal{D}(\mathbf{s}) d\mathbf{x} + \int_{\Omega \cup \Gamma} \int_{\Omega \cup \Gamma} (v' - v)\mathbf{s} \cdot \boldsymbol{\alpha} d\mathbf{x}' d\mathbf{x} = \int_{\Gamma} v\mathcal{N}(\mathbf{s}) d\mathbf{x}$$

- Let \mathcal{G} denote the linear operator mapping functions $v : \Omega \cup \Gamma \rightarrow \mathbb{R}$ into functions defined over $\Omega \cup \Gamma \times \Omega \cup \Gamma$ given by

$$\mathcal{G}(v) = (v' - v)\boldsymbol{\alpha} \quad \text{for } \mathbf{x}, \mathbf{x}' \in \Omega \cup \Gamma$$

- Then, we obtain

$$\int_{\Omega} v \mathcal{D}(\mathbf{s}) d\mathbf{x} + \int_{\Omega \cup \Gamma} \int_{\Omega \cup \Gamma} \mathbf{s} \cdot \mathcal{G}(v) d\mathbf{x}' d\mathbf{x} = \int_{\Gamma} v \mathcal{N}(\mathbf{s}) d\mathbf{x}$$

- this is the nonlocal analog of the classical result

$$\int_{\Omega} v \nabla \cdot \mathbf{q} d\mathbf{x} + \int_{\Omega} \nabla v \cdot \mathbf{q} d\mathbf{x} = \int_{\partial\Omega} v \mathbf{q} \cdot \mathbf{n} dA$$

- the particular choice $v = \text{constant}$ results in

$$\int_{\Omega} \mathcal{D}(\mathbf{s}) d\mathbf{x} = \int_{\Gamma} \mathcal{N}(\mathbf{s}) d\mathbf{x}$$

i.e., the nonlocal Gauss's theorem for \mathbf{s}

- One sees that

$$\int_{\Omega} v \mathcal{D}(\mathbf{s}) \, d\mathbf{x} + \int_{\Omega \cup \Gamma} \int_{\Omega \cup \Gamma} \mathbf{s} \cdot \mathcal{G}(v) \, d\mathbf{x}' d\mathbf{x} = \int_{\Gamma} v \mathcal{N}(\mathbf{s}) \, d\mathbf{x}$$

can be written as

$$(v, \mathcal{D}(\mathbf{s}))_{L^2(\Omega)} - (-\mathcal{G}(v), \mathbf{s})_{[L^2((\Omega \cup \Gamma) \times (\Omega \cup \Gamma))]^d} = (v, \mathcal{N}(\mathbf{s}))_{L^2(\Gamma)}$$

where

$(\cdot, \cdot)_X$ denotes the inner product on the Hilbert space X

- mimicking the classical theory for local differential operators, we see that \mathcal{D} and $-\mathcal{G}$ are adjoint operators

NONLINEAR, NONLOCAL BOUNDARY-VALUE PROBLEMS

- Let

$U(\Omega \cup \Gamma)$ and $V(\Omega \cup \Gamma)$ denote Banach spaces

$$\Gamma = \Gamma_e + \Gamma_n \quad \text{with} \quad \Gamma_e \cap \Gamma_n = \emptyset$$

$$V_e(\Omega \cup \Gamma) = \{v \in V(\Omega \cup \Gamma) \quad : \quad v = 0 \text{ for } \mathbf{x} \in \Gamma_e\}$$

- Define the data functions

$$b : \Omega \rightarrow \mathfrak{R}$$

$$h_e : \Gamma_e \rightarrow \mathfrak{R}$$

$$h_n : \Gamma_n \rightarrow \mathfrak{R}$$

- For $u \in U(\Omega \cup \Gamma)$, let

$$s(\mathbf{x}, \mathbf{x}') = \mathcal{W}(u)$$

for a possibly nonlinear operator \mathcal{W} which also may depend explicitly on \mathbf{x} and \mathbf{x}'

- Consider the variational problem

seek $u \in U(\Omega \cup \Gamma)$ such that

$$u = h_e \quad \text{for } \mathbf{x} \in \Gamma_e$$

and

$$\int_{\Omega \cup \Gamma} \int_{\Omega \cup \Gamma} \mathcal{W}(u) \cdot \mathcal{G}(v) d\mathbf{x}' d\mathbf{x} = \int_{\Omega} v b d\mathbf{x} + \int_{\Gamma_n} v h_n d\mathbf{x} \quad \forall v \in V_e(\Omega \cup \Gamma)$$

- The nonlocal Gauss's theorem and its consequences show that the variational formulation can be viewed as a weak formulation of the nonlocal “boundary-value” problem

$$\begin{aligned} -\mathcal{D}(\mathcal{W}(u)) &= b & \text{for } \mathbf{x} \in \Omega \\ u &= h_e & \text{for } \mathbf{x} \in \Gamma_e \\ \mathcal{N}(\mathcal{W}(u)) &= h_n & \text{for } \mathbf{x} \in \Gamma_n \end{aligned}$$

- the second equation is a “Dirichlet boundary” conditions that is essential for the variational principle
- the third equation is a “Neumann boundary” condition that is natural for the variational principle

— if $\Gamma_e = \emptyset$, then

- the space of test functions $V_e(\Omega \cup \Gamma)$ is replaced by $V(\Omega \cup \Gamma)/\mathfrak{R}$

- the compatibility condition

$$\int_{\Omega} b d\mathbf{x} + \int_{\Gamma} h_n d\mathbf{x} = 0$$

must hold

- this is entirely analogous to the classical case

NONLOCAL LINEAR OPERATORS AND GREEN'S IDENTITIES

- We now specialize to the case of $U(\Omega \cup \Gamma) = V(\Omega \cup \Gamma)$ and to linear operators
- For a tensor-valued mapping $\mathbb{K}(\mathbf{x}, \mathbf{x}')$, let

$$\mathbf{s} = \mathcal{W}(u) = \mathbb{K} \cdot \mathcal{G}(u) = (u' - u)\mathbb{K} \cdot \boldsymbol{\alpha}$$

— this is a **constitutive relation**

- From the nonlocal Gauss's theorem, we then obtain the **nonlocal Green's first identity**

$$\int_{\Omega} v \mathcal{D}(\mathbb{K} \cdot \mathcal{G}(u)) d\mathbf{x} + \int_{\Omega \cup \Gamma} \int_{\Omega \cup \Gamma} \mathcal{G}(v) \cdot \mathbb{K} \cdot \mathcal{G}(u) d\mathbf{x}' d\mathbf{x} = \int_{\Gamma} v \mathcal{N}(\mathbb{K} \cdot \mathcal{G}(u)) d\mathbf{x}$$

— this is the nonlocal analog of the classical Green's first identity

$$\int_{\Omega} v \nabla \cdot (\mathbb{D} \nabla u) d\mathbf{x} + \int_{\Omega} \nabla v \cdot \mathbb{D} \cdot \nabla u d\mathbf{x} = \int_{\partial\Omega} v \mathbf{n} \cdot (\mathbb{D} \nabla u) dA$$

- One can immediately obtain a **nonlocal Green's second identity**

$$\begin{aligned} \int_{\Omega} v \mathcal{D}(\mathbb{K} \cdot \mathcal{G}(u)) \, d\mathbf{x} - \int_{\Omega} u \mathcal{D}(\mathbb{K} \cdot \mathcal{G}(v)) \, d\mathbf{x} \\ = \int_{\Gamma} \left(v \mathcal{N}(\mathbb{K} \cdot \mathcal{G}(u)) - u \mathcal{N}(\mathbb{K} \cdot \mathcal{G}(v)) \right) d\mathbf{x} \end{aligned}$$

- this is the nonlocal analog of the classical Green's second identity

$$\begin{aligned} \int_{\Omega} v \nabla \cdot (\mathbb{D} \nabla u) \, d\mathbf{x} - \int_{\Omega} u \nabla \cdot (\mathbb{D} \nabla v) \, d\mathbf{x} \\ = \int_{\partial\Omega} v \mathbf{n} \cdot (\mathbb{D} \nabla u) \, dA - \int_{\partial\Omega} u \mathbf{n} \cdot (\mathbb{D} \nabla v) \, dA \end{aligned}$$

- A nonlocal Green's third identity will come later

LINEAR, NONLOCAL BOUNDARY-VALUE PROBLEMS

- For $s = \mathcal{W}(u) = \mathbb{K} \cdot \mathcal{G}(u) = (u' - u)\mathbb{K} \cdot \boldsymbol{\alpha}$ and

$$U(\Omega \cup \Gamma) = V(\Omega \cup \Gamma) = L^2(\Omega \cup \Gamma)$$

the variational problem reduces to

seek $u \in V(\Omega \cup \Gamma)$ such that

$$u = h_e \quad \text{for } \mathbf{x} \in \Gamma_e$$

and

$$\begin{aligned} \int_{\Omega \cup \Gamma} \int_{\Omega \cup \Gamma} \mathcal{G}(v) \cdot \mathbb{K} \cdot \mathcal{G}(u) \, d\mathbf{x}' d\mathbf{x} \\ = \int_{\Omega} v b \, d\mathbf{x} + \int_{\Gamma_n} v h_n \, d\mathbf{x} \quad \forall v \in L_e^2(\Omega \cup \Gamma) \end{aligned}$$

where

$$L_e^2(\Omega \cup \Gamma) = \{v \in L^2(\Omega \cup \Gamma) : v = 0 \text{ on } \Gamma_e\}$$

- The corresponding “boundary-value” problem reduces to the linear problem

$$\begin{aligned} -\mathcal{D}(\mathbb{K} \cdot \mathcal{G}(u)) &= b & \text{for } \mathbf{x} \in \Omega \\ u &= h_e & \text{for } \mathbf{x} \in \Gamma_e \\ \mathcal{N}(\mathbb{K} \cdot \mathcal{G}(u)) &= h_n & \text{for } \mathbf{x} \in \Gamma_n \end{aligned}$$

- We have the explicit relations

$$\begin{aligned} \int_{\Omega \cup \Gamma} \int_{\Omega \cup \Gamma} \mathcal{G}(v) \cdot \mathbb{K} \cdot \mathcal{G}(u) \, d\mathbf{x}' d\mathbf{x} &= \int_{\Omega \cup \Gamma} \int_{\Omega \cup \Gamma} (v' - v) \boldsymbol{\alpha} \cdot \mathbb{K} \cdot \boldsymbol{\alpha} (u' - u) \, d\mathbf{x}' d\mathbf{x} \\ \mathcal{D}(\mathbb{K} \cdot \mathcal{G}(u)) &= 2 \int_{\Omega \cup \Gamma} (u' - u) \boldsymbol{\alpha} \cdot \mathbb{K} \cdot \boldsymbol{\alpha} \, d\mathbf{x}' & \text{for } \mathbf{x} \in \Omega \\ \mathcal{N}(\mathbb{K} \cdot \mathcal{G}(u)) &= -2 \int_{\Omega \cup \Gamma} (u' - u) \boldsymbol{\alpha} \cdot \mathbb{K} \cdot \boldsymbol{\alpha} \, d\mathbf{x}' & \text{for } \mathbf{x} \in \Gamma_n \end{aligned}$$

- The linear nonlocal “boundary-value” problem may be expressed in the form

$$\text{seek } u \in L^2(\Omega \cup \Gamma) \text{ such that } u = h_e \text{ for } \mathbf{x} \in \Gamma_e \text{ and} \\ B(u, v) = F(v) \quad \forall v \in L_e^2(\Omega \cup \Gamma),$$

where, for all $u, v \in L^2(\Omega \cup \Gamma)$, we have the bilinear form

$$B(u, v) := \int_{\Omega \cup \Gamma} \int_{\Omega \cup \Gamma} \mathcal{G}(v) \cdot \mathbb{K} \cdot \mathcal{G}(u) d\mathbf{x}' d\mathbf{x} \\ = \int_{\Omega \cup \Gamma} \int_{\Omega \cup \Gamma} (v' - v) \boldsymbol{\alpha} \cdot \mathbb{K} \cdot \boldsymbol{\alpha}(u' - u) d\mathbf{x}' d\mathbf{x}$$

and the linear functional

$$F(v) := \int_{\Omega} v b d\mathbf{x} + \int_{\Gamma_n} v h_n d\mathbf{x}$$

- The analogous classical problem has

$$B(u, v) = \int_{\Omega} \nabla v \cdot \mathbb{D} \cdot \nabla u \, d\mathbf{x}$$

WELL POSEDENESS OF NONLOCAL LINEAR BOUNDARY-VALUE PROBLEMS

- We now assume that the constitutive tensor \mathbb{K} is symmetric and positive definite and that its elements are symmetric mappings and that

$$\int_{\Omega \cup \Gamma} \boldsymbol{\alpha} \cdot \mathbb{K} \cdot \boldsymbol{\alpha} \, d\mathbf{x}' \leq K_1 \quad \text{and} \quad \int_{\Gamma_e} \boldsymbol{\alpha} \cdot \mathbb{K} \cdot \boldsymbol{\alpha} \, d\mathbf{x}' \geq K_2 \quad \forall \mathbf{x} \in \Omega \cup \Gamma$$

- We assume that $\Gamma_n = \emptyset$ and $h_e = 0$ and $b \in L^2(\Omega)$
 - so we treat the homogeneous “Dirichlet” problem

- One easily sees that

$$|F(v)| \leq \|b\|_{L^2(\Omega)} \|v\|_{L^2(\Omega \cup \Gamma)} \quad \forall v \in L^2(\Omega \cup \Gamma)$$

so that $F(v)$ is a bounded linear functional on $L^2(\Omega \cup \Gamma)$

- It can be shown that

$$B(u, v) = B(v, u) \quad \forall u, v \in L^2(\Omega \cup \Gamma)$$

$$|B(u, v)| \leq 4K_1 \|u\|_{L^2(\Omega \cup \Gamma)} \|v\|_{L^2(\Omega \cup \Gamma)} \quad \forall u, v \in L^2(\Omega \cup \Gamma)$$

$$B(u, u) \geq K_2 \|u\|_{L^2(\Omega \cup \Gamma)}^2 \quad \forall u \in L_e^2(\Omega \cup \Gamma)$$

so that the bilinear form $B(\cdot, \cdot)$ is symmetric, continuous, and coercive with respect to $L_e^2(\Omega \cup \Gamma)$

- By the Lax-Milgram theorem, we then have that the variational problem has a unique solution $u \in L_e^2(\Omega \cup \Gamma)$ and, moreover, that solution satisfies

$$\|u\|_{L^2(\Omega \cup \Gamma)} \leq \frac{1}{K_2} \|b\|_{L^2(\Omega)}$$

- note that, unlike the classical elliptic PDE case, there is no smoothing from the data to the solution

- Related papers that give more extensive analyses, including making connections between the function space $V(\Omega \cup \Gamma)$ and fractional Sobolev spaces with index $0 \leq s \leq 1$

Q. DU AND K. ZHOU, Mathematical analysis for the peridynamic nonlocal continuum theory; submitted.

K. ZHOU AND Q. DU, Mathematical and numerical analysis of linear peridynamic models with nonlocal boundary conditions; submitted.

Q. DU, M. GUNZBURGER, R. LEHOUCQ, AND K. ZHOU, A vector nonlocal calculus with application to the peridynamic model; in preparation

ADDITIONAL RESULTS

- **Green's functions and Green's third identity**

- fundamental solutions and Green's function corresponding to the linear nonlocal boundary value problem can be defined
- a **nonlocal Green's third identity** can then be derived from the Green's second identity (with G denoting a free-space Green's function)

$$u(\mathbf{y}) = \int_{\Omega} G(\mathbf{x}; \mathbf{y}) \mathcal{D}(\mathbb{K} \cdot \mathcal{G}(u(\mathbf{x}))) d\mathbf{x} \\ - \int_{\Gamma} \left(G(\mathbf{x}; \mathbf{y}) \mathcal{N}(\mathbb{K} \cdot \mathcal{G}(u(\mathbf{x}))) - u(\mathbf{x}) \mathcal{N}(\mathbb{K} \cdot \mathcal{G}(G(\mathbf{x}; \mathbf{y}))) \right) d\mathbf{x} \quad \forall \mathbf{y} \in \Omega$$

- this is the analog of the classical Green's third identity (with $\mathbb{D} = \mathbb{I}$)

$$u(\mathbf{y}) = \int_{\Omega} G(\mathbf{x}; \mathbf{y}) \Delta u(\mathbf{x}) d\mathbf{x} - \int_{\partial\Omega} \left(G(\mathbf{x}; \mathbf{y}) \frac{\partial u(\mathbf{x})}{\partial n} - u(\mathbf{x}) \frac{\partial G(\mathbf{x}; \mathbf{y})}{\partial n} \right) dA$$

- from the nonlocal Green's third identity, the solution of the nonlocal “boundary-value” problem is given by

$$\begin{aligned}
 u(\mathbf{y}) = & - \int_{\Omega} G(\mathbf{x}; \mathbf{y}) b(\mathbf{x}) d\mathbf{x} \\
 & + \int_{\Gamma_e} h_e(\mathbf{x}) \mathcal{N}(\mathbb{K} \cdot \mathcal{G}(G(\mathbf{x}; \mathbf{y}))) d\mathbf{x} - \int_{\Gamma_n} G(\mathbf{x}; \mathbf{y}) h_n(\mathbf{x}) d\mathbf{x} \\
 & \forall \mathbf{y} \in \Omega \cup \Gamma_n
 \end{aligned}$$

- the classical analog is

$$u(\mathbf{y}) = - \int_{\Omega} G(\mathbf{x}; \mathbf{y}) b(\mathbf{x}) d\mathbf{x} + \int_{\Gamma_e} h_e \frac{\partial G}{\partial n} dA - \int_{\Gamma_n} h_n G dA \quad \forall \mathbf{y} \in \Omega$$

• Local smooth limits

- We now see what happens if we assume:
 1. solutions of the nonlocal “boundary-value”-problems are smooth
 2. the nonlocal operators are asymptotically local
- we emphasize that these assumptions are made only to make the connection to classical problems for partial differential equations and are not required for the well posedness of the nonlocal “boundary-value”-problems
- in addition, the nonlocal “boundary-value”-problems admit solutions that are not solutions, even in the usual sense of weak solutions, of the partial differential equations
- thus, one can view solutions of the nonlocal “boundary-value”-problems as further generalizations of solutions of the partial differential equations, generalized in two ways: they are nonlocal and they lack the smoothness needed for them to be standard weak solutions

- **smoothness assumption:** assume that the solution $u(\mathbf{x})$ of the nonlocal “boundary-value”-problem satisfies

$$u(\mathbf{x}') = u(\mathbf{x}) + \nabla u(\mathbf{x}) \cdot (\mathbf{x}' - \mathbf{x}) + o(\varepsilon^2) \quad \text{if } \|\mathbf{x}' - \mathbf{x}\| \leq \varepsilon$$

where $\varepsilon^{-2}o(\varepsilon^2) \rightarrow 0$ as $\varepsilon \rightarrow 0$

- **locality assumption:** assume that, with $\mathbf{z} = \mathbf{x}' - \mathbf{x}$

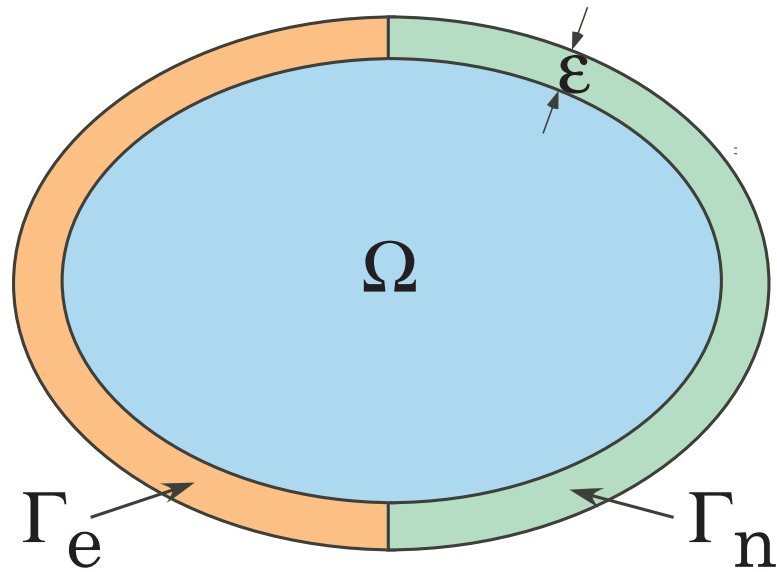
$$\alpha(\mathbf{x}, \mathbf{x}') = \frac{\mathbf{x}' - \mathbf{x}}{|\mathbf{x} - \mathbf{x}'|} \beta(|\mathbf{x} - \mathbf{x}'|) = \frac{\mathbf{z}}{|\mathbf{z}|} \beta(|\mathbf{x} - \mathbf{x}'|)$$

where, for given ε

$$\beta(|\mathbf{z}|) = 0 \quad \text{whenever } |\mathbf{z}| \geq \varepsilon$$

- several other assumptions are made to insure that integrals are finite and also about the smoothness of the data

— we consider the following geometric situation



and then see what happens as $\varepsilon \rightarrow 0$

— what happens is that, as $\varepsilon \rightarrow 0$, the nonlocal variational problem

seek $u \in L^2(\Omega \cup \Gamma)$ such that

$$u = h_e \quad \text{for } \mathbf{x} \in \Gamma_e$$

and

$$\int_{\Omega \cup \Gamma} \int_{\Omega \cup \Gamma} \mathcal{G}(v) \cdot \mathbb{K} \cdot \mathcal{G}(u) d\mathbf{x}' d\mathbf{x} = \int_{\Omega} v b d\mathbf{x} + \int_{\Gamma_n} v h_n d\mathbf{x} \quad \forall v \in L_e^2(\Omega \cup \Gamma)$$

reduces to the classical local variational problem

$$\begin{cases} \int_{\Omega} \nabla v \cdot \mathbb{D} \cdot \nabla u d\mathbf{x} = \int_{\Omega} v b d\mathbf{x} + \int_{\partial\Omega_n} v \tilde{h}_n d\mathbf{x} & \text{in } \Omega \\ u = \tilde{h}_e & \text{on } \partial\Omega_e \end{cases}$$

where

$$\mathbb{D}(\mathbf{x}) = \lim_{\varepsilon \rightarrow 0} \int_{\Omega \cup \Gamma} \mathbf{z} \otimes \mathbf{z} \frac{\mathbf{z} \cdot \mathbb{K}(\mathbf{x}, \mathbf{x}') \cdot \mathbf{z}}{|\mathbf{z}|^2} (\beta(|\mathbf{z}|))^2 d\mathbf{x}'$$

— also,

as $\varepsilon \rightarrow 0$, the corresponding nonlocal “boundary-value” problem

$$\begin{aligned} -\mathcal{D}(\mathbb{K} \cdot \mathcal{G}(u)) &= b && \text{for } \mathbf{x} \in \Omega \\ u &= h_e && \text{for } \mathbf{x} \in \Gamma_e \\ \mathcal{N}(\mathbb{K} \cdot \mathcal{G}(u)) &= h_n && \text{for } \mathbf{x} \in \Gamma_n \end{aligned}$$

reduces to classical boundary-value problem

$$\begin{cases} -\nabla \cdot (\mathbb{D} \cdot \nabla u) = b & \text{in } \Omega \\ u = \tilde{h}_e & \text{on } \partial\Omega_e \\ (\mathbb{D} \cdot \nabla u) \cdot \mathbf{n} = \tilde{h}_n & \text{on } \partial\Omega_n \end{cases}$$

- **Nonlocal linear convection-diffusion-reaction problems**

- let $\mathbf{a}(\mathbf{x}, \mathbf{x}')$ and $\omega(\mathbf{x}, \mathbf{x}')$ denote **anti-symmetric** and **symmetric** functions, respectively
- consider the nonlocal variational principle

seek $u \in V(\Omega \cup \Gamma)$ such that

$$u = h_e \quad \text{for } \mathbf{x} \in \Gamma$$

and

$$\begin{aligned} & \int_{\Omega \cup \Gamma} \int_{\Omega \cup \Gamma} \mathcal{G}(v) \cdot \mathbb{K} \cdot \mathcal{G}(u) d\mathbf{x}' d\mathbf{x} + \int_{\Omega \cup \Gamma} v \int_{\Omega \cup \Gamma} \mathbf{a} \cdot \mathcal{G}(u) d\mathbf{x}' d\mathbf{x} \\ & + \int_{\Omega \cup \Gamma} v \int_{\Omega \cup \Gamma} \omega \mathcal{A}(u) d\mathbf{x}' d\mathbf{x} = \int_{\Omega} v b d\mathbf{x} \quad \forall v \in V_e(\Omega \cup \Gamma), \end{aligned}$$

- the corresponding nonlocal “Dirichlet boundary-value” problem is given by

$$\begin{aligned} -\mathcal{D}(\mathbb{K} \cdot \mathcal{G}(u)) + \mathbf{a} \cdot \mathcal{G}(u) + \omega \mathcal{A}(u) &= b & \text{for } \mathbf{x} \in \Omega \\ u &= h_e & \text{for } \mathbf{x} \in \Gamma \end{aligned}$$

- we then have that the local smooth limit of general nonlocal “Dirichlet boundary-value” problem reduces to the general linear convection-diffusion-reaction problem

$$-\nabla \cdot (\mathbb{D} \cdot \nabla u) + \mathbf{w} \cdot \nabla u + cu = b$$

along with a Dirichlet boundary condition

- \mathbf{w} and c are related to \mathbf{a} and ω in analogous ways to how \mathbb{D} is related to \mathbb{K}

FINITE ELEMENT METHODS

- Discretization of nonlocal “boundary-value” problems are usually effected by applying a quadrature rule to the “strong” form of the equations
 - for example, the nonlocal equation

$$-\mathcal{D}(\mathbb{K} \cdot \mathcal{G}(u)) = b \quad \text{for } \mathbf{x} \in \Omega$$

which is equivalent to

$$-2 \int_{\Omega \cup \Gamma} (u' - u) \boldsymbol{\alpha} \cdot \mathbb{K} \cdot \boldsymbol{\alpha} d\mathbf{x}' = b \quad \text{for } \mathbf{x} \in \Omega$$

is discretized into

$$-2 \sum_{j=1}^N w_j (u(\mathbf{x}_j) - u(\mathbf{x}_i)) \boldsymbol{\alpha}(\mathbf{x}_i, \mathbf{x}_j) \cdot \mathbb{K}(\mathbf{x}_i, \mathbf{x}_j) \cdot \boldsymbol{\alpha}(\mathbf{x}_i, \mathbf{x}_j) = b(\mathbf{x}_i)$$

for $i = 1, \dots, M$

for some chosen set $\{\mathbf{x}_j, w_j\}_{j=1}^N$ of quadrature points and weights and some chosen set $\{\mathbf{x}_i\}_{i=1}^M$ of collocation points

- this amounts to a particle discretization and, indeed, for general peridynamic material models, such discretizations have been implemented at Sandia into LAMPPS, an existing molecular dynamics code
- We want to develop, analyze, implement, and test finite element discretizations of the nonlocal boundary value problems
 - we have a variational form of the “boundary-value” problems which we can use as the setting for developing Galerkin finite element methods
- The fact that the variational problem is well posed in $L^2(\Omega \cup \Gamma)$ means that discontinuous finite element spaces are conforming
 - in particular, unlike what is the case for elliptic PDEs, we can easily develop DG methods that do not involve accounting for fluxes across element boundaries
 - ⇒ nonlocal problems of the type we study are perfectly suited for DG methods

- In fact, in the Lax-Milgram setting we developed for the nonlocal “boundary-value” problems we have that if

u denotes the exact solution of the nonlocal “boundary-value” problem

$S^h \subset L^2(\Omega \cup \Gamma)$ denotes a finite element space

u^h denotes the finite element approximation

then

$$\|u - u^h\|_{L^2(\Omega \cup \Gamma)} \leq C \inf_{v^h \in S^h} \|u - v^h\|_{L^2(\Omega \cup \Gamma)}$$

- Of course, continuous finite element spaces are obviously conforming as well, so that we also can use them
 - a big advantage of discontinuous spaces is that the best approximation can be computed locally, i.e., one just has to determine the best approximation on each element
 - this is not possible for continuous spaces; we will see what implications these observations have

1D model problems and their discretization

- Consider the “boundary-value” problem

$$\begin{cases} \frac{1}{\delta^2} \int_{x-\delta}^{x+\delta} \frac{u(x) - u(x')}{|x - x'|} dx' = b(x) & \text{for } x \in \Omega \\ u(x) = g(x) & \text{for } x \in \Gamma \end{cases}$$

where

$$\Omega = (0, 1) \quad \Gamma = (-\delta, 0) \cup (1, 1 + \delta)$$

- δ plays the role of the localization parameter ε used earlier
- for peridynamics, it is referred to as the [horizon](#)

- We then have the Galerkin formulation

seek $u \in L^2((-\delta, 1 + \delta))$ such that

$$u(x) = g(x) \quad \text{for } x \in (-\delta, 0) \quad \text{and} \quad x \in (1, 1 + \delta)$$

and

$$\frac{1}{\delta^2} \int_0^1 \int_{x-\delta}^{x+\delta} (v(x') - v(x)) (u(x') - u(x)) \frac{1}{|x - x'|} dx' dx = \int_0^1 b(x) dx$$

$$\forall v \in L_e^2((-\delta, 1 + \delta))$$

- We then choose

$$S^h \subset L^2((-\delta, 1 + \delta))$$

$$S_e^h \subset L_e^2((-\delta, 1 + \delta))$$

$g^h(x) \in S^h|_{(-\delta, 0) \cup (1, 1 + \delta)}$ to be an approximation of $g(x)$

e.g., the L^2 projection of $g(x)$ onto $S^h|_{(-\delta, 0) \cup (1, 1 + \delta)}$

- We then define the discrete problem

seek $u^h \in S^h$ such that

$$u^h(x) = g^h(x) \quad \text{for } x \in (-\delta, 0) \quad \text{and} \quad x \in (1, 1 + \delta)$$

and

$$\frac{1}{\delta^2} \int_0^1 \int_{x-\delta}^{x+\delta} (v^h(x') - v^h(x)) (u^h(x') - u^h(x)) \frac{1}{|x - x'|} dx' dx = \int_0^1 b(x) dx$$

$$\forall v \in S_e^h$$

- This is equivalent to a linear system of algebraic equations for the coefficients of the expansion of u^h in terms of a basis for S^h
- Note that δ may be such that $(x - \delta, x + \delta)$ spans several finite element intervals
 - as a result, we have that, in general, the coefficient matrix of the linear system is banded but is not necessarily tridiagonal

- We consider two exact solutions

- a smooth solution

$$u(x) = x^2(1 - x^2) \quad \text{for which} \quad b(x) = 6x^2 + \frac{1}{2}\delta^2 - 1$$

- a solution with a jump discontinuity at $x = 0.5$

$$u(x) = \begin{cases} x & \text{for } x < 0.5 \\ x^2 & \text{for } x > 0.5 \end{cases}$$

for which

$$b(x) = \begin{cases} 0 & \text{for } x \in [0, 0.5 - \delta) \\ \frac{1}{2}\delta^2 - \delta + \frac{3}{8} + (2\delta - \frac{3}{2} - \ln \delta)x & \\ \quad + (\frac{3}{2} + \ln \delta)x^2 - (x^2 - x) \ln(\frac{1}{2} - x) & \text{for } x \in [0.5 - \delta, 0.5) \\ \frac{1}{2}\delta^2 - \delta + \frac{3}{8} + (2\delta + \frac{3}{2} + \ln \delta)x & \\ \quad - (\frac{3}{2} + \ln \delta)x^2 + (x^2 - x) \ln(x - \frac{1}{2}) & \text{for } x \in (0.5, 0.5 + \delta) \\ 1 & \text{for } x \in [0.5 + \delta, 1.0] \end{cases}$$

- We use three **conforming** finite element spaces defined (mostly) with respect to a uniform grid of size h
 - continuous piecewise linears
 - discontinuous piecewise constants
 - discontinuous piecewise linears
- One interesting thing to examine is the relation between the horizon δ and the grid size h
 - some advocate choosing $\delta = Mh$ for some integer M
 - this has the advantage that the **bandwidth** of the matrix **remains fixed** as h is reduced
 - others view δ to be a **model parameter** so that its value should not depend on h
 - in this case, the **bandwidth will increase** as h is reduced because more intervals will interact with a given interval

- For the first set of computational results, we cheat
 - for all h , we place a grid point at the location of the jump discontinuity
 - of course, one does not, in general, know where the jump discontinuity occurs
 - however, it is still instructive to compare the three different finite element discretizations in this “best-case” scenario
 - if a method is “bad” in this setting, it will be even worse in the general setting

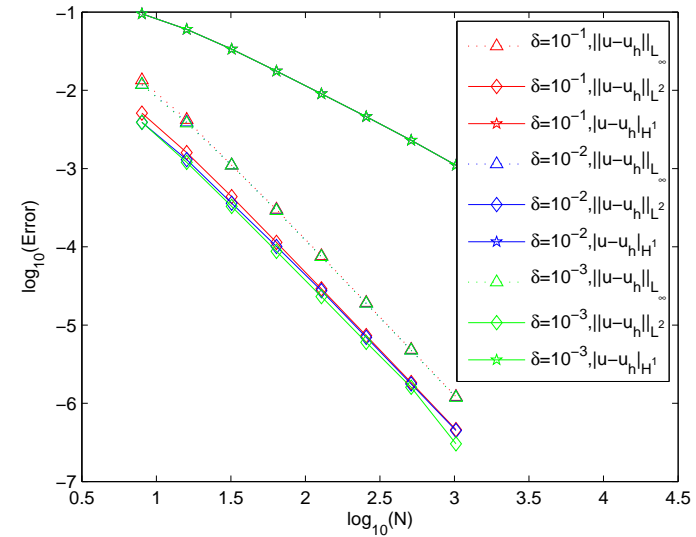
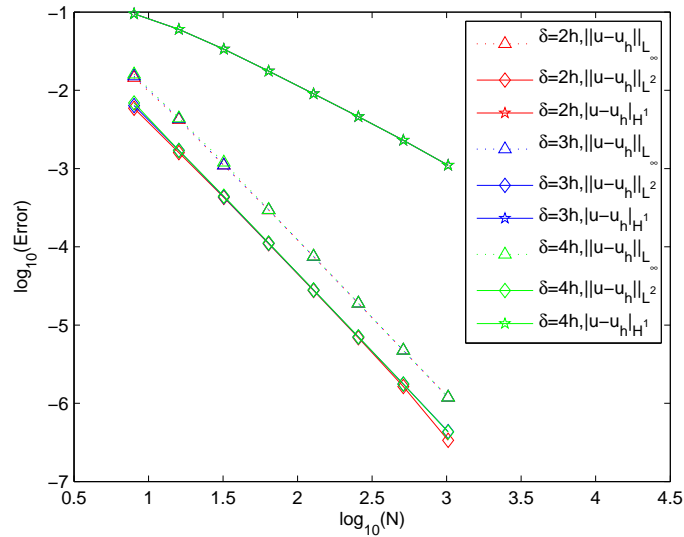
Continuous piecewise-linear finite elements in the best case scenario

h	L^2		L^∞		H^1	
	Error	Rate	Error	Rate	Error	Rate
2^{-3}	6.40E-3	–	1.52E-2	–	9.51E-2	–
2^{-4}	1.70E-3	1.91	4.30E-3	1.82	6.02E-2	0.66
2^{-5}	4.36E-4	1.96	1.10E-3	1.97	3.35E-2	0.85
2^{-6}	1.11E-4	1.97	2.96E-4	1.89	1.76E-2	0.93
2^{-7}	2.80E-5	1.99	7.51E-5	1.98	9.00E-3	0.98
2^{-8}	7.03E-6	1.99	1.89E-5	1.99	4.60E-3	0.97
2^{-9}	1.76E-6	2.00	4.75E-6	1.99	2.30E-3	1.00
2^{-10}	4.34E-7	2.02	1.19E-6	2.00	1.10E-3	1.06

Errors and convergence rates of continuous *piecewise-linear* approximations for $\delta = 3h$ for the *smooth* exact solution

	L^2		L^∞		H^1	
h	Error	Rate	Error	Rate	Error	Rate
2^{-3}	3.90E-3	–	1.18E-2	–	9.50E-2	–
2^{-4}	1.30E-3	1.70	3.80E-3	1.63	6.02E-2	0.66
2^{-5}	3.28E-4	1.87	1.10E-3	1.79	3.35E-2	0.85
2^{-6}	8.76E-5	1.90	2.88E-4	1.93	1.76E-2	0.93
2^{-7}	2.31E-5	1.92	7.43E-5	1.96	9.00E-3	0.97
2^{-8}	6.01E-6	1.94	1.88E-5	1.98	4.60E-3	0.97
2^{-9}	1.60E-6	1.91	4.78E-6	1.99	2.30E-3	1.00
2^{-10}	3.77E-7	2.09	1.18E-6	2.01	1.20E-3	0.94

Errors and convergence rates of *continuous piecewise-linear* approximations for $\delta = 0.001$ for the *smooth* exact solution



L^2 , L^∞ , and H^1 errors vs. $N = 1/h$ for *continuous piecewise-linear* approximations for the exact *smooth* exact solution

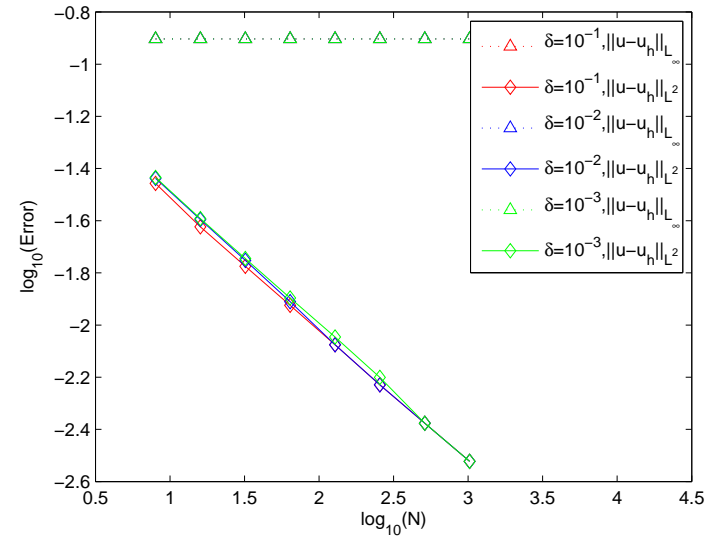
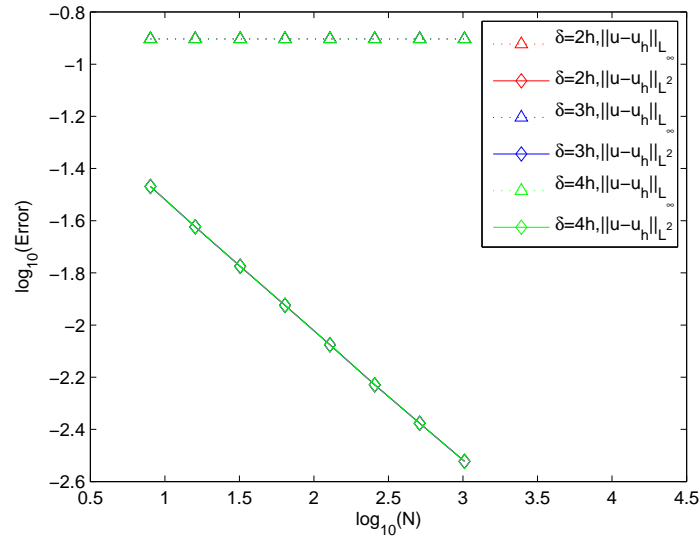
left: $\delta = 2h$, $3h$, and $4h$

right: $\delta = 0.1$, 0.01 , and 0.001

note that $\delta > h$ for some δ and h but that $\delta < h$ for some others

h	$\delta = 3h$				$\delta = 0.001$			
	L^2		L^∞		L^2		L^∞	
	Error	Rate	Error	Rate	Error	Rate	Error	Rate
2^{-3}	3.40E-2	–	1.25E-1	–	3.68E-2	–	1.25E-1	–
2^{-4}	2.38E-2	0.52	1.25E-1	0	2.56E-2	0.52	1.25E-1	0
2^{-5}	1.68E-2	0.52	1.25E-1	0	1.80E-2	0.51	1.25E-1	0
2^{-6}	1.19E-2	0.50	1.25E-1	0	1.27E-2	0.50	1.25E-1	0
2^{-7}	0.84E-2	0.50	1.25E-1	0	0.90E-2	0.50	1.25E-1	0
2^{-8}	0.59E-2	0.50	1.25E-1	0	0.63E-2	0.52	1.25E-1	0
2^{-9}	0.42E-2	0.49	1.25E-1	0	0.44E-2	0.52	1.25E-1	0
2^{-10}	0.30E-2	0.49	1.25E-1	0	0.30E-2	0.55	1.25E-1	0

Errors and convergence rates of *continuous piecewise-linear* approximations for the *discontinuous* exact solution



L^2 and L^∞ errors vs. $N = 1/h$ for continuous *piecewise linear approximations* for the *discontinuous* exact solution

left: $\delta = 2h, 3h, \text{ and } 4h$

right: $\delta = 0.1, 0.01, \text{ and } 0.001$

note that $\delta > h$ for some δ and h but that $\delta < h$ for some others

- For the **smooth solution**, continuous piecewise-linear finite element approximations are optimally accurate with respect to functions in H^2
 - this is true for both $\delta = Mh$ and δ independent of h
 - this is true for both $\delta < h$ and $\delta > h$
 - the convergence rates are the same as for finite element methods for elliptic PDEs
- For the solution having a **jump discontinuity**, continuous piecewise-linear finite element approximations are still optimally accurate
 - unfortunately, the optimal rate of convergence in L^2 is $0.5 - \epsilon$ because the exact solution merely belongs to $H^{1/2-\epsilon}$
 - this is true for both $\delta = Mh$ or δ fixed and for $\delta < h$ and $\delta > h$
 - again the convergence rates are the same as for finite element methods for elliptic PDEs

- Conclusion for continuous piecewise linears in the best case scenario
 - from the perspective of rates of convergence, there seems to be no advantage to continuous finite element methods for the nonlocal model compared to using the same finite elements methods for local models
 - because all results hold for $\delta < h$, we might as well choose such a $\delta - h$ combination
 - in this case the nonlocal model reduces to a local model, as is evidenced by the fact that the coefficient matrix is tridiagonal
 - this shows that for smooth solutions, δ is not a modeling parameter

Discontinuous finite elements in the best case scenario

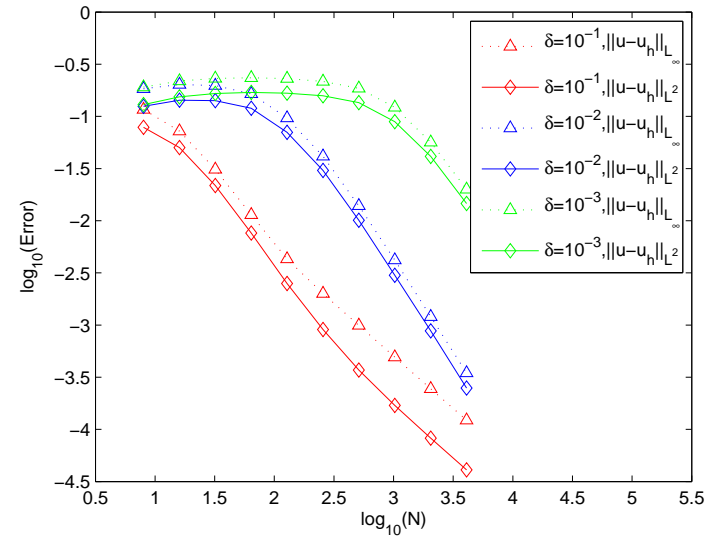
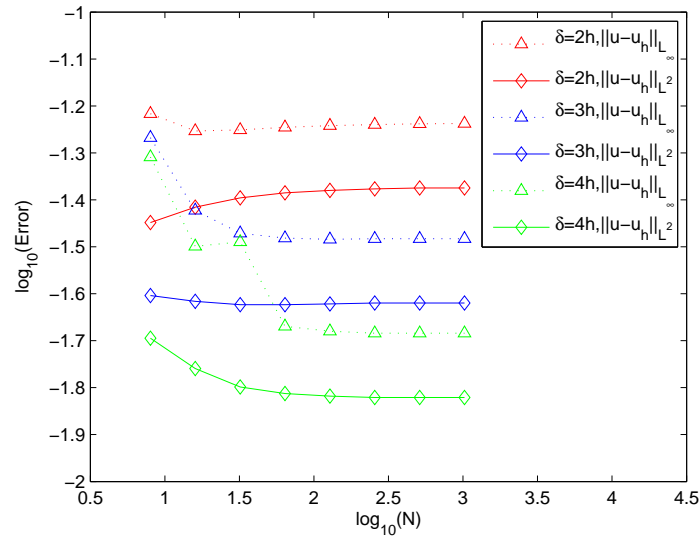
h	$\delta = 2h$		$\delta = 3h$		$\delta = 4h$	
	L^2 error	L^∞ error	L^2 error	L^∞ error	L^2 error	L^∞ error
2^{-3}	3.56E-2	6.07E-2	2.49E-2	2.02E-2	2.02E-2	4.91E-2
2^{-4}	3.84E-2	5.58E-2	2.42E-2	3.78E-2	1.74E-2	3.17E-2
2^{-5}	4.02E-2	5.61E-2	2.38E-2	3.38E-2	1.59E-2	2.34E-2
2^{-6}	4.12E-2	5.68E-2	2.38E-2	3.30E-2	1.54E-2	2.14E-2
2^{-7}	4.17E-2	5.73E-2	2.39E-2	3.28E-2	1.52E-2	2.09E-2
2^{-8}	4.20E-2	5.76E-2	2.40E-2	3.29E-2	1.51E-2	2.07E-2
2^{-9}	4.22E-2	5.78E-2	2.40E-2	3.29E-2	1.51E-2	2.07E-2
2^{-10}	4.22E-2	5.79E-2	2.40E-2	3.29E-2	1.51E-2	2.07E-2

L^2 and L^∞ errors of *discontinuous piecewise-constant* approximations for the *smooth* exact solution and for δ *proportional to* h

$\delta = 0.1$					$\delta = 0.01$			
h	L^2		L^∞		L^2		L^∞	
	Error	Rate	Error	Rate	Error	Rate	Error	Rate
2^{-3}	7.85E-2	–	1.16E-1	–	1.25E-1	–	1.84E-1	–
2^{-4}	5.02E-2	0.65	7.21E-2	0.69	1.43E-1	–	2.02E-1	–
2^{-5}	2.17E-2	1.21	3.10E-2	1.22	1.42E-1	0.01	1.97E-1	0.04
2^{-6}	7.60E-3	1.51	1.14E-2	1.44	1.19E-1	0.25	1.65E-1	0.26
2^{-7}	2.50E-3	1.60	4.30E-3	1.41	7.02E-2	0.76	9.65E-2	0.77
2^{-8}	9.05E-4	1.47	2.00E-3	1.10	3.03E-2	1.47	4.15E-2	1.10
2^{-9}	3.70E-4	1.29	9.91E-4	1.01	1.01E-2	1.29	1.39E-2	1.01
2^{-10}	1.70E-4	1.12	4.92E-4	1.01	3.00E-3	1.12	4.29E-3	1.01
2^{-11}	8.24E-5	1.04	2.45E-4	1.01	8.78E-4	1.04	1.20E-3	1.01
2^{-12}	4.09E-5	1.01	1.22E-4	1.00	2.49E-4	1.01	3.47E-4	1.00

$\delta = 0.001$				
h	L^2		L^∞	
	Error	Rate	Error	Rate
2^{-3}	1.30E-1	–	1.91E-1	–
2^{-4}	1.54E-1	–	2.16E-1	–
2^{-5}	1.66E-1	–	2.31E-1	–
2^{-6}	1.70E-1	–	2.34E-1	–
2^{-7}	1.67E-1	0.02	2.30E-1	0.02
2^{-8}	1.58E-1	0.08	2.16E-1	0.09
2^{-9}	1.35E-1	0.22	1.86E-1	0.22
2^{-10}	8.90E-2	0.61	1.22E-1	0.61
2^{-11}	4.13E-2	1.11	5.65E-2	1.11
2^{-12}	1.46E-2	1.50	2.00E-2	1.50

Errors and convergence rates of *discontinuous piecewise-constant* approximations for the *smooth* exact solution and for δ fixed independent of h



L^2 and L^∞ errors vs. $N = 1/h$ for *discontinuous piecewise-constant* approximations for the *smooth* exact solution

left: $\delta = 2h, 3h$, and $4h$

right: $\delta = 0.1, 0.01$, and 0.001

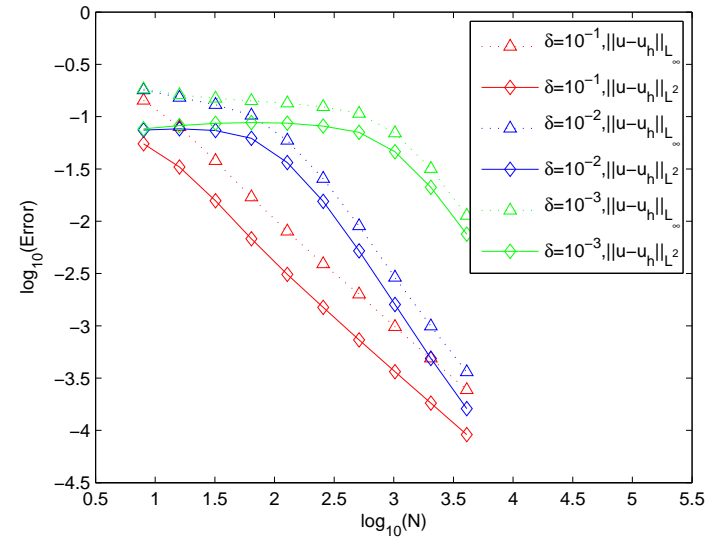
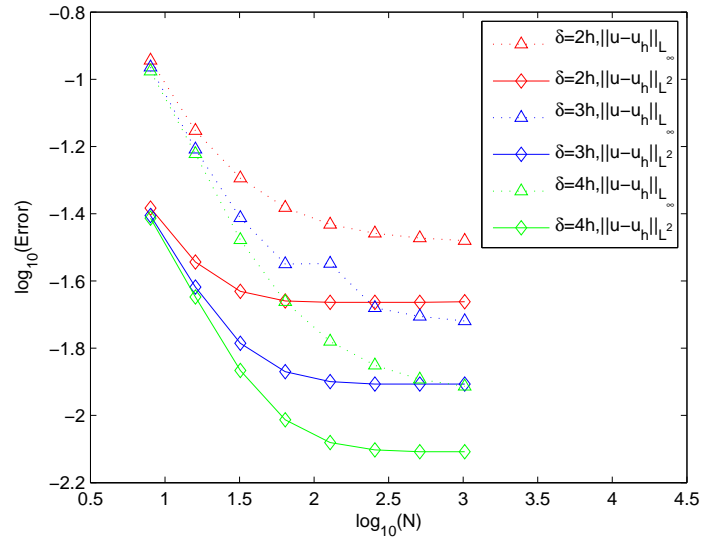
	$\delta = 2h$		$\delta = 3h$		$\delta = 4h$	
h	L^2 error	L^∞ error	L^2 error	L^∞ error	L^2 error	L^∞ error
2^{-3}	4.14E-2	1.14E-1	3.93E-2	1.09E-1	3.86E-2	1.06E-1
2^{-4}	2.86E-2	7.03E-2	2.41E-2	6.19E-2	2.25E-2	6.00E-2
2^{-5}	2.34E-2	5.08E-2	1.64E-2	3.87E-2	1.36E-2	3.33E-2
2^{-6}	2.19E-2	4.15E-2	1.35E-2	2.82E-2	9.74E-3	2.18E-2
2^{-7}	2.17E-2	3.70E-2	1.26E-2	2.33E-2	8.34E-3	1.66E-2
2^{-8}	2.17E-2	3.48E-2	1.24E-2	2.09E-2	7.91E-3	1.41E-2
2^{-9}	2.17E-2	3.37E-2	1.24E-2	1.97E-2	7.84E-3	1.28E-2
2^{-10}	2.18E-2	3.31E-2	1.24E-2	1.91E-2	7.82E-3	1.22E-2

L^2 and L^∞ errors of discontinuous piecewise-constant approximations for the *discontinuous* exact solution and for δ proportional to h

$\delta = 0.1$					$\delta = 0.01$			
h	L^2		L^∞		L^2		L^∞	
	Error	Rate	Error	Rate	Error	Rate	Error	Rate
2^{-3}	5.49E-2	–	1.43E-1	–	7.43E-2	–	1.79E-1	–
2^{-4}	3.30E-2	0.73	8.00E-2	0.84	7.64E-2	–	1.52E-1	0.24
2^{-5}	1.57E-2	1.07	3.79E-2	1.08	7.37E-2	0.01	1.30E-1	0.23
2^{-6}	6.80E-3	1.21	1.70E-2	1.16	6.21E-2	0.25	1.03E-1	0.34
2^{-7}	3.10E-3	1.13	8.00E-3	1.09	3.64E-2	0.77	5.93E-2	0.79
2^{-8}	1.50E-3	1.05	3.90E-3	1.04	1.55E-2	1.23	2.55E-2	1.22
2^{-9}	7.32E-4	1.03	2.00E-3	0.96	5.20E-3	1.58	9.00E-3	1.50
2^{-10}	3.65E-4	1.01	9.79E-4	1.03	1.60E-3	1.70	2.90E-3	1.63
2^{-11}	1.82E-4	1.00	4.89E-4	1.00	4.88E-4	1.71	9.93E-4	1.55
2^{-12}	9.10E-5	1.00	2.44E-4	1.00	1.61E-4	1.60	3.62E-4	1.46

$\delta = 0.001$				
h	L^2		L^∞	
	Error	Rate	Error	Rate
2^{-3}	7.65E-2	–	1.83E-1	–
2^{-4}	8.20E-2	–	1.61E-1	0.18
2^{-5}	8.62E-2	–	1.49E-1	0.18
2^{-6}	8.77E-2	–	1.42E-1	0.07
2^{-7}	8.65E-2	0.02	1.35E-1	0.07
2^{-8}	8.13E-2	0.09	1.24E-1	0.12
2^{-9}	7.07E-2	0.20	1.07E-1	0.21
2^{-10}	4.61E-2	0.62	6.95E-2	0.62
2^{-11}	2.11E-2	1.28	3.18E-2	1.13
2^{-12}	7.50E-3	1.49	1.13E-2	1.49

Errors and convergence rates of *discontinuous piecewise-constant* approximations for the *discontinuous* exact solution and for δ fixed independent of h



L^2 and L^∞ errors vs. $N = 1/h$ for discontinuous piecewise-constant approximations for the discontinuous exact solution

left: $\delta = 2h, 3h$, and $4h$

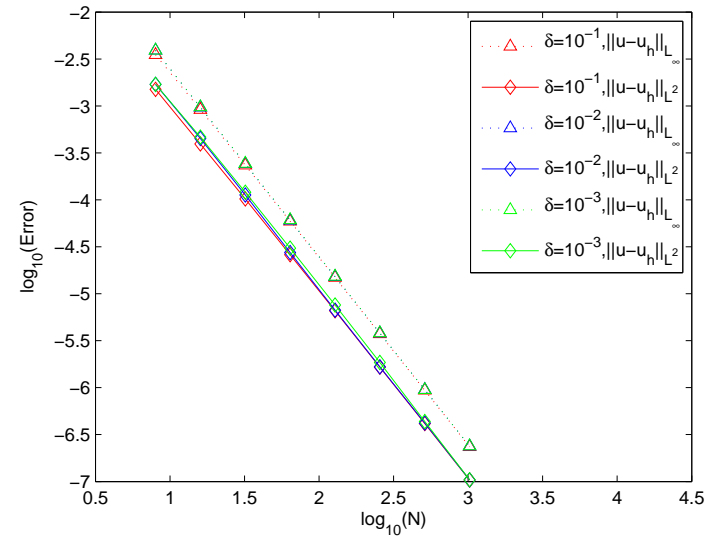
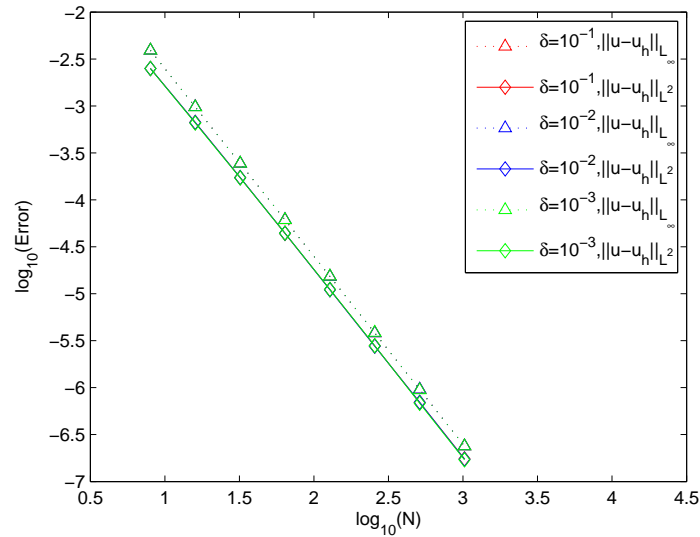
right: $\delta = 0.1, 0.01$, and 0.001

h	L^2		L^∞		H^1	
	Error	Rate	Error	Rate	Error	Rate
2^{-3}	2.50E-3	–	3.90E-3	–	6.25E-2	–
2^{-4}	6.58E-4	1.93	9.71E-4	2.01	3.38E-2	0.89
2^{-5}	1.71E-4	1.94	2.44E-4	1.99	1.75E-2	0.95
2^{-6}	4.41E-5	1.96	6.13E-5	1.99	8.90E-3	0.98
2^{-7}	1.11E-5	1.99	1.53E-5	2.00	4.50E-3	0.98
2^{-8}	2.80E-6	1.99	3.85E-6	1.99	2.20E-3	1.03
2^{-9}	6.82E-7	2.04	9.44E-7	2.03	1.10E-3	1.00
2^{-10}	1.70E-7	2.00	2.38E-7	1.99	5.63E-4	0.97

Errors and convergence rates of *discontinuous piecewise-linear* approximations for the *smooth* exact solution and for $\delta = 0.001$

	L^2		L^∞	
h	Error	Rate	Error	Rate
2^{-3}	1.70E-03	1.77	3.90E-03	2.01
2^{-4}	4.65E-04	1.87	9.71E-04	2.01
2^{-5}	1.20E-04	1.95	2.44E-04	2.00
2^{-6}	3.06E-05	1.98	6.10E-05	2.00
2^{-7}	7.58E-06	2.01	1.52E-05	2.00
2^{-8}	1.86E-06	2.03	3.81E-06	2.00
2^{-9}	4.37E-07	2.09	9.45E-07	2.01
2^{-10}	1.04E-07	2.06	2.38E-07	1.99

Errors and convergence rates of *discontinuous piecewise-linear* approximations for the *discontinuous* exact solution and for $\delta = 0.001$



L^2 and L^∞ errors vs. $N = 1/h$ for *discontinuous piecewise-linear* approximations for $\delta = 0.1, 0.01$, and 0.001

left: *smooth* exact solution

right: *discontinuous* exact solution

- If the horizon $\delta = Mh$ is chosen proportional to the grid size h , piecewise-constant approximations fail to converge for both smooth and discontinuous exact solutions
- On the other hand, if δ is fixed independent of h , piecewise-constant approximations converge for both smooth and discontinuous exact solutions, provided h is sufficiently small relative to δ ; seemingly, one needs $h < \delta$
- If δ is fixed independent of h , discontinuous piecewise-linear approximations converge at optimal rates for both smooth and discontinuous exact solutions
 - note that because we have placed a grid point at the location of the jump discontinuity, the rates of convergence for discontinuous finite element approximations are the same for both smooth functions and for functions containing a jump discontinuity

- Conclusion for discontinuous approximations in the best case scenario

- it seems that piecewise-constant approximations are not robust with respect to the relative sizes of the horizon δ and the grid size h
- it seems that discontinuous piecewise-linear approximations are robust, not only with respect to the relative sizes of δ and h , but also to the smoothness of the solution
- the observation that discontinuous piecewise-linear approximations lead to optimally accurate results for smooth solutions is not surprising, given that they are conforming for the nonlocal model and that they contain as a subspace the continuous piecewise-linear functions
- again, for smooth solutions, δ can be interpreted as being an available parameter that can be chosen for convenience

- the observation that discontinuous piecewise-linear approximations lead to optimally accurate results for the **discontinuous** solution illustrates the potential of nonlocal models:
 - one can obtain accurate results for problems with discontinuities for which finite element methods for classical local models involving derivatives have difficulty

A hybrid continuous-discontinuous finite element method

- Discontinuous finite element methods are better than continuous finite element methods for the nonlocal “boundary-value” problem, but for the same grid, they result in more degrees of freedom

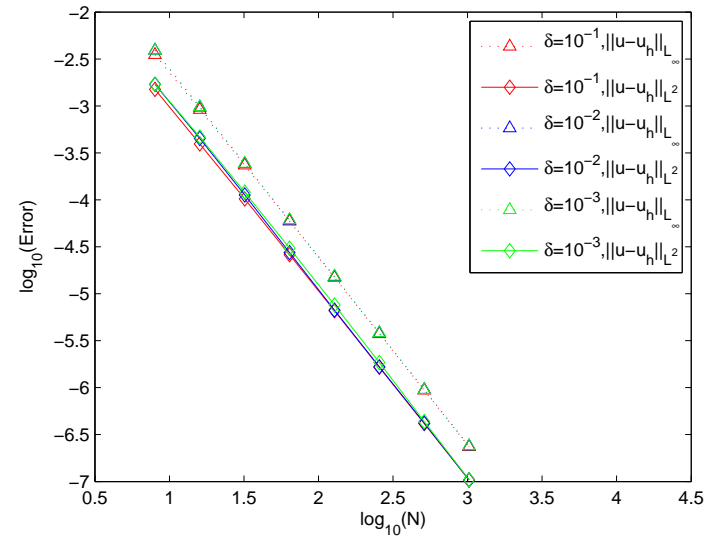
	CL	DC	DL
L^2 errors	$O(N^{-1/2})$	$O(N^{-1})$	$O(N^{-2})$
number of unknowns	N	$N + 1$	$2N + 2$
dimensions of matrix	$N \times N$	$(N + 1) \times (N + 1)$	$(2N + 2) \times (2N + 2)$
half bandwidth of matrix	$M + 1$	M	$2M + 1$

For the exact solution having a jump discontinuity, a comparison of the L^2 rates of convergence and matrix properties for continuous-linear (CL), discontinuous-constant (DC), and discontinuous-linear (DL) finite element approximations for $h = 1/(N + 1)$ and $\delta = Mh$, where N and M are positive integers

- However, for the same number of degrees of freedom, say N , the accuracy of the discontinuous linears is much better than continuous linears
- Even so, it would be nice to take advantage of the fact that continuous approximations of the nonlocal model should be perfectly fine in regions where the solution is smooth
- So why not use discontinuous piecewise linears only in a “small” neighborhood of the jump discontinuity and use continuous piecewise linear everywhere else
- We see that even though we use continuous approximations almost everywhere, the hybrid approximation results in optimally accurate rates of convergence; note that this is achieved without any need for grid refinement

h	L^2		L^∞	
	Error	Rate	Error	Rate
2^{-3}	1.50E-03	1.74	3.50E-03	1.97
2^{-4}	3.94E-04	1.93	9.12E-04	1.94
2^{-5}	1.02E-04	1.95	2.34E-04	1.97
2^{-6}	2.60E-05	1.97	5.91E-05	1.98
2^{-7}	6.57E-06	1.99	1.49E-05	1.99
2^{-8}	1.65E-06	1.99	3.73E-06	1.99
2^{-9}	4.14E-07	2.00	9.36E-07	2.00
2^{-10}	1.04E-07	2.00	2.34E-07	2.00

*Errors and convergence rates of hybrid discontinuous/continuous piecewise-linear approximations for the **discontinuous** exact solution and for $\delta = 0.1$*



L^2 and L^∞ errors vs. $N = 1/h$ for hybrid discontinuous/continuous piecewise-linear approximations for the *discontinuous* exact solution with $\delta = 0.1, 0.01$, and 0.001

- Now, let's see what happens if we stop cheating

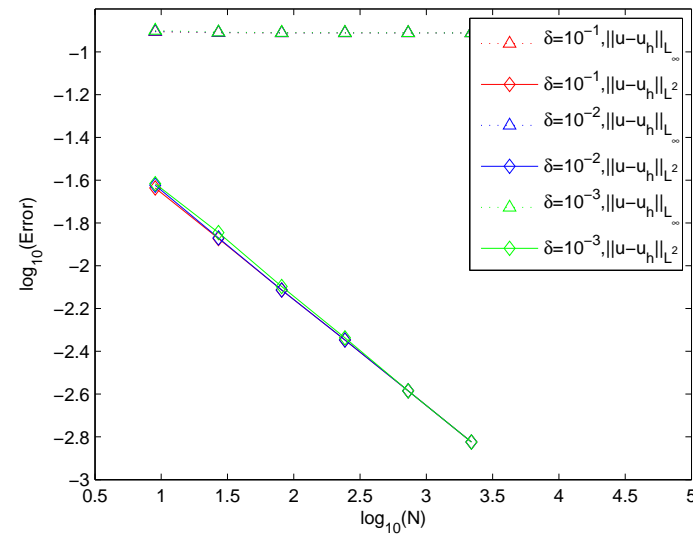
The case of grid points and points of discontinuities not coinciding

h	$\delta = 0.1$				
	L^2		L^∞		
	Error	Rate	Error	Rate	
3^{-2}	2.23E-2	–	1.33E-1	–	
3^{-3}	1.29E-2	0.50	1.35E-1	–	
3^{-4}	0.75E-2	0.50	1.36E-1	–	
3^{-5}	0.43E-2	0.50	1.36E-1	–	
3^{-6}	0.25E-2	0.50	1.36E-1	–	
3^{-7}	0.14E-2	0.50	1.36E-1	–	

h	$\delta = 0.01$				
	L^2		L^∞		
	Error	Rate	Error	Rate	
3^{-2}	2.38E-2	–	1.23E-1	–	
3^{-3}	1.33E-2	0.53	1.28E-1	–	
3^{-4}	0.74E-2	0.53	1.35E-1	–	
3^{-5}	0.43E-2	0.50	1.35E-1	–	
3^{-6}	0.25E-2	0.50	1.36E-1	–	
3^{-7}	0.14E-2	0.50	1.36E-1	–	

h	$\delta = 0.001$				
	L^2		L^∞		
	Error	Rate	Error	Rate	
3^{-2}	2.41E-2	–	1.24E-1	–	
3^{-3}	1.3E-2	0.41	1.23E-1	–	
3^{-4}	0.79E-2	0.51	1.24E-1	–	
3^{-5}	0.44E-2	0.53	1.27E-1	–	
3^{-6}	0.25E-2	0.54	1.35E-1	–	
3^{-7}	0.14E-2	0.50	1.36E-1	–	

*Errors and convergence rates of discontinuous piecewise-linear approximations for the **discontinuous** exact solution for the case in which there is **no grid point** located at the point of discontinuity of the solution*



L^2 and L^∞ errors vs. $N = 1/h$ for discontinuous piecewise-linear approximations for the **discontinuous** exact solution for the case in which there is **no grid point** located at the point of discontinuity of the solution

- These results are actually optimal because we have that for any discontinuous finite element space,
 - i.e., regardless of the degree of polynomial used within the individual elements,

$$\inf_{v^h \in S^h} \|u - v^h\|_{L^2(\Omega)} = O(h^{1/2}) \quad \text{and} \quad \inf_{v^h \in S^h} \|u - v^h\|_{L^\infty(\Omega)} = O(h^0)$$

- We can save the situation by taking advantage of the following four facts:

- if u^h denotes the finite element solution, then

$$\|u - u^h\|_{L^2(\Omega)} \leq C \inf_{v^h \in S^h} \|u - v^h\|_{L^2(\Omega)}$$

- for discontinuous finite element spaces, the error in the best approximation can be determined element by element, i.e.,

$$\inf_{v^h \in S^h} \|u - v^h\|_{L^2(\Omega)}^2 = \sum_{elements} \inf_{v^h \in S^h|_{element}} \|u - v^h\|_{L^2(element)}^2$$

- for elements in which the exact solution u is smooth, we have (using discontinuous piecewise linears)

$$\inf_{v^h \in S^h|_{element}} \|u - v^h\|_{L^2(element)} = O(h_{element}^2)$$

- for elements in which the exact solution u has a jump discontinuity

$$\inf_{v^h \in S^h|_{element}} \|u - v^h\|_{L^2(element)} = O(h_{element}^{1/2})$$

- So,

- if we let h denote the grid size of the elements in which the exact solution u is smooth

and

- if we then choose the grid size of the elements containing the jump discontinuity in the exact solution to be h^4

we then have that

$$\|u - u^h\|_{L^2(\Omega)} = O(h^2)$$

- Thus, we can get the accuracy we want by doing totally local, i.e., abrupt, grid refinement

h	Error(L_2)	rate	Error(L_∞)	rate
2^{-2}	6.33E-3	-	1.24E-1	-
2^{-3}	1.77E-3	1.84	1.23E-1	-
2^{-4}	4.60E-4	1.94	1.22E-1	-
2^{-5}	1.18E-4	1.96	1.22E-1	-
2^{-6}	3.01E-5	1.98	1.22E-1	-
2^{-7}	7.62E-6	1.98	1.22E-1	-

*Errors and convergence rates of discontinuous piecewise-linear approximations for the **discontinuous** exact solution for the case in which there is **no grid point located at the point of discontinuity** of the solution; all intervals are of size h except the interval containing the discontinuity which is of size h^4 ; here $\delta = 0.1$*

- We saved the L^2 error but not the L^∞ error
- It is true that best L^∞ approximations are always local because

$$\max_{\text{all elements}} |v| = \max_{\text{over the elements}} \left(\max_{\text{each element}} |v| \right)$$

- but not only do we **do not** have that

$$\|u - u^h\|_{L^\infty(\Omega)} \leq C \|u - w^h\|_{L^\infty(\Omega)}$$

for w^h the best L^∞ approximation to u

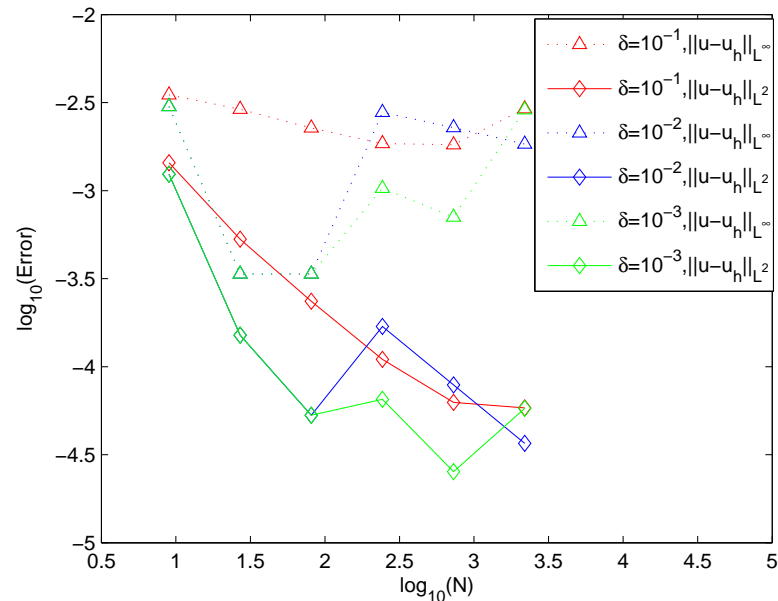
- but we also **do** have that the error in the best L^∞ approximation is of $O(h^0)$ regardless of how small we make the interval containing the point of discontinuity

- But

h	Error(L_2)	rate	Error(L_∞)	rate
3^{-2}	4.99E-3	-	1.39E-2	-
3^{-3}	1.49E-3	1.74	3.50E-3	1.99
3^{-4}	3.97E-4	1.91	9.06E-4	1.95
3^{-5}	1.02E-4	1.96	2.33E-4	1.96
3^{-6}	2.60E-5	1.97	5.91E-5	1.98
3^{-7}	6.61E-6	1.98	1.49E-5	1.99

*Errors **determined by ignoring the interval containing the discontinuity** and the corresponding convergence rates of discontinuous piecewise-linear approximations for the discontinuous exact solution for the case in which there is no grid point located at the point of discontinuity of the solution; all intervals are of size h except the interval containing the discontinuity which is of size h^4 ; here $\delta = 0.1$*

- Grid refinement at the point of discontinuity is still necessary



Errors determined by ignoring the interval containing the discontinuity and the corresponding convergence rates of discontinuous piecewise-linear approximations for the discontinuous exact solution for the case in which there is no grid point located at the point of discontinuity of the solution; all intervals are of size h including the interval containing the discontinuity

- What does this all mean in 2D and 3D?
- What else can be said in 2D and 3D about DG for nonlocal equations of the type we study here?

- When using discontinuous finite element spaces, it is not too difficult to identify the elements within which jump discontinuities in the solution occur
 - thus, an adaptive strategy can be devised to recursively refine those elements until the surface at which the solution is discontinuous is localized to elements of small enough size, e.g., h^4 in the above example, so that the desired L^2 accuracy is recovered
 - refined elements that do not contain that surface may be de-refined so that the only small elements are those containing that surface
- Hanging nodes (having a vertex of an element be on an edge of a neighboring element) are no problem
 - this makes mesh refinement much easier

- Abrupt changes in the mesh size is OK
 - no need to smoothly transition from a coarse mesh to a fine mesh
 - this also makes mesh refinement much easier
- All of the above means that one should be able to devise an adaptive grid refinement–grid coarsening strategy that results in:
 - a grid for which the only tiny elements are those that contain surfaces at which jump discontinuities in the solution occur
 - away from the surface-following layers of tiny elements, the grid changes abruptly to a coarse grid
 - that surface is surrounded by a layer of tiny elements that is mostly one element thick

- One can use **elements of any shape**, not just triangles, quadrilaterals, tetrahedra, and hexahedra
 - e.g., Voronoi or even non-polygonal elements can be used
 - using Voronoi instead of Delauney in 3D is really important because Voronoi regions always have "good" shape whereas Delauney can easily have slivers
- One can easily use different degree polynomials in different elements
 - do not have to worry about matching them on the boundary between elements
- One can easily define truly **meshless methods** which are much simpler than those for PDEs
 - e.g., there is no need to make the basis functions continuous

- There is no need to put points on the boundary
 - in our notation, we mean the boundary between Ω and Γ
 - one can just grid $\Omega \cup \Gamma$ and completely ignore $\partial\Omega$
 - this has important implications for complicated geometries

CURRENT AND FUTURE WORK

- With Q. Du, R. Lehoucq, and K. Zhou
 - fusing the nonlocal calculus to the connections made by Du and Zhou to Sobolev spaces
 - extension of the nonlocal calculus to the vector-valued case
 - application to the peridynamic model of materials
 - extension to nonlinear problems
- With M. Parks and P. Seleson
 - extension to material interface problems
 - systematic development of atomistic-to-continuum coupling methods
- With a bunch of people
 - further development and analysis of finite element approximations