A NONLOCAL VECTOR CALCULUS

AND

FINITE ELEMENT METHODS FOR NONLOCAL DIFFUSION AND MECHANICS

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- The talk is based on the three papers

[1] M. Gunzburger and R. Lehoucq; A nonlocal vector calculus with application to nonlocal boundary value problems,
Multiscale Modeling and Simulation **8** 2010, 1581-1598

[2] M. Gunzburger, Q. Du, R. Lehoucq, and K. Zhou; A nonlocal vector calculus, nonlocal volume-constrained problems, and nonlocal balance laws,
submitted to *Archive for Rational Mechanics and Analysis*

[3] X. Chen and M. Gunzburger; Continuous and discontinuous finite element methods for a peridynamics model of mechanics,
to appear in *Computer Methods in Applied Mechanics and Engineering*,
`doi:10.1016/j.cma.2010.10.014`

- We also reference the related papers

[4] Q. Du and K. Zhou; Mathematical analysis for the peridynamic nonlocal continuum theory, *Mathematical Modeling and Numerical Analysis* 2010, `doi:10.1051/m2an/2010040`

[5] K. Zhou and Q. Du; Mathematical and numerical analysis of linear peridynamic models with nonlocal boundary conditions,
SIAM Journal on Numerical Analysis **48** 2010, 1759-1780

[6] E. Emmrich and O. Weckner; On the well-posedness of the linear peridynamic model and its convergence towards the Navier equation of linear elasticity,
Communications in Mathematical Sciences **5** 2007, 851-864

A NONLOCAL VECTOR CALCULUS

NONLOCAL DIVERGENCE, GRADIENT, AND CURL OPERATORS

- $\mathbf{x}$, $\mathbf{y}$, $\mathbf{z}$ denote points in $\mathbb{R}^d$

- Point functions – functions from $\Omega \subset \mathbb{R}^d \longrightarrow \mathbb{R}^{n\times k}$ or $\mathbb{R}^n$ or $\mathbb{R}$

  point tensor functions $\mathbf{U}(\mathbf{x})$
  point vectors functions $\mathbf{u}(\mathbf{x})$
  point scalar functions $u(\mathbf{x})$

- Two-point functions – functions from $\Omega \times \Omega \longrightarrow \mathbb{R}^{n\times k}$, or $\mathbb{R}^n$, or $\mathbb{R}$

  point tensor functions $\boldsymbol{\Psi}(\mathbf{x},\mathbf{y})$
  point vectors functions $\boldsymbol{\psi}(\mathbf{x},\mathbf{y})$
  point scalar functions $\psi(\mathbf{x},\mathbf{y})$

  – symmetric two-point functions $\Leftarrow \quad \psi(\mathbf{x},\mathbf{y}) = \psi(\mathbf{y},\mathbf{x})$
  – antisymmetric two-point functions $\Leftarrow \quad \psi(\mathbf{x},\mathbf{y}) = -\psi(\mathbf{y},\mathbf{x})$

- Point operators map two-point functions to point functions
  - they are nonlocal operators because they involve integrals of two-point functions

- Two-point operators map point functions to two-point functions
  - they are nonlocal operators because they explicitly involve pairs of point functions

- The nonlocal divergence, gradient, and curl operators are point operators

- The nonlocal divergence operator maps two-point vector functions to point scalar functions

$$\mathcal{D}\big(\boldsymbol{\nu}\big)(\mathbf{x}) := -\int_{\Omega} \big(\boldsymbol{\nu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\nu}(\mathbf{y},\mathbf{x})\big) \cdot \boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\, d\mathbf{y} \quad \text{for } \mathbf{x} \in \Omega$$

where $\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})$ is a given anti-symmetric two-point vector function

- The nonlocal gradient operator maps two-point scalar functions to point vector functions

$$\mathcal{G}\big(\eta\big)(\mathbf{x}) := -\int_{\Omega} \big(\eta(\mathbf{x},\mathbf{y}) + \eta(\mathbf{y},\mathbf{x})\big)\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\, d\mathbf{y} \quad \text{for } \mathbf{x} \in \Omega$$

- In $\mathbb{R}^3$, nonlocal curl operator maps two-point vector functions into point vector functions

$$\mathcal{C}\big(\boldsymbol{\mu}\big)(\mathbf{x}) := -\int_{\Omega} \big(\boldsymbol{\mu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\mu}(\mathbf{y},\mathbf{x})\big) \times \boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\, d\mathbf{y} \quad \text{for } \mathbf{x} \in \Omega$$

– using the wedge product, curl operators can be defined in higher dimensions

– in two dimensions, one can reduce the curl operator to two curl operators, one operating on scalars, the other on vectors

- Notational simplification

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

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

and so on

– for example

$$\mathcal{D}(\boldsymbol{\nu}) = \int_\Omega (\boldsymbol{\nu} + \boldsymbol{\nu}') \cdot \boldsymbol{\alpha} \, d\mathbf{y}$$

NONLOCAL INTEGRAL THEOREMS

- One easily obtains the nonlocal integral theorems

nonlocal Gauss theorem: $$\int_\Omega \mathcal{D}(\boldsymbol{\nu})\,d\mathbf{x} = 0$$

$$\int_\Omega \mathcal{G}(\eta)\,d\mathbf{x} = 0$$

nonlocal Stokes theorem: $$\int_\Omega \mathcal{C}(\boldsymbol{\mu})\,d\mathbf{x} = 0$$

– for example, we have

$$\int_\Omega \mathcal{D}(\boldsymbol{\nu})\,d\mathbf{x} = -\int_\Omega\int_\Omega (\boldsymbol{\nu}+\boldsymbol{\nu}')\cdot\boldsymbol{\alpha}\,d\mathbf{y}\,d\mathbf{x} = 0$$

- From the nonlocal integral theorems, one obtains the nonlocal integration by parts formulas

$$\int_\Omega u\mathcal{D}\big(\boldsymbol{\nu}\big)\,d\mathbf{x} - \int_\Omega\int_\Omega \big((u'-u)\boldsymbol{\alpha}\big)\cdot\boldsymbol{\nu}\,d\mathbf{y}d\mathbf{x} = 0$$

$$\int_\Omega \mathbf{v}\cdot\mathcal{G}\big(\eta\big)\,d\mathbf{x} - \int_\Omega\int_\Omega \big((\mathbf{v}'-\mathbf{v})\cdot\boldsymbol{\alpha}\big)\eta\,d\mathbf{y}d\mathbf{x} = 0$$

$$\int_\Omega \mathbf{w}\cdot\mathcal{C}\big(\boldsymbol{\mu}\big)\,d\mathbf{x} + \int_\Omega\int_\Omega \big((\mathbf{w}'-\mathbf{w})\times\boldsymbol{\alpha}\big)\cdot\boldsymbol{\mu}\,d\mathbf{y}d\mathbf{x} = 0$$

NONLOCAL ADJOINT OPERATORS

- Adjoint operators are nonlocal two-point operators corresponding to the nonlocal point operators
  - given a point operator $\mathcal{L}$ that maps two-point functions F to point functions defined over Ω, the adjoint operator $\mathcal{L}^*$ is a two-point operator that maps point functions G to two-point functions defined over $\Omega \times \Omega$ that satisfies

$$\big(G, \mathcal{L}(F)\big)_{\Omega} - \big(\mathcal{L}^*(G), F\big)_{\Omega\times\Omega} = 0$$

  - $(\cdot, \cdot)$ denotes $L^2(\Omega)$ or $L^2(\Omega \times \Omega)$ inner products
  - F and G may denote pairs of vector-scalar, scalar-vector, or vector-vector functions

- The integration by parts formulas can be used to immediately determine the nonlocal adjoint operators corresponding to the nonlocal divergence, gradient, and curl operators

  – the adjoint of $\mathcal{D}$ is the two-point operator such that

$$\mathcal{D}^*\big(u\big)(\mathbf{x},\mathbf{y}) = (u' - u)\boldsymbol{\alpha} \quad \text{for } \mathbf{x},\mathbf{y} \in \Omega$$

  – the adjoint of $\mathcal{G}$ is the two-point operator such that

$$\mathcal{G}^*\big(\mathbf{v}\big)(\mathbf{x},\mathbf{y}) = (\mathbf{v}' - \mathbf{v}) \cdot \boldsymbol{\alpha} \quad \text{for } \mathbf{x},\mathbf{y} \in \Omega$$

  – the adjoint of $\mathcal{C}$ is the two-point operator such that

$$\mathcal{C}^*\big(\mathbf{w}\big)(\mathbf{x},\mathbf{y}) = -(\mathbf{w}' - \mathbf{w}) \times \boldsymbol{\alpha} \quad \text{for } \mathbf{x},\mathbf{y} \in \Omega$$

- We can then rewrite the nonlocal integration by parts formulas in terms of the nonlocal adjoint operators

$$\int_\Omega u\mathcal{D}(\boldsymbol{\nu})\,d\mathbf{x} - \int_\Omega\int_\Omega \mathcal{D}^*(u)\cdot\boldsymbol{\nu}\,d\mathbf{y}\,d\mathbf{x} = 0$$

$$\int_\Omega \mathbf{v}\cdot\mathcal{G}(\eta)\,d\mathbf{x} - \int_\Omega\int_\Omega \mathcal{G}^*(\mathbf{v})\eta\,d\mathbf{y}\,d\mathbf{x} = 0$$

$$\int_\Omega \mathbf{w}\cdot\mathcal{C}(\boldsymbol{\mu})\,d\mathbf{x} - \int_\Omega\int_\Omega \mathcal{C}^*(\mathbf{w})\cdot\boldsymbol{\mu}\,d\mathbf{y}\,d\mathbf{x} = 0$$

NONLOCAL GREEN'S IDENTITIES

- A nonlocal Green's first identity can be derived by setting $F = \Theta\mathcal{L}^*(H)$ in the defining relation for adjoint operators
  - $\mathcal{L}^*(H)$ may be a scalar or vector or second-order tensor function
  - correspondingly, Θ is a scalar or second-order tensor or fourth-order tensor function

  leading to the nonlocal Green's first identity

$$\big(G, \mathcal{L}(\Theta\mathcal{L}^*(H))\big)_\Omega - \big(\mathcal{L}^*(G), \Theta\mathcal{L}^*(H)\big)_{\Omega\times\Omega} = 0$$

- If Θ is a symmetric tensor, one can then easily obtain the nonlocal Green's second identity

$$\Big(G, \mathcal{L}\big(\Theta\mathcal{L}^*(H)\big)\Big)_\Omega - \Big(H, \mathcal{L}\big(\Theta\mathcal{L}^*(G)\big)\Big)_\Omega = 0$$

- For the nonlocal divergence, gradient, and curl operators and the corresponding nonlocal adjoint operators we then have nonlocal Green's first identities

$$\int_\Omega u\mathcal{D}\big(\mathbf{\Theta}_2\cdot\mathcal{D}^*(v)\big)\,d\mathbf{x}-\int_\Omega\int_\Omega \mathcal{D}^*(u)\cdot\mathbf{\Theta}_2\cdot\mathcal{D}^*(v)\,d\mathbf{y}d\mathbf{x}=0$$

$$\int_\Omega \mathbf{v}\cdot\mathcal{G}\big(\theta\mathcal{G}^*(\mathbf{u})\big)\,d\mathbf{x}-\int_\Omega\int_\Omega \theta\mathcal{G}^*(\mathbf{v})\mathcal{G}^*(\mathbf{u})\,d\mathbf{y}d\mathbf{x}=0$$

$$\int_\Omega \mathbf{w}\cdot\mathcal{C}\big(\mathbf{\Theta}_4:\mathcal{C}^*(\mathbf{u})\big)\,d\mathbf{x}-\int_\Omega\int_\Omega \mathcal{C}^*(\mathbf{w}):\mathbf{\Theta}_4:\mathcal{C}^*(\mathbf{u})\,d\mathbf{y}d\mathbf{x}=0$$

  - in the first equation, $\mathbf{\Theta}_2(\mathbf{x},\mathbf{y})\colon\Omega\times\Omega\to\mathbb{R}^{n\times n}$ denotes a two-point second-order tensor function
  - in the second equation, $\theta(\mathbf{x},\mathbf{y})\colon\Omega\times\Omega\to\mathbb{R}$ denotes a two-point scalar function
  - in the third equation, $\mathbf{\Theta}_4(\mathbf{x},\mathbf{y})\colon\Omega\times\Omega\to\mathbb{R}^{3\times3\times3\times3}$ denotes a two-point fourth-order tensor function

- We also obtain the nonlocal Green's second identities

$$\int_\Omega u\mathcal{D}\big(\boldsymbol{\Theta}\cdot\mathcal{D}^*(v)\big)\,d\mathbf{x} - \int_\Omega v\mathcal{D}\big(\boldsymbol{\Theta}\cdot\mathcal{D}^*(u)\big)\,d\mathbf{x} = 0$$

$$\int_\Omega \mathbf{v}\cdot\mathcal{G}\big(\theta\mathcal{G}^*(\mathbf{u})\big)\,d\mathbf{x} - \int_\Omega \mathbf{u}\cdot\mathcal{G}\big(\theta\mathcal{G}^*(\mathbf{v})\big)\,d\mathbf{x} = 0$$

$$\int_\Omega \mathbf{w}\cdot\mathcal{C}\big(\boldsymbol{\Theta}:\mathcal{C}^*(\mathbf{u})\big)\,d\mathbf{x} - \int_\Omega \mathbf{u}\cdot\mathcal{C}\big(\boldsymbol{\Theta}:\mathcal{C}^*(\mathbf{w})\big)\,d\mathbf{x} = 0$$

A NONLOCAL DIVERGENCE FOR TENSOR FUNCTIONS

- A nonlocal divergence operator for tensor functions is defined by applying the nonlocal divergence operator to each of the rows of the tensor
  - thus, if $\mathbf{\Psi} : \Omega \times \Omega \to \mathbb{R}^{n\times k}$ is a two-point tensor function, we have

$$\mathcal{D}_t(\mathbf{\Psi})(\mathbf{x}) := -\int_\Omega \big(\mathbf{\Psi} + \mathbf{\Psi}'\big) \cdot \boldsymbol{\alpha}\, d\mathbf{y} \quad \text{for } \mathbf{x} \in \Omega$$

- A nonlocal Gauss theorem for tensor functions and the corresponding integration by parts formula and Green's identities can be derived for the operator $\mathcal{D}_t$
  - in particular, for a point function $\mathbf{v}(\mathbf{x}) : \Omega \to \mathbb{R}^n$, we have the adjoint operator

$$\mathcal{D}_t^*(\mathbf{v})(\mathbf{x},\mathbf{y}) = (\mathbf{v}' - \mathbf{v}) \otimes \boldsymbol{\alpha} \quad \text{for } \mathbf{x},\mathbf{y} \in \Omega$$

NONLOCAL VECTOR IDENTITIES

- The nonlocal divergence, gradient, and curl operators and the corresponding adjoint operators satisfy

$$
\begin{aligned}
\mathcal{D}\big(\mathcal{C}^*(\mathbf{u})\big) &= 0 && \text{for } \mathbf{u}\colon \Omega \longrightarrow \mathbb{R}^3 \\
\mathcal{C}\big(\mathcal{D}^*(u)\big) &= \mathbf{0} && \text{for } u\colon \Omega \longrightarrow \mathbb{R} \\
\mathcal{G}^*(\mathbf{u}) &= \mathrm{tr}\big(\mathcal{D}_t^*(\mathbf{u})\big) && \text{for } \mathbf{u}\colon \Omega \longrightarrow \mathbb{R}^n \\
\mathcal{D}_t\big(\mathcal{D}_t^*(\mathbf{u})\big) - \mathcal{G}\big(\mathcal{G}^*(\mathbf{u})\big) &= \mathcal{C}\big(\mathcal{C}^*(\mathbf{u})\big) && \text{for } \mathbf{u}\colon \Omega \longrightarrow \mathbb{R}^3
\end{aligned}
$$

- Functions of the form $\mathcal{C}^*(\mathbf{u})$ do not entirely comprise the null space of the operator $\mathcal{D}$
  - in fact, for any anti-symmetric $\boldsymbol{\nu}(\mathbf{x},\mathbf{y})$, we have $\mathcal{D}\big(\boldsymbol{\nu}\big) = 0$
  - however, functions of the form $\mathcal{C}^*(\mathbf{u})$ are the only symmetric two-point functions belonging to the null space of $\mathcal{D}$
  - analogous statements can be made for the null space of the operator $\mathcal{C}$ and two-point functions of the form $\mathcal{D}^*(u)$

- The four identities are analogous to vector identities associated with the differential divergence, gradient and curl operator
  - this suggest that $\mathcal{D}^*$, $\mathcal{G}^*$, and $\mathcal{C}^*$ can also be viewed as nonlocal analogs of the differential gradient, divergence, and curl operators operating on point functions
  - note however that $\mathcal{G}^*\big(\mathcal{C}(\boldsymbol{\mu})\big) \neq 0$ and $\mathcal{C}^*\big(\mathcal{G}(\eta)\big) \neq 0$
- We also have that, if b and $\mathbf{b}$ denote a constant scalar and vector, respectively, then

$$\mathcal{D}^*(b) = 0 \qquad \mathcal{G}^*(\mathbf{b}) = \mathbf{0} \qquad \mathcal{C}^*(\mathbf{b}) = \mathbf{0}$$

  - moreover, these three relationships are equivalent to the three nonlocal integral theorems
  - similar results do not hold for the point divergence, gradient, and curl operators, e.g., in general, we have that

$$\mathcal{D}(\mathbf{b}) \neq 0 \qquad \mathcal{G}(b) \neq 0 \qquad \mathcal{C}(\mathbf{b}) \neq 0$$

    for constants b and constant vectors $\mathbf{b}$

WHY DOES THE NONLOCAL VECTOR CALCULUS NOT ALWAYS LOOK LIKE THE LOCAL DIFFERENTIAL CALCULUS?

- In addition to

  – the divergence, gradient, and curl operators and

  – integrals over a region in $\mathbb{R}^n$

  the theorems and identities of the vector calculus for differential operators also involve

  – operators acting on functions defined on the boundary of that region and

  – integrals over that boundary surface

– for example, given a region $\Omega \subset \mathbb{R}^n$ having boundary $\partial\Omega$, the divergence theorem for a vector-valued function $\mathbf{u}$ states that

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

and the Green's (generalized) first identity for scalar functions u and v states that, for tensor-valued "constitutive" functions Θ,

$$\int_\Omega u\nabla \cdot (\Theta\nabla v)\, d\mathbf{x} + \int_\Omega \nabla u \cdot (\Theta\nabla v)\, d\mathbf{x} = \int_{\partial\Omega} u(\Theta\nabla v) \cdot \mathbf{n}\, d\mathbf{x}$$

– however, neither the nonlocal divergence theorem

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

nor the nonlocal Green's first identity

$$\int_\Omega u\mathcal{D}\big(\boldsymbol{\Theta}_2 \cdot \mathcal{D}^*(v)\big)\, d\mathbf{x} - \int_\Omega \int_\Omega \mathcal{D}^*(u) \cdot \boldsymbol{\Theta}_2 \cdot \mathcal{D}^*(v)\, d\mathbf{y} d\mathbf{x}$$

contain terms that correspond to the boundary integrals

– Where are the boundary integrals? Where are the boundary operators?

- This is a fundamental difference between the nonlocal vector calculus and the local differential vector calculus

- However, by viewing boundary operators in the vector calculus for differential operators as constraint operators defined on lower-dimensional constraint manifolds, it is a simple matter to rewrite the nonlocal vector theorems and identities so that they do include such terms

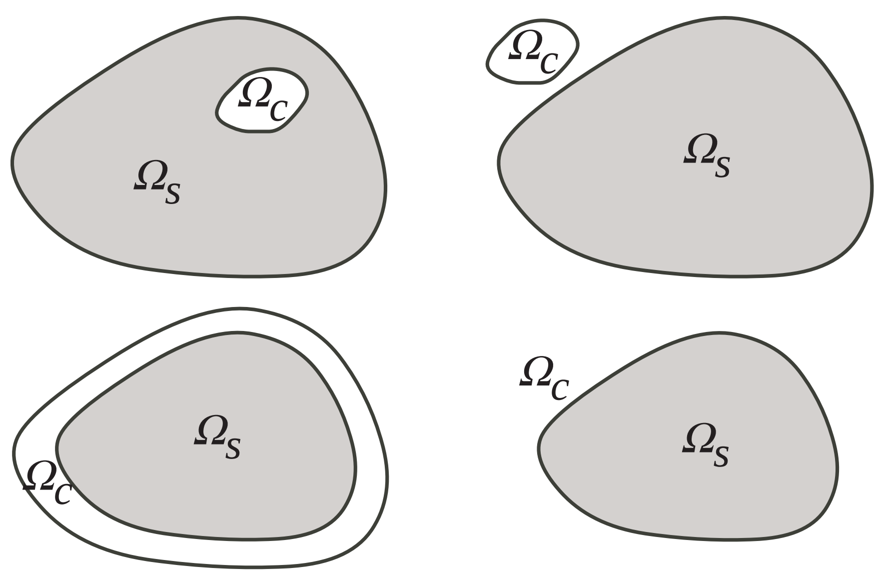
  – the reason it was not necessary to introduce constraint operators and "boundary" integrals in the theorems and identities of the nonlocal vector calculus is that, in the nonlocal case, "boundary" operators must operate on functions defined over measurable volumes, and not on lower-dimensional manifolds

  – as a result, the actions of these operators are, in a real sense, indistinguishable from those of the nonlocal operators we have already defined, except for the resulting domains

- In addition to trying to mimic more closely the theorems and identities of the vector calculus for differential operators, we introduce constraint regions and constraint operators because they are needed to describe nonlocal volume-constrained problems and showing their well posedness

CONSTRAINT REGIONS

- We divide the region Ω into disjoint, covering open subsets Ω_s and Ω_c
  - Ω_s is the solution domain
  - Ω_c is the constraint domain
- Note that no relation is assumed between Ω_s and Ω_c
  - for example, these four configurations, as well as others, are possible



CONSTRAINT OPERATORS

- The first thing we do is restrict the domains resulting from the action of the nonlocal operators
  - for example, we now define the nonlocal divergence operator by

$$\mathcal{D}(\boldsymbol{\nu})(\mathbf{x}) := -\int_\Omega \big(\boldsymbol{\nu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\nu}(\mathbf{y},\mathbf{x})\big) \cdot \boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\, d\mathbf{y} \quad \text{for } \mathbf{x} \in \Omega_s$$

- We then define the corresponding point constraint operator $\mathcal{N}(\boldsymbol{\nu})\colon \Omega_c \to \mathbb{R}$ by

$$\mathcal{N}(\boldsymbol{\nu})(\mathbf{x}) := \int_\Omega (\boldsymbol{\nu} + \boldsymbol{\nu}') \cdot \boldsymbol{\alpha}\, d\mathbf{y} \qquad \text{for } \mathbf{x} \in \Omega_c$$

  - note that the the point operator $\mathcal{D}$ and the corresponding point constraint operator $\mathcal{N}$ are defined using the same integral formulas but

    $\mathcal{D}(\boldsymbol{\nu})$ is defined for $\mathbf{x} \in \Omega_s$

    $\mathcal{N}(\boldsymbol{\nu})$ is defined for $\mathbf{x} \in \Omega_c$

- Similarly, we define the point constraint operator

$$\boxed{\mathcal{S}(\eta)(\mathbf{x}) := \int_{\Omega} (\eta + \eta')\boldsymbol{\alpha}\, d\mathbf{y} \qquad \text{for } \mathbf{x} \in \Omega_c}$$

corresponding to the nonlocal gradient operator $\mathcal{G}$ and the point constraint operator

$$\boxed{\mathcal{T}(\boldsymbol{\mu})(\mathbf{x}) := \int_{\Omega} (\boldsymbol{\mu} + \boldsymbol{\mu}') \times \boldsymbol{\alpha}\, d\mathbf{y} \qquad \text{for } \mathbf{x} \in \Omega_c}$$

corresponding to the nonlocal curl operator $\mathcal{C}$

- It is now a trivial matter to rewrite the nonlocal integral theorems, the nonlocal integration by parts formulas, and the nonlocal Green's identities so that they look more like the ones for the differential vector calculus

- Nonlocal integral theorems

nonlocal Gauss theorem: $$\int_{\Omega_s} \mathcal{D}(\boldsymbol{\nu})\, d\mathbf{x} = \int_{\Omega_c} \mathcal{N}(\boldsymbol{\nu})$$

$$\int_{\Omega} \mathcal{G}(\eta)\, d\mathbf{x} = \int_{\Omega_c} \mathcal{S}(\eta)\, d\mathbf{x}$$

nonlocal Stokes theorem: $$\int_{\Omega_s} \mathcal{C}(\boldsymbol{\mu})\, d\mathbf{x} = \int_{\Omega_c} \mathcal{T}(\boldsymbol{\mu})\, d\mathbf{x}$$

- Nonlocal integration by parts formulas

$$\int_{\Omega_s} u\mathcal{D}(\boldsymbol{\nu})\,d\mathbf{x} - \int_{\Omega}\int_{\Omega} \mathcal{D}^*(u)\cdot\boldsymbol{\nu}\,d\mathbf{y}d\mathbf{x} = \int_{\Omega_c} u\mathcal{N}(\boldsymbol{\nu})\,d\mathbf{x}$$

$$\int_{\Omega_s} \mathbf{v}\cdot\mathcal{G}(\eta)\,d\mathbf{x} - \int_{\Omega}\int_{\Omega} \mathcal{G}^*(\mathbf{v})\eta\,d\mathbf{y}d\mathbf{x} = \int_{\Omega_c} \mathbf{v}\cdot\mathcal{S}(\eta)\,d\mathbf{x}$$

$$\int_{\Omega_s} \mathbf{w}\cdot\mathcal{C}(\boldsymbol{\mu})\,d\mathbf{x} - \int_{\Omega}\int_{\Omega} \mathcal{C}^*(\mathbf{w})\cdot\boldsymbol{\mu}\,d\mathbf{y}d\mathbf{x} = \int_{\Omega_c} \mathbf{w}\cdot\mathcal{T}(\boldsymbol{\mu})\,d\mathbf{x}$$

- Nonlocal Green's first identities

$$\int_{\Omega_s} u\mathcal{D}\big(\mathbf{\Theta}_2 \cdot \mathcal{D}^*(v)\big)\,d\mathbf{x} - \int_{\Omega}\int_{\Omega} \mathcal{D}^*(u)\cdot\mathbf{\Theta}_2\cdot\mathcal{D}^*(v)\boldsymbol{\nu}\,d\mathbf{y}d\mathbf{x} = \int_{\Omega_c} u\mathcal{N}\big(\mathbf{\Theta}_2\cdot\mathcal{D}^*(v)\big)\,d\mathbf{x}$$

$$\int_{\Omega_s} \mathbf{v}\cdot\mathcal{G}\big(\theta\mathcal{G}^*(\mathbf{u})\big)\,d\mathbf{x} - \int_{\Omega}\int_{\Omega} \theta\mathcal{G}^*(\mathbf{v})\mathcal{G}^*(\mathbf{u})\,d\mathbf{y}d\mathbf{x} = \int_{\Omega_c} \mathbf{v}\cdot\mathcal{S}\big(\theta\mathcal{G}^*(\mathbf{u})\big)\,d\mathbf{x}$$

$$\int_{\Omega_s} \mathbf{w}\cdot\mathcal{C}\big(\mathbf{\Theta}_4 : \mathcal{C}^*(\mathbf{u})\big)\,d\mathbf{x} - \int_{\Omega}\int_{\Omega} \mathcal{C}^*(\mathbf{w}) : \mathbf{\Theta}_4 : \mathcal{C}^*(\mathbf{u})\,d\mathbf{y}d\mathbf{x} = \int_{\Omega_c} \mathbf{w}\cdot\mathcal{T}\big(\mathbf{\Theta}_4 : \mathcal{C}^*(\mathbf{u})\big)\,d\mathbf{x}$$

- Nonlocal Green's second identities

$$\int_{\Omega_s} u\mathcal{D}_s\big(\mathbf{\Theta}_2 \cdot \mathcal{D}^*(v)\big)\,d\mathbf{x} - \int_{\Omega_s} v\mathcal{D}_s\big(\mathbf{\Theta}_2 \cdot \mathcal{D}^*(u)\big)\,d\mathbf{x}$$
$$= \int_{\Omega_c} u\mathcal{N}_s\big(\mathbf{\Theta}_2 \cdot \mathcal{D}^*(v)\big)\,d\mathbf{x} - \int_{\Omega_c} v\mathcal{N}_s\big(\mathbf{\Theta}_2 \cdot \mathcal{D}^*(u)\big)\,d\mathbf{x}$$

$$\int_{\Omega_s} \mathbf{v}\cdot\mathcal{G}\big(\theta\mathcal{G}^*(\mathbf{u})\big)\,d\mathbf{x} - \int_{\Omega_s} \mathbf{u}\cdot\mathcal{G}\big(\theta\mathcal{G}^*(\mathbf{v})\big)\,d\mathbf{x}$$
$$= \int_{\Omega_c} \mathbf{v}\cdot\mathcal{S}\big(\theta\mathcal{G}^*(\mathbf{u})\big)\,d\mathbf{x} - \int_{\Omega_c} \mathbf{u}\cdot\mathcal{S}\big(\theta\mathcal{G}^*(\mathbf{v})\big)\,d\mathbf{x}$$

$$\int_{\Omega_s} \mathbf{w}\cdot\mathcal{C}\big(\mathbf{\Theta}_4 : \mathcal{C}^*(\mathbf{u})\big)\,d\mathbf{x} - \int_{\Omega_s} \mathbf{u}\cdot\mathcal{C}\big(\mathbf{\Theta}_4 : \mathcal{C}^*(\mathbf{w})\big)\,d\mathbf{x}$$
$$= \int_{\Omega_c} \mathbf{w}\cdot\mathcal{T}\big(\mathbf{\Theta}_4 : \mathcal{C}^*(\mathbf{u})\big)\,d\mathbf{x} - \int_{\Omega_c} \mathbf{u}\cdot\mathcal{T}\big(\mathbf{\Theta}_4 : \mathcal{C}^*(\mathbf{v})\big)\,d\mathbf{x}$$

EXAMPLES OF VOLUME-CONSTRAINED PROBLEMS

- We divide the constraint region Ω_c into two disjoint, covering subregions
  - the "Dirichlet" subregion Ω_{c1}
  - the "Neumann" subregion Ω_{c2}

- Let $\boldsymbol{\Theta}_4$ denote a fourth-order tensor two-point function
  $\boldsymbol{\Theta}_2$ denote a second-order tensor two-point function
  θ denote a scalar two-point function

- The nonlocal volume-constrained problems

$$\begin{cases} \mathcal{D}\big(\mathbf{\Theta}_2 \cdot \mathcal{D}^*(u)\big) = f & \text{in } \Omega \\ u = g & \text{in } \Omega_{c1} \\ \mathcal{N}\big(\mathbf{\Theta}_2 \cdot \mathcal{D}^*(u)\big) = h & \text{in } \Omega_{c2} \end{cases}$$

$$\begin{cases} \mathcal{D}_t\big(\mathbf{\Theta}_4 : \mathcal{D}_t^*(\mathbf{u})\big) = \mathbf{f} & \text{in } \Omega \\ \mathbf{u} = \mathbf{g} & \text{in } \Omega_{c1} \\ \mathcal{N}_t\big(\mathbf{\Theta}_4 : \mathcal{D}_t^*(\mathbf{u})\big) = \mathbf{h} & \text{in } \Omega_{c2} \end{cases}$$

$$\begin{cases} \mathcal{C}\big(\mathbf{\Theta}_4 : \mathcal{C}^*(\mathbf{u})\big) + \mathcal{G}\big(\theta \mathcal{G}^*(\mathbf{u})\big) = \mathbf{f} & \text{in } \Omega \\ \mathbf{u} = \mathbf{g} & \text{in } \Omega_{c1} \\ \mathcal{T}\big(\mathbf{\Theta}_4 : \mathcal{C}^*(\mathbf{u})\big) + \mathcal{S}\big(\theta \mathcal{G}^*(\mathbf{u})\big) = \mathbf{h} & \text{in } \Omega_{c2} \end{cases}$$

are analogous to the second-order differential boundary-value problems

$$\begin{cases} -\nabla \cdot \big(\mathbf{K}_2 \cdot \nabla u\big) = f & \text{in } \Omega \\ u = g & \text{on } \partial\Omega_1 \\ \big(\mathbf{K}_2 \cdot \nabla u\big) \cdot \mathbf{n} = h & \text{on } \partial\Omega_2 \end{cases}$$

$$\begin{cases} -\nabla \cdot \big(\mathbf{K}_4 : \nabla \mathbf{u}\big) = \mathbf{f} & \text{in } \Omega \\ \mathbf{u} = \mathbf{g} & \text{on } \partial\Omega_1 \\ \big(\mathbf{K}_4 : \nabla \mathbf{u}\big) \cdot \mathbf{n} = \mathbf{h} & \text{on } \partial\Omega_2 \end{cases}$$

$$\begin{cases} \nabla \times \big(\mathbf{K}_4 : \nabla \times \mathbf{u}\big) - \nabla\big(k \nabla \cdot \mathbf{u}\big) = \mathbf{f} & \text{in } \Omega \\ \mathbf{u} = \mathbf{g} & \text{on } \partial\Omega_1 \\ \left.\begin{array}{r} \mathbf{n} \times \big(\mathbf{K}_4 : \nabla \times \mathbf{u}\big) = \mathbf{h}_1 \\ k \nabla \cdot \mathbf{u} = h_2 \end{array}\right\} & \text{on } \partial\Omega_2, \end{cases}$$

respectively, where $\partial\Omega = \partial\Omega_1 \cup \partial\Omega_2$ denotes the boundary of Ω with $\partial\Omega_1 \cap \partial\Omega_2 = \emptyset$ and where $\mathbf{K}_4$, $\mathbf{K}_2$, and k denote fourth-order tensor, second-order tensor, and scalar point functions, respectively

- A special form of the first nonlocal volume-constrained problem is studied in [1] by appealing to a variational formulation
  - well-posedness results are provided there for the case in which the natural energy space is equivalent to $L^2(\Omega)$
  - no smoothing of the solution with respect to the data results
  - rigorous connection to the corresponding differential boundary-value problem is demonstrated

- More generally, as shown in [2], the natural energy space associated with the nonlocal operators used in the first costrained-value problem may be a strict subspace of $L^2(\Omega)$
  - for instance a fractional Sobolev space
  - the nonlocal variational problems possess smoothing properties akin to that for elliptic partial differential equations but with reduced order

- The nonlocal point operators, the corresponding nonlocal adjoint operators, and the corresponding nonlocal constraint operators can be used to define other nonlocal volume-constrained problems, including problems in solid and fluid mechanics

IDENTIFICATION, IN A DISTRIBUTIONAL SENSE, OF NONLOCAL OPERATORS WITH DIFFERENTIAL OPERATORS

- We want to somehow identify the nonlocal point divergence operator $\mathcal{D}$ with the differential divergence operator $\nabla\cdot$
  - of course, this identification is subject to the understanding that the former operates on two-point functions while the latter operates on point functions

- Let $\boldsymbol{\nu} \in \mathcal{C}_0^\infty(\Omega \times \Omega)$ and select the (antisymmetric) distribution

$$\boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) = \nabla_{\mathbf{y}}\delta(\mathbf{y}-\mathbf{x})$$

- Then,

$$\mathcal{D}\big(\boldsymbol{\nu}\big)(\mathbf{x}) = \nabla_{\mathbf{x}} \cdot \boldsymbol{\nu}(\mathbf{x},\mathbf{x})$$

  - in particular, we have

$$\mathcal{D}\Big(\mathbf{u}(\mathbf{x}) + \mathbf{u}(\mathbf{y})\Big)(\mathbf{x}) = \nabla_{\mathbf{x}} \cdot \mathbf{u}(\mathbf{x})$$

- For functions that are compactly supported within Ω, the nonlocal Gauss theorem reduces to ??????

$$\int_{\partial\Omega} \boldsymbol{\nu}(\mathbf{x}, \mathbf{x}) \cdot \mathbf{n}_{\mathbf{x}} = 0$$

which is exactly the classical Gauss theorem

- We can also identify the action of $\mathcal{D}^*$ on a point function with the action of $-\nabla$ on that function

  – let $u \in \mathcal{C}_0^\infty(\Omega)$

  – then,

$$\boxed{\int_{\Omega} \mathcal{D}^*(u)\, d\mathbf{y} = -\nabla_{\mathbf{x}} u}$$

- Now consider $\mathcal{D}\big(\mathcal{D}^*\big)$, the composition of the nonlocal divergence operator and its adjoint
  - let $u \in \mathcal{C}_0^\infty(\Omega)$
  - select $|\alpha(\mathbf{x},\mathbf{y})|^2 = \dfrac{1}{2}\Delta_{\mathbf{y}}\delta(\mathbf{y}-\mathbf{x})$, where Δ denotes the differential Laplace operator
  - then,
$$\mathcal{D}\big(\mathcal{D}^* u(\mathbf{x})\big) = -\Delta_{\mathbf{x}} u(\mathbf{x})$$
  - an immediate application is to use the nonlocal Green's first identity with $\mathbf{\Theta}_2 = \mathbf{I}$ to obtain
$$\int_\Omega \nabla_{\mathbf{x}} u \cdot \nabla_{\mathbf{x}} v \, d\mathbf{x} = \int_\Omega \int_\Omega \mathcal{D}^*(u) \cdot \mathcal{D}^*(v) \, d\mathbf{y} d\mathbf{x}$$

- We have focused on the nonlocal divergence operator $\mathcal{D}$
  - similar results hold for the nonlocal gradient operator $\mathcal{G}$, the nonlocal curl operator $\mathcal{C}$, and the nonlocal divergence operator on tensors $\mathcal{D}_t$

RELATIONS BETWEEN WEIGHTED NONLOCAL OPERATORS AND WEAK REPRESENTATIONS OF DIFFERENTIAL OPERATORS

- The nonlocal point operators $\mathcal{D}$, $\mathcal{G}$, and $\mathcal{C}$ induce new operators, referred to as weighted operators
  - letting $\omega(\mathbf{x},\mathbf{y})\colon \Omega\times\Omega \longrightarrow \mathbb{R}$ denote a non-negative scalar-valued two-point function, the weighted nonlocal divergence of a point function $u(\mathbf{x})$ is defined by

$$\mathcal{D}_\omega(\mathbf{u})(\mathbf{x}) := \mathcal{D}\big(\omega(\mathbf{x},\mathbf{y})\mathbf{u}(\mathbf{x})\big)(\mathbf{x}) = -\int_\Omega (\omega\mathbf{u} + \omega'\mathbf{u}')\boldsymbol{\alpha}\,d\mathbf{y} \quad \text{for } \mathbf{x}\in\Omega$$

  - the adjoint operator corredponding to the weighted operator $\mathcal{D}_\omega$ is given by the weighted integral of the nonlocal adjoint operator $\mathcal{D}^*$ $\Rightarrow$

$$\mathcal{D}^*_\omega(v)(\mathbf{x}) = \int_\Omega \mathcal{D}^*(v)(\mathbf{x},\mathbf{y})\,\omega(\mathbf{x},\mathbf{y})\,d\mathbf{y} \quad \text{for } \mathbf{x}\in\Omega$$

  - similar results hold for the nonlocal gradient operator $\mathcal{G}$, the nonlocal curl operator $\mathcal{C}$, and the nonlocal divergence operator on tensors $\mathcal{D}_t$

- Let $\Omega = \mathbb{R}^d$,

$$B_\varepsilon(\mathbf{x}) := \{\mathbf{y} \in \mathbb{R}^d \ : \ |\mathbf{y} - \mathbf{x}| < \varepsilon\} \qquad \text{for } \varepsilon > 0$$

and

$$\begin{cases} \boldsymbol{\alpha}(\mathbf{x}, \mathbf{y}) = \dfrac{\mathbf{y} - \mathbf{x}}{|\mathbf{y} - \mathbf{x}|} \qquad \text{for } \mathbf{x} \neq \mathbf{y} \\ \omega(|\mathbf{x} - \mathbf{y}|) = \begin{cases} |\mathbf{y} - \mathbf{x}|\phi(|\mathbf{y} - \mathbf{x}|) & \mathbf{y} \in B_\varepsilon(\mathbf{x}) \\ 0 & \text{otherwise} \end{cases} \end{cases}$$

with ϕ a positive radial function satisfying a normalization condition

$$\int_{B_\varepsilon(\mathbf{x})} |\mathbf{y} - \mathbf{x}|^2 \phi(|\mathbf{y} - \mathbf{x}|)\, d\mathbf{y} = d,$$

where d denotes the space dimension

  - note that $\boldsymbol{\alpha}$ is an antisymmetric function whereas ω is a symmetric function

– then, the components of the weighted gradient $\mathcal{G}_\omega(u)$ and weighted adjoint divergence $\mathcal{D}^*_\omega(u)$ of a scalar function u are given by, for $j = 1, \ldots, d$,

$$\mathsf{d}_j u(\mathbf{x}) = -\int_{B_\varepsilon(\mathbf{0})} \big(u(\mathbf{x}+\mathbf{z}) + u(\mathbf{x})\big)\, z_j\, \phi(|\mathbf{z}|)\, d\mathbf{z}$$
$$\mathsf{d}^*_j u(\mathbf{x}) = \int_{B_\varepsilon(\mathbf{0})} \big(u(\mathbf{x}+\mathbf{z}) - u(\mathbf{x})\big)\, z_j\, \phi(|\mathbf{z}|)\, d\mathbf{z},$$

where z_j denotes the j-th component of $\mathbf{z}$

– it follows that

$$\mathsf{d}_j u = -\mathsf{d}^*_j u$$

so that

$$\mathcal{D}_\omega = -\mathcal{G}^*_\omega, \qquad \mathcal{G}_\omega = -\mathcal{D}^*_\omega, \qquad \mathcal{C}_\omega = \mathcal{C}^*_\omega$$

– if we select

$$\mathbf{z}_j \phi(|\mathbf{z}|) = -\partial_j \delta(\mathbf{z}),$$

where $\partial_j u$ denotes the weak derivative of u with respect to x_j, then,

$$\mathsf{d}_j = \partial_j \qquad \textit{and} \qquad \mathsf{d}^*_j = -\partial_j.$$

- Keeping the same ω,
  - the weighted operators d_j and d_j^* are bounded linear operators from $H^1(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$
  - if $u \in H^1(\mathbb{R}^d)$, then as $\varepsilon \to 0$,

$$\|\mathsf{d}_j u - \partial_j u\|_{L^2(\mathbb{R}^d)} \to 0$$
$$\|\mathsf{d}_j^* u + \partial_j u\|_{L^2(\mathbb{R}^d)} \to 0,$$

  - if

$$\int_{B_\varepsilon(0)} |\mathbf{z}|^{1+s} \phi(|\mathbf{z}|)\, d\mathbf{z} < \infty \quad \text{for some } 0 \le s \le 1,$$

    then, for $j = 1, \ldots, d$, the weighted operators d_j and d_j^* are bounded linear operators from $H^t(\mathbb{R}^d)$ to $H^{t-s}(\mathbb{R}^d)$ for any $t \ge 0$
  - if $s = 0$, then the weighted operators are bounded operators from $L^2(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$
  - if $s > 0$, the operators d_j and d_j^* actually map a subspace of $L^2(\mathbb{R}^d)$, for instance $H^s(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$, or even map $L^2(\mathbb{R}^d)$ to $H^{-s}(\mathbb{R}^d)$; see also [4]

- As a direct consequence, we have that
  - the weighted operators $\mathcal{D}_\omega$, $\mathcal{G}_\omega$, and $\mathcal{C}_\omega$ and their adjoint operators $\mathcal{D}^*_\omega$, $\mathcal{G}^*_\omega$, and $\mathcal{C}^*_\omega$ are bounded linear operators from $H^t(\mathbb{R}^d)$ to $H^{t-s}(\mathbb{R}^d)$ for $0 \le s \le 1$
  - if $u \in H^1(\mathbb{R}^d)$ and $\mathbf{u} \in [H^1(\mathbb{R}^d)]^d$,

$$\begin{aligned}
&\mathcal{D}_\omega(\mathbf{u}) \to \nabla \cdot \mathbf{u} &\qquad& \mathcal{D}^*_\omega(u) \to -\nabla u \\
&\mathcal{G}_\omega(u) \to \nabla u &\qquad& \mathcal{G}^*_\omega(\mathbf{u}) \to -\nabla \cdot \mathbf{u} \\
&\mathcal{C}_\omega(\mathbf{u}) \to \nabla \times \mathbf{u} &\qquad& \mathcal{C}^*_\omega(\mathbf{u}) \to \nabla \times \mathbf{u},
\end{aligned}$$

    where the convergence as $\varepsilon \to 0$ is with respect to $L^2(\mathbb{R}^d)$

- let $u \in H^1(\mathbb{R}^d)$, $\mathbf{u} \in [H^1(\mathbb{R}^d)]^d$, $\mathbf{C}_1 : \mathbb{R}^d \to \mathbb{R}^d \times \mathbb{R}^d$ in $L^\infty(\mathbb{R}^d \times \mathbb{R}^d)$, and $c_2 : \mathbb{R}^d \to \mathbb{R}$ in $L^\infty(\mathbb{R}^d)$, then

$$\begin{aligned}
&\mathcal{D}_\omega\big(\mathbf{C}_1 \cdot \mathcal{D}^*_\omega(u)\big) \to -\nabla \cdot (\mathbf{C}_1 \cdot \nabla u)\\
&\mathcal{G}_\omega\big(c_2 \mathcal{G}^*_\omega(\mathbf{u})\big) \to -\nabla(c_2 \nabla \cdot \mathbf{u})\\
&\mathcal{C}_\omega\big(\mathbf{C}_1 \cdot \mathcal{C}^*_\omega(\mathbf{u})\big) \to \nabla \times \big(\mathbf{C}_1 \cdot (\nabla \times \mathbf{u})\big),
\end{aligned}$$

  where the convergence as $\varepsilon \to 0$ is with respect to $H^{-1}(\mathbb{R}^d)$

- similar results can be obtained for the nonlocal divergence operator on tensors; in particular, we have that $\mathcal{D}_{t,\omega}(\mathbf{C}_3 : \mathcal{D}^*_{t,\omega}(\mathbf{u})) \to -\nabla \cdot (\mathbf{C}_3 : \nabla \mathbf{u})$ with $\mathbf{C}_3 : \mathbb{R}^d \to \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d$ in $L^\infty(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d)$

- Let $\mathcal{Q}$ denote a linear operator that commutes with the differential and non-local operators
  - then, if $\mathcal{Q}\mathbf{u} \in H^1(\mathbb{R}^d)$,

$$\begin{aligned} \mathcal{D}_\omega(\mathcal{Q}\mathbf{u}) &\to \nabla \cdot \mathcal{Q}\mathbf{u} & \qquad \mathcal{D}^*_\omega(\mathcal{Q}\mathbf{u}) &\to -\nabla \mathcal{Q}\mathbf{u} \\ \mathcal{G}_\omega(\mathcal{Q}\mathbf{u}) &\to \nabla \mathcal{Q}\mathbf{u} & \qquad \mathcal{G}^*_\omega(\mathcal{Q}\mathbf{u}) &\to -\nabla \cdot \mathcal{Q}\mathbf{u} \\ \mathcal{C}_\omega(\mathcal{Q}\mathbf{u}) &\to \nabla \times \mathcal{Q}\mathbf{u} & \qquad \mathcal{C}^*_\omega(\mathcal{Q}\mathbf{u}) &\to \nabla \times \mathcal{Q}\mathbf{u}, \end{aligned}$$

    where the convergence as $\varepsilon \longrightarrow 0$ is with respect to $L^2(\mathbb{R}^d)$.
  - if $\mathcal{Q}$ is selected as a differential operator with constant coefficients, or its formal inverse, we can observe convergence in either stronger or weaker norms

PERIDYNAMICS

- We demonstrate the connection between the nonlocal vector calculus and the peridynamic nonlocal model of continuum mechanics

- We have that, for a vector point function $\mathbf{u}$,

$$-\frac{1}{2}\mathcal{D}_t\Big(\big(\mathcal{D}_t^*(\mathbf{u})\big)^T\Big) = \int_\Omega (\boldsymbol{\alpha}\otimes\boldsymbol{\alpha})\cdot(\mathbf{u}'-\mathbf{u})\,d\mathbf{y}$$

  - a mechanical perspective indicates that

    $\big(\mathcal{D}_t^*(\mathbf{u})\big)^T$ describes the deformation of $\mathbf{u}$

    a constitutive relation maps the deformation to the force density given by the integral operator

  - because the integrand is antisymmetric with respect to the arguments $\mathbf{x}$ and $\mathbf{y}$, this operator induces an interaction – that of force between subregions

- If we require that the integral operator to contain only rigid motions in its null space, that is,

$$\mathcal{D}_t\Big(\big(\mathcal{D}_t^*(\mathbf{u})\big)^T\Big) = 0 \quad \Longleftrightarrow \quad \mathbf{u} = \mathbf{A}\mathbf{x} + \mathbf{c}$$

with $\mathbf{A}$ a constant skew-symmetric matrix and $\mathbf{c}$ a constant vector, then a necessary and sufficient condition is that

$$\boldsymbol{\alpha}(\mathbf{x}, \mathbf{y}) = \big(\mathbf{y} - \mathbf{x}\big)\zeta(|\mathbf{y} - \mathbf{x}|)$$

where $\zeta : \mathbb{R}^+ \to \mathbb{R}$

- We then have, with $\sigma := \zeta^{-2}$,

$$-\frac{1}{2}\mathcal{D}_t\Big(\big(\mathcal{D}_t^*(\mathbf{u})\big)^T\Big) = \int_\Omega \frac{\big(\mathbf{y} - \mathbf{x}\big) \otimes \big(\mathbf{y} - \mathbf{x}\big)}{\sigma(|\mathbf{y} - \mathbf{x}|)} \cdot \big(\mathbf{u}(\mathbf{y}) - \mathbf{u}(\mathbf{x})\big)\, d\mathbf{y}$$

  – this is the linearized peridynamic bond-based operator

- When $\Omega \equiv \mathbb{R}^d$, [4] provides analytical conditions on σ describing the amount of smoothing associated with the integral operator and the well-posedness of the balance of linear momentum and associated equilibrium equation
  - that paper also demonstrates that as the peridynamic horizon goes to zero,

$$-\frac{1}{2}\mathcal{D}_t\big((\mathcal{D}_t^*\mathbf{u})^T\big) \rightarrow -\mu\nabla\cdot(\nabla\mathbf{u}) - 2\mu\nabla(\nabla\cdot\mathbf{u}),$$

    which is the Navier operator of linear elasticity with Poisson ratio $= 1/4$; see also [6]
  - in [5], volume-constrained problems on bounded domains in $\mathbb{R}$ and squares in $\mathbb{R}^2$ are considered

- We can also formulate the state-based peridynamic model in terms of the nonlocal operators, but now the weighted operators are needed
  - let $\boldsymbol{\alpha}$ and ω be given as in the discussion of weighted operators
  - then, the linear state-based peridynamic integral operator is given by

$$-\mathcal{D}_{t,\omega}\Big(\eta\big(\mathcal{D}^*_{t,\omega}(\mathbf{u})\big)^T + \big(\lambda\mathcal{G}^*_\omega(\mathbf{u})\big)\,\mathbf{I}\Big)$$

    where η and λ are materials constants
  - the scalar $\mathcal{G}^*_\omega(\mathbf{u})$ measures the volumetric change, or dilatation, in the material

    so that $\mathcal{G}^*_\omega(\mathbf{u})\,\mathbf{I}$ is a diagonal tensor representing volumetric stress
  - this allows us to readily apply the nonlocal calculus to study the well-posedness of both free-space and volume-constrained linear peridynamic state-based balance laws
  - it also suggests why, in the limit as $\varepsilon \longrightarrow 0$, the above operator leads to the linear Navier operator of elasticity for linear isotropic materials with general Poisson ratios

FINITE ELEMENT METHODS

FINITE ELEMENT METHODS

- Discretization of nonlocal volume problems are usually effected by applying a quadrature rule to the "strong" form of the equations
  - for example, the nonlocal equation

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

which is equivalent to

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

is discretized into

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

$$\text{for } i=1,\ldots,M$$

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
    $\Longrightarrow$ 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

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

- 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

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

where

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

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

- We the have the Galerkin formulation

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

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

and

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

- 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

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

and

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

- 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

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

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

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

for which

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

- 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

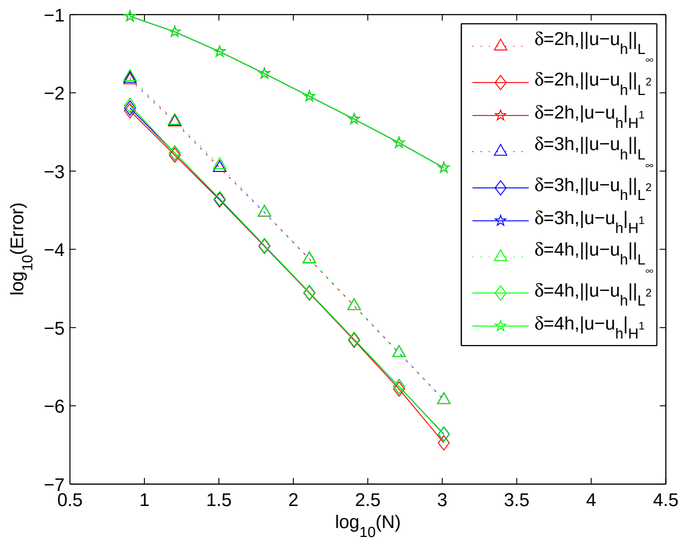
Continuous piecewise-linear finite elements in the best case scenario

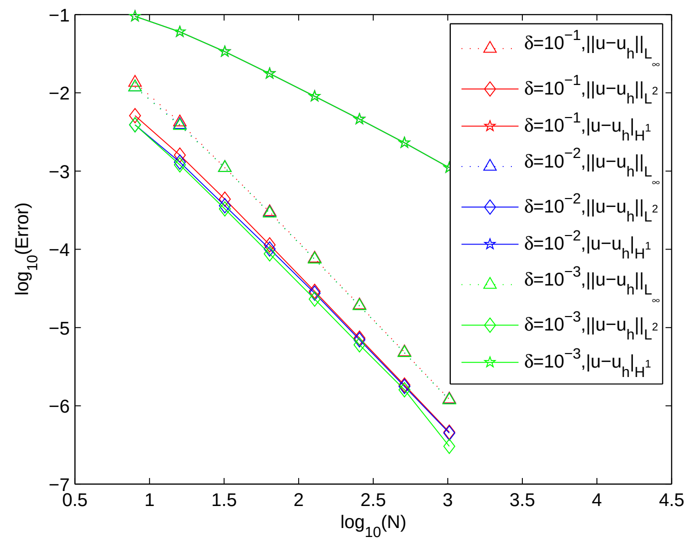
h	L^2 Error	L^2 Rate	L^∞ Error	L^∞ Rate	H^1 Error	H^1 Rate
2^{-3}	6.40E-3	–	1.52E-2	–	9.51E-2	–
2^{-4}	1.70E-3	1.91	4.30E-3	1.82	6.02E-2	0.66
2^{-5}	4.36E-4	1.96	1.10E-3	1.97	3.35E-2	0.85
2^{-6}	1.11E-4	1.97	2.96E-4	1.89	1.76E-2	0.93
2^{-7}	2.80E-5	1.99	7.51E-5	1.98	9.00E-3	0.98
2^{-8}	7.03E-6	1.99	1.89E-5	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

h	L^2 Error	L^2 Rate	L^∞ Error	L^∞ Rate	H^1 Error	H^1 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

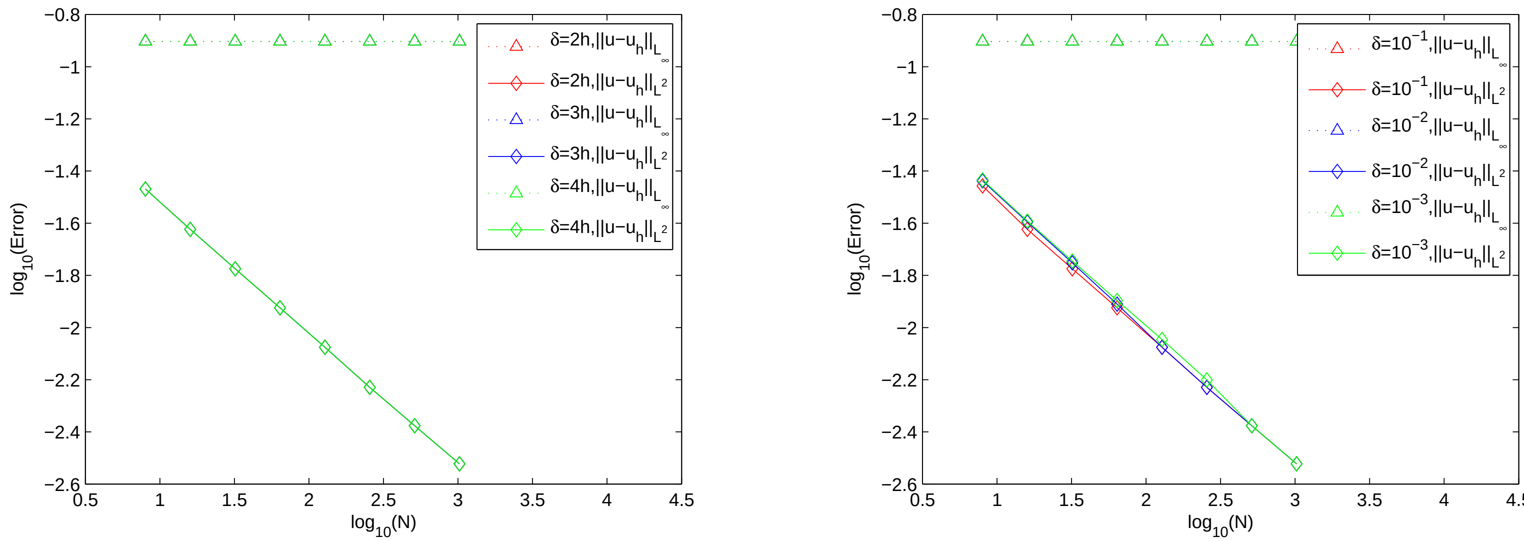
left: $\delta = 2h$, $3h$, and $4h$

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: $\delta = 2h$, $3h$, *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

- 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

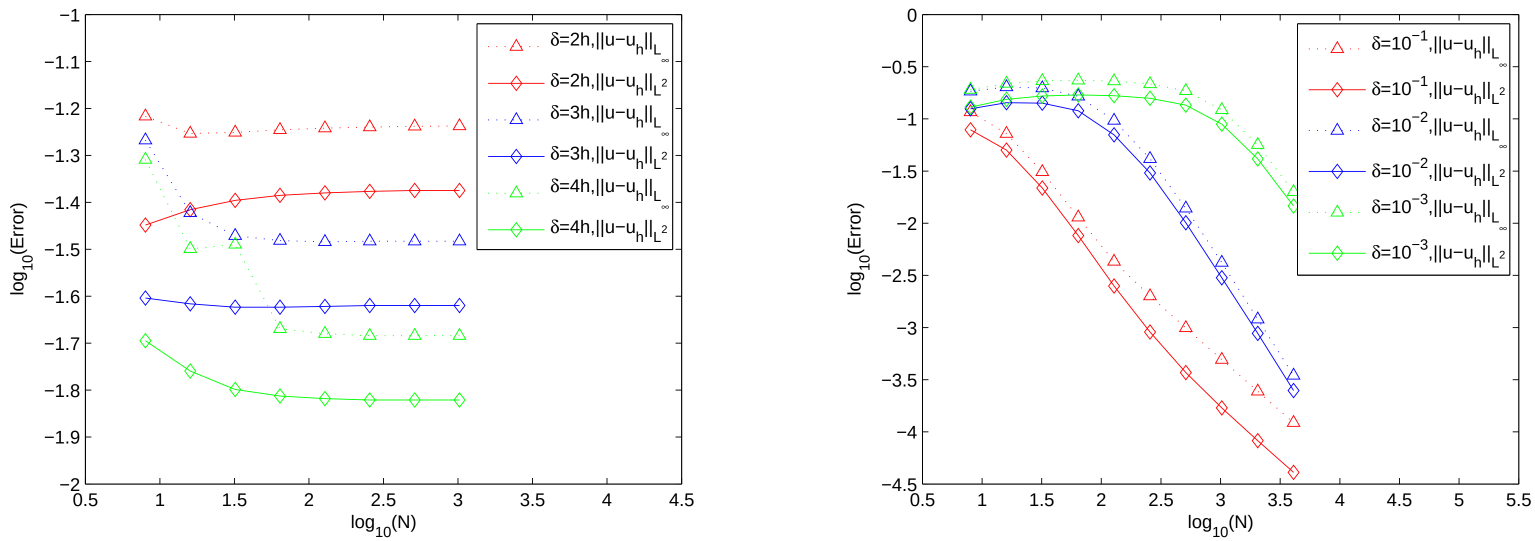
h	$\delta = 2h$		$\delta = 3h$		$\delta = 4h$	
	L^2 error	L^∞ error	L^2 error	L^∞ error	L^2 error	L^∞ error
2^{-3}	3.56E-2	6.07E-2	2.49E-2	2.02E-2	2.02E-2	4.91E-2
2^{-4}	3.84E-2	5.58E-2	2.42E-2	3.78E-2	1.74E-2	3.17E-2
2^{-5}	4.02E-2	5.61E-2	2.38E-2	3.38E-2	1.59E-2	2.34E-2
2^{-6}	4.12E-2	5.68E-2	2.38E-2	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

h	$\delta = 0.1$				$\delta = 0.01$			
	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

h	$\delta = 0.001$			
	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

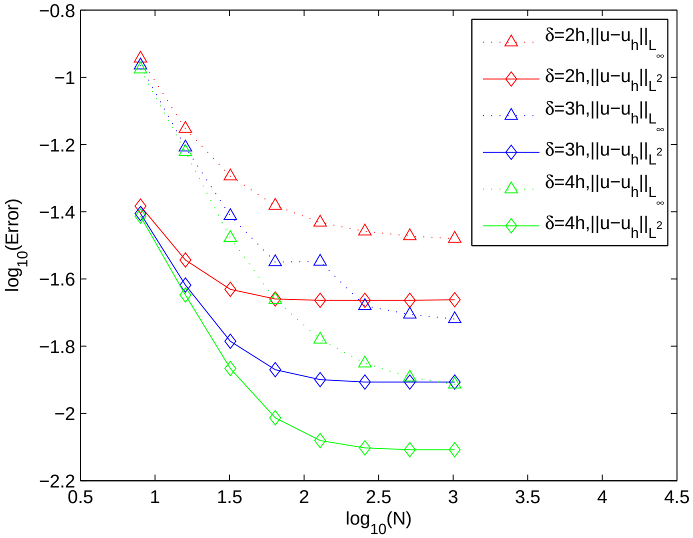
h	$\delta = 2h$		$\delta = 3h$		$\delta = 4h$	
	L^2 error	L^∞ error	L^2 error	L^∞ error	L^2 error	L^∞ error
2^{-3}	4.14E-2	1.14E-1	3.93E-2	1.09E-1	3.86E-2	1.06E-1
2^{-4}	2.86E-2	7.03E-2	2.41E-2	6.19E-2	2.25E-2	6.00E-2
2^{-5}	2.34E-2	5.08E-2	1.64E-2	3.87E-2	1.36E-2	3.33E-2
2^{-6}	2.19E-2	4.15E-2	1.35E-2	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

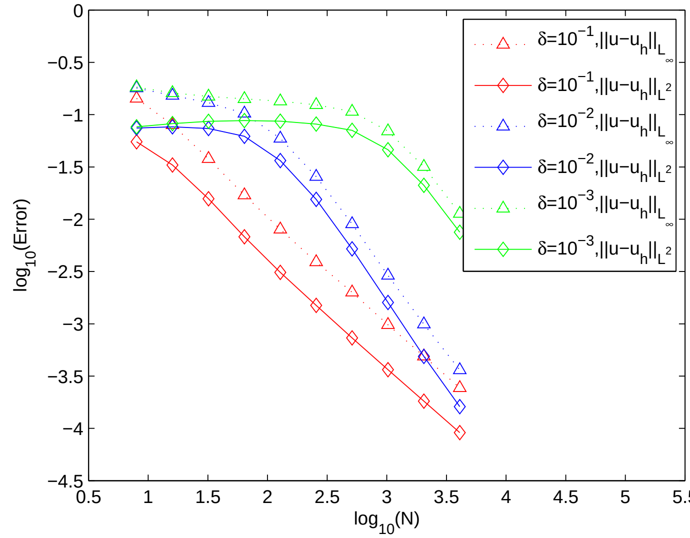
L^2 *and* L^∞ *errors of* discontinuous piecewise-constant *approximations for the discontinuous exact solution and for* δ *proportional to* h

h	$\delta = 0.1$ L^2 Error	L^2 Rate	L^∞ Error	L^∞ Rate	$\delta = 0.01$ L^2 Error	L^2 Rate	L^∞ Error	L^∞ 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

h	$\delta = 0.001$ L^2 Error	L^2 Rate	L^∞ Error	L^∞ 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 $4h$

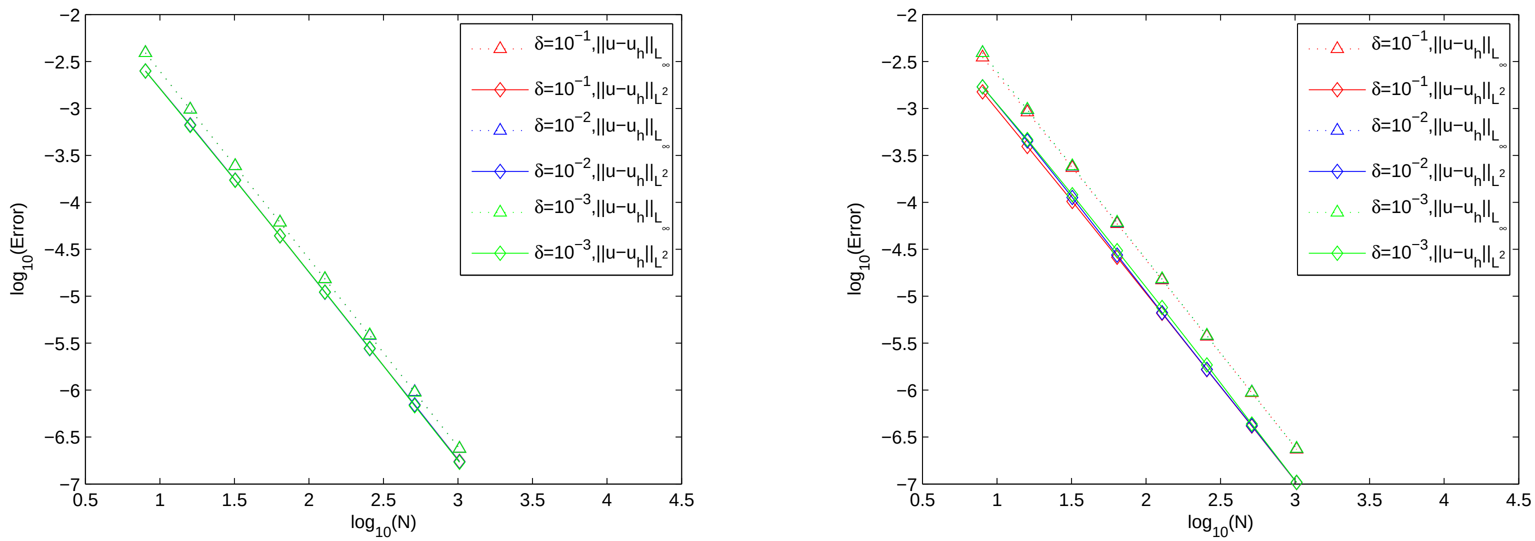
right: $\delta = 0.1$, 0.01, and 0.001

h	L^2 Error	L^2 Rate	L^∞ Error	L^∞ Rate	H^1 Error	H^1 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 $\delta = 0.001$

h	L^2 Error	L^2 Rate	L^∞ Error	L^∞ 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

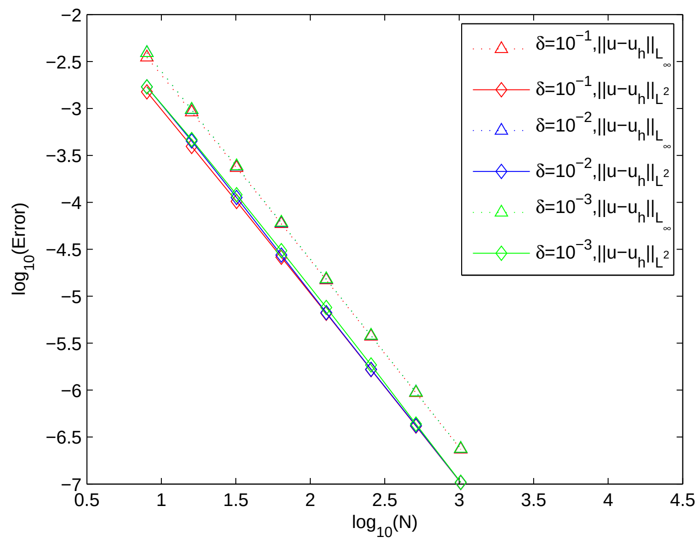
- Even so, it would be nice to take advantage of the fact that continuous approximations of the nonlocal model should be perfectly fine in regions where the solution is smooth

- 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 Error	L^2 Rate	L^∞ Error	L^∞ 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

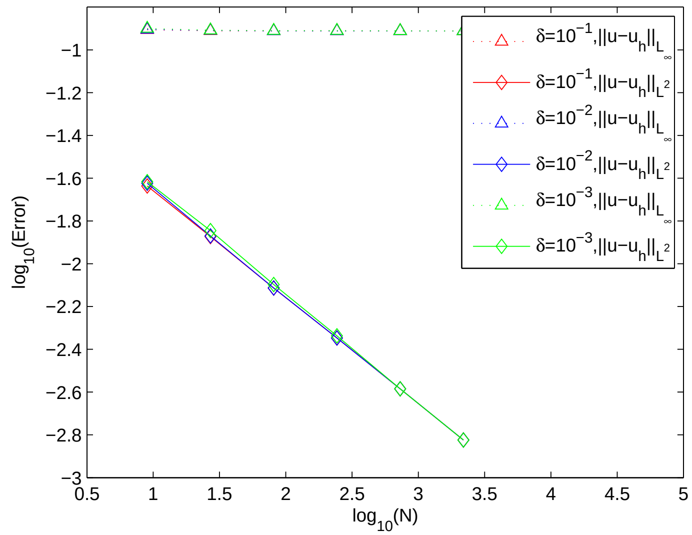
- Now, let's see what happens if we stop cheating

The case of grid points and points of discontinuities not coinciding

h	$\delta = 0.1$, L^2 Error	$\delta = 0.1$, L^2 Rate	$\delta = 0.1$, L^∞ Error	$\delta = 0.1$, L^∞ Rate	$\delta = 0.01$, L^2 Error	$\delta = 0.01$, L^2 Rate	$\delta = 0.01$, L^∞ Error	$\delta = 0.01$, L^∞ Rate
3^{-2}	2.23E-2	–	1.33E-1	–	2.38E-2	–	1.23E-1	–
3^{-3}	1.29E-2	0.50	1.35E-1	–	1.33E-2	0.53	1.28E-1	–
3^{-4}	0.75E-2	0.50	1.36E-1	–	0.74E-2	0.53	1.35E-1	–
3^{-5}	0.43E-2	0.50	1.36E-1	–	0.43E-2	0.50	1.35E-1	–
3^{-6}	0.25E-2	0.50	1.36E-1	–	0.25E-2	0.50	1.36E-1	–
3^{-7}	0.14E-2	0.50	1.36E-1	–	0.14E-2	0.50	1.36E-1	–

h	$\delta = 0.001$, L^2 Error	$\delta = 0.001$, L^2 Rate	$\delta = 0.001$, L^∞ Error	$\delta = 0.001$, L^∞ 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,

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

- 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.,

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

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

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

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

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

- 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

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

  – 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

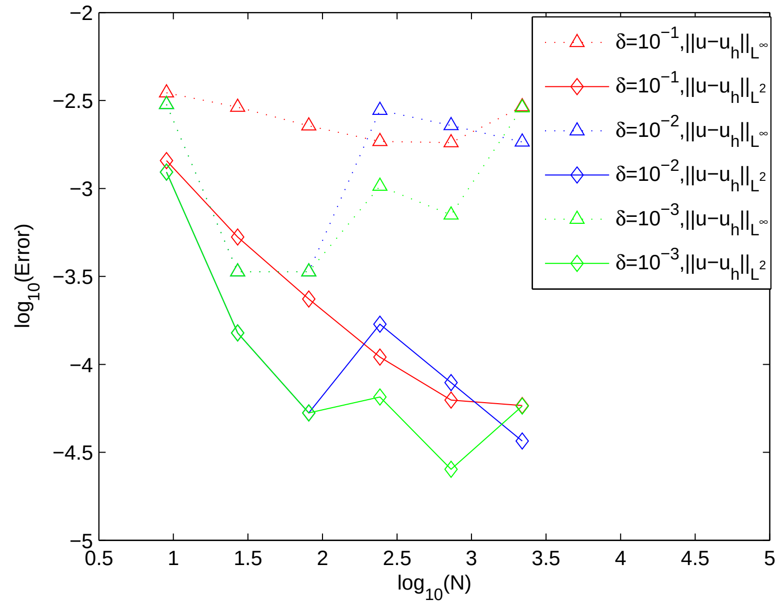
  – but we also do have that the error in the best L^∞ approximation is of $O(h^0)$ regardless of how small we make the interval containing the point of discontinuity

- 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