A NONLOCAL VECTOR CALCULUS

AND

THE ANALYSIS AND APPROXIMATION OF NONLOCAL MODELS FOR DIFFUSION AND MECHANICS

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BACKGROUND

We are interested in

- building (computational) multiscale models that work as a bridge between

  models that are valid at small scales but are not tractable at large scales

  and

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- building computational multiscale monomodels
  - single models that work across a wide very rage of scales

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  and

  models that are tractable at large scales but are not valid at small scales

- building computational multiscale monomodels

  – single models that work across a wide very rage of scales

- in particular, we are interested in computational multiscale models for the mechanics of solids

- but I'm not going talk about any of this today

- “We” includes

  Rich Lehoucq and Mike Parks at Sandia

  Qiang Du at Penn State and his student Kun Zhou

  Pablo Seleson (postoc) at University of Texas at Austin

  Miro Stoyanov (postdoc) and Xi Chen and Guannan Zhang (students) at Florida State

  Yanzhi Zhang at Missouri Institute of Science and Technology

- Closely related talk at 5:20 this afternoon:

  Mathematical Analysis of the Nonlocal State Based Peridynamic Models

  Kun Zhou

  Penn State University

NONLOCAL VOLUME-CONSTRAINED PROBLEMS

- Let $\mathcal{L}$ denote the linear integral operator

$$\mathcal{L}u(\mathbf{x}) := 2\int_{\Omega} \big(u(\mathbf{y}) - u(\mathbf{x})\big)\,\gamma(\mathbf{x},\mathbf{y})\,d\mathbf{y} \qquad \mathbf{x} \in \widetilde{\Omega} \subseteq \Omega \subseteq \mathbb{R}^d$$

where

$u, b\colon \Omega \to \mathbb{R}$

the kernel $\gamma(\mathbf{x},\mathbf{y})\colon \Omega \times \Omega \to \mathbb{R}$ is a non-negative symmetric mapping $\Rightarrow \gamma(\mathbf{x},\mathbf{y}) = \gamma(\mathbf{y},\mathbf{x})$

$\widetilde{\Omega}$ has non-zero volume

– $\mathcal{L}$ is nonlocal because the value of $\mathcal{L}u$ at a point $\mathbf{x}$ requires knowledge of u at points $\mathbf{y} \neq \mathbf{x}$

- Consider the nonlocal volume-constrained problem

$$\begin{cases} -\mathcal{L}u = b & \text{on } \widetilde{\Omega} \subset \Omega \\ \mathcal{V}u = 0 & \text{on } \Omega \setminus \widetilde{\Omega} \end{cases}$$

where

$\mathcal{V}$ denotes a linear operator of volume constraints
on the non-zero volume $\Omega \setminus \widetilde{\Omega}$

– this problem is the spatial contribution to a nonlocal diffusion equation and a nonlocal wave equation

– choosing $\gamma(\mathbf{x},\mathbf{y}) = \frac{\partial^2}{\partial \mathbf{y}^2}\delta(\mathbf{x}-\mathbf{y})$,

where δ denotes the Dirac delta measure,

results, in the sense of distributions, in $\mathcal{L} \equiv \Delta$, the Laplace operator

– we study volume-constrained problems for other kernels

- In particular, we
  - discuss how the operator $\mathcal{L}$ arises in applications
  - develop variational formulations of volume-constrained problems
  - examine the well posedness of volume-constrained problems
  - develop conforming finite element methods including, for appropriate kernels γ, discontinuous Galerkin methods
  - study the convergence and the condition number of finite element approximations of u and $\mathcal{L}$, respectively
  - discuss implementation issues related to finite element discretizations

- Our study is based on a nonlocal vector calculus we have developed
  - thus, after discussing applications, we briefly review the nonlocal vector calculus

- We draw comparisons and parallels between
  - the nonlocal vector calculus and the classical vector calculus for differential operators

  and

  - volume-constrained problems and the second-order scalar elliptic boundary-value problem

$$\begin{cases} -\nabla \cdot \mathbf{D}\nabla u = b & \text{on } \Omega \\ \mathcal{B}u = 0 & \text{on } \partial\Omega \end{cases}$$

where

$\mathbf{D} : \mathbb{R} \to \mathbb{R}^{d\times d}$ denotes a tensor

$\mathcal{B}$ denotes a linear operator acting on the boundary $\partial\Omega$ of Ω

APPLICATIONS OF NONLOCAL OPERATOR $\mathcal{L}$

- The operator $\mathcal{L}$ arises in many applications such as

  - nonlocal diffusion and as a proxy for fractional diffusion
  - graphs
  - image analyses
  - machine learning
  - nonlocal Dirichlet forms
  - the peridynamic model for solid mechanics
  - nonlocal heat conduction

— we briefly discuss some of the these applications

- but we postpone discussion of nonlocal diffusion until after our discussions of applications and of the nonlocal vector calculus

Peridynamics and a nonlocal wave equation

- Stewart Silling derived the linearized peridynamic balance of linear momentum

$$\mathbf{u}_{tt}(\mathbf{x},t) = \mathbf{\Lambda}(\mathbf{x},t) + \mathbf{u}(\mathbf{x},t) \qquad \mathbf{x} \in \mathbb{R}^d, t > 0$$

where $\mathbf{u} : \Omega \to \mathbb{R}^d$ and

$$\mathbf{\Lambda}(\mathbf{x},t) := \int_\Omega \frac{(\mathbf{y}-\mathbf{x}) \otimes (\mathbf{y}-\mathbf{x})}{\sigma(|\mathbf{y}-\mathbf{x}|)} \big(\mathbf{u}(\mathbf{y},t) - \mathbf{u}(\mathbf{x},t)\big)\, d\mathbf{y}$$

- the operators $\mathcal{L}$ and $\mathbf{\Lambda}$ coincide when $d = 1$ and

$$\gamma(x,y) = (y-x)^2/\sigma(|y-x|)$$

- Du and Zhou provide well-posedness results for both the peridynamics balance law and the associated equilibrium equation $\Lambda + b = \mathbf{0}$ on unbounded domains and also analyze specialized 1D and 2D volume-constrained problems; see also related work by Julio Rossi and co-workers

- As a special case of the peridynamics balance law we obtain the nonlocal wave equation

$$
\begin{cases}
u_{tt}(\mathbf{x},t) = \mathcal{L}u(\mathbf{x},t) & \mathbf{x} \in \mathbb{R}^d, t \geq 0 \\
u(\mathbf{x},0) = u_0(\mathbf{x}) & \mathbf{x} \in \mathbb{R}^d, \\
u_t(\mathbf{x},0) = v_0(\mathbf{x}) & \mathbf{x} \in \mathbb{R}^d
\end{cases}
$$

- Forthcoming papers (by Du, G., Lehoucq, and Zhou) will provide further analyses and numerical analyses for the peridynamic model
  - see Kun Zhou's talk this afternoon

Graph Laplacian

- Lov'asz and Szegedy introduce a precise notion of the limit of a sequence of dense graphs
  - the limit is a symmetric measurable function $W : [0,1] \times [0,1] \mapsto [0,1]$ and represents the continuum analog of an adjacency matrix for a simple unweighted graph

- The operator $\mathcal{L}$ then represents the continuum analog of the graph Laplacian for the simple unweighted graph when $W \equiv \gamma$ and $(0,1) \equiv \Omega$
  - this allows consideration of many properties of a graph associated with its Laplacian matrix to be independent of the graph's size and connectivity
  - this includes diffusion and the relationship between the eigenvectors and eigenfunctions of the graph Laplacian and $\mathcal{L}$ induced by W
  - the latter topic is the subject of work by Rich Lehoucq and co-workers that is to be reported elsewhere

Fractional Laplacian

- The fractional Laplacian is defined to be the pseudo-differential operator $\mathcal{F}$ that satisfies

$$\mathcal{F}\big((-\Delta)^s u\big)(\xi) = |\xi|^{2s}\widehat{u}(\xi), \qquad 0 < s < 1$$

where $\widehat{u}$ denotes the Fourier transform of u

- Suppose that $u \in L^2(\mathbb{R}^d)$ and that

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}(u(\mathbf{x}) - u(\mathbf{y}))^2|\mathbf{y}-\mathbf{x}|^{-(d+2s)}d\mathbf{y}\,d\mathbf{x} < \infty$$

  – then the Fourier transform can be used to show that an equivalent characterization of the fractional Laplacian is given by

$$(-\Delta)^s u = C_{d,s}\int_{\mathbb{R}^d}\frac{u(\mathbf{x}) - u(\mathbf{y})}{|\mathbf{y}-\mathbf{x}|^{d+2s}}d\mathbf{y}, \qquad 0 < s < 1$$

  for some normalizing constant$C_{d,s}$

– then, when $\widetilde{\Omega} = \Omega \equiv \mathbb{R}^d$ and $\gamma(\mathbf{x}, \mathbf{y}) \equiv |\mathbf{y} - \mathbf{x}|^{-(d+2s)}$, we have that

$$\boxed{\mathcal{L} = -\big(-\Delta\big)^s, \qquad 0 < s < 1}$$

which shows that

the fractional Laplacian is a special case of the operator $\mathcal{L}$

- more on this later

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 $\Omega \subset \mathbb{R}^d \to \mathbb{R}^{n\times k}$ or $\mathbb{R}^n$ or $\mathbb{R}$

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

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

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

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

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

- 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

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

- 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

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

- For the sake of economy, we will focus mostly on the divergence operator
  - everything we say has corresponding analogs for the gradient and curl operators

NONLOCAL INTEGRAL THEOREMS, ADJOINT OPERATORS, AND GREEN'S AND OTHER IDENTITIES

- One easily obtains the nonlocal integral theorem

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

  - that is

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

- From the nonlocal integral theorem, one obtains the nonlocal integration by parts formula

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

Nonlocal adjoint operators

- Given an operator $\mathcal{L}$ that maps two-point functions F to point functions defined over Ω, the adjoint operator $\mathcal{L}^*$ that maps point functions G to two-point functions defined over $\Omega \times \Omega$ 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 (or appropriate duality pairings)

- 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 operator

  – the adjoint of $\mathcal{D}$ is given by

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

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

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

Nonlocal Green's identities

- A nonlocal Green's first identity can be derived by setting $F = \Theta\mathcal{F}^*(H)$ in the defining relation for adjoint operators ($\mathcal{F} = \mathcal{D}$, or $\mathcal{G}$, or $\mathcal{V}$)
  - $\mathcal{L}^*(H)$ 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

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

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

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

- For the nonlocal divergence operator and the corresponding nonlocal adjoint operator we then have nonlocal Green's first identity

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

  – $\mathbf{\Theta}(\mathbf{x},\mathbf{y}):\,\Omega\times\Omega\to\mathbb{R}^{n\times n}$ denotes a two-point second-order tensor function

- We also obtain the nonlocal Green's second identity

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

Nonlocal vector identities

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

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

- 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 $\mathcal{C}^*\big(\mathcal{G}(\eta)\big) \neq 0$

Why doesn't the nonlocal vector calculus always look like the local differential vector calculus?

- In addition to

  – the divergence, gradient, and curl operators

  and

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

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

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

and the Green's (generalized) first identity for scalar functions u and v states that, for tensor-valued "constitutive" functions $\mathbf{D}$,

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

– however, neither the nonlocal divergence theorem

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

nor the nonlocal Green's first identity

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

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 "boundary"-like terms

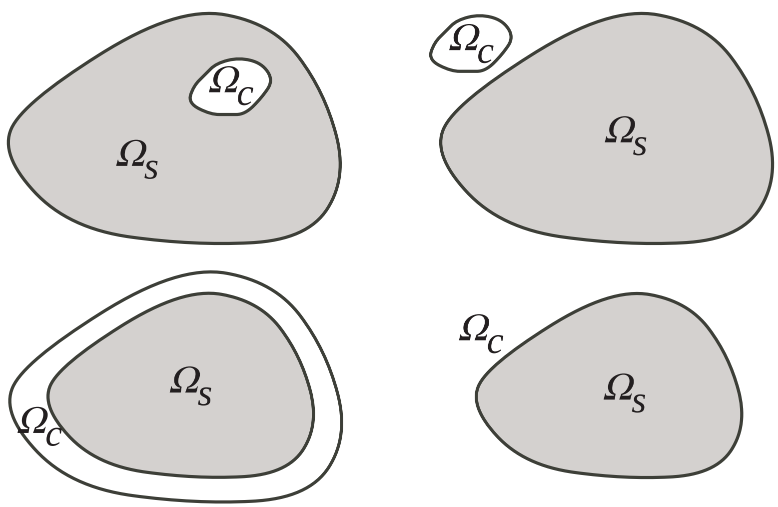
  – the reason it was not necessary to introduce constraint operators and "boundary" integrals in the theorems and identities of the nonlocal vector calculus is that, in the nonlocal case, constraint operators operate on functions defined over measurable volumes, and not on lower-dimensional manifolds

  – 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 their 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 AND OPERATORS

- We divide the region Ω into disjoint, covering open subsets $\widetilde{\Omega}$ and $\Omega \setminus \widetilde{\Omega}$
  - $\widetilde{\Omega}$ is the solution domain
  - $\Omega \setminus \widetilde{\Omega}$ is the constraint domain
- Note that no relation is assumed between $\widetilde{\Omega}$ and $\Omega \setminus \widetilde{\Omega}$
  - for example, these four configurations, as well as others, are possible



$\Omega_s = \widetilde{\Omega} \qquad \Omega_c = \Omega \setminus \widetilde{\Omega}$

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

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

- We then define the corresponding constraint operator $\mathcal{N}(\boldsymbol{\nu})$ by

$$\mathcal{N}(\boldsymbol{\nu})(\mathbf{x}) := -\int_\Omega \big(\boldsymbol{\nu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\nu}(\mathbf{y},\mathbf{x})\big) \cdot \boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) \qquad \text{for } \mathbf{x} \in \Omega \setminus \widetilde{\Omega}$$

  - 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 $\mathbf{x} \in \widetilde{\Omega}$

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

- 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 Gauss' theorem

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

- Nonlocal integration by parts formula

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

- Nonlocal Green's first identity

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

- Nonlocal Green's second identity

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

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

NONLOCAL DIFFUSION

- Before we discuss nonlocal diffusion, we review diffusion in the classical context

CLASSICAL LOCAL DIFFUSION

- $\Omega \subseteq \mathbb{R}^d$ denotes an open region

  $\Omega_1 \subset \Omega$ and $\Omega_2 \subset \Omega$ denote two disjoint open regions

  $\partial\Omega_{12} = \overline{\Omega}_1 \cap \overline{\Omega}_2$ common boundary of Ω_1 and Ω_2

- If $\partial\Omega_{12}$ is nonempty

classical local flux out of Ω_1 into Ω_2 $\Rightarrow$ $\displaystyle\int_{\partial\Omega_{12}} \mathbf{q} \cdot \mathbf{n}_1 \, dA$

$\mathbf{q}$ = flux density

$\mathbf{n}_1$ = unit normal on $\partial\Omega_{12}$ pointing outward from Ω_1

- Note that
  - the flux from Ω_1 into Ω_2 occurs across their common boundary $\partial\Omega_{12}$
  - if the two disjoint regions have no common boundary, then the flux from one to the other is zero
  - the classical flux is then deemed local since there is no interaction between Ω_1 and Ω_2 when separated by a finite distance

- The classical flux satisfies action-reaction

$$\int_{\partial\Omega_{12}} \mathbf{q}\cdot\mathbf{n}_1\,dA + \int_{\partial\Omega_{21}} \mathbf{q}\cdot\mathbf{n}_2\,dA = \int_{\partial\Omega_{12}} \mathbf{q}\cdot\mathbf{n}_1\,dA - \int_{\partial\Omega_{12}} \mathbf{q}\cdot\mathbf{n}_1\,dA = 0$$

  - in words,

    the flux from Ω_1 into Ω_2

    is equal and opposite to

    the flux from Ω_2 into Ω_1

Local diffusion

- Ω denote a bounded, open set in $\mathbb{R}^d$

- Then, classical balance laws have the form

$$\frac{d}{dt}\int_{\widehat{\Omega}} u(\mathbf{x},t)\,dx = \int_{\widehat{\Omega}} b\,d\mathbf{x} - \int_{\partial\widehat{\Omega}} \mathbf{q}\cdot\mathbf{n}\,dA \qquad \forall\,\widehat{\Omega}\subseteq\Omega$$

$\mathbf{n} =$ unit normal vector on $\partial\widehat{\Omega}$ pointing outwards from $\widehat{\Omega}$

$b =$ source density for u in $\widehat{\Omega}$

$\mathbf{q} =$ now denotes the flux density along $\partial\widehat{\Omega}$ corresponding to u

– in words,

the temporal rate of change of the quantity $\int_{\widehat{\Omega}} u(\mathbf{x},t)\,dx$

is given by

the amount of u created within $\widehat{\Omega}$ by the source b

minus

the flux of u out of $\widehat{\Omega}$ through its boundary $\partial\widehat{\Omega}$

- The classical diffusion flux for a quantity u arises when the flux density

$$\boxed{\mathbf{q} \equiv -\mathbf{D}\nabla u}$$

$\mathbf{D}$ = a symmetric, positive definite second-order tensor

– substitution into the balance law yields that

$$\frac{d}{dt}\int_{\widehat{\Omega}} u(\mathbf{x},t)\,dx = \int_{\widehat{\Omega}} b\,d\mathbf{x} + \int_{\partial\widehat{\Omega}} (\mathbf{D}\nabla u)\cdot\mathbf{n}\,dA \qquad \forall\,\widehat{\Omega}\subseteq\Omega$$

- Because $\widehat{\Omega}\subseteq\Omega$ is arbitrary, using Gauss' theorem, on obtains

classical diffusion equation $\Rightarrow \qquad u_t - \nabla\cdot(\mathbf{D}\nabla u) = b \qquad \forall\,\mathbf{x}\in\Omega\,,\ t>0$

– to uniquely determine u, one must also require u to satisfy an initial condition

$$u(\mathbf{x},0) = u_0(\mathbf{x}) \qquad \forall\, \mathbf{x} \in \Omega$$

and a boundary condition

$$\mathcal{B}u = g \qquad \forall\, \mathbf{x} \in \partial\Omega\,,\ t > 0$$

$\mathcal{B} =$ an operator acting on functions defined on $\partial\Omega$

– common choices include

$$\begin{array}{lcl} \mathcal{B}v = v & \Rightarrow & \text{Dirichlet} \\ \mathcal{B}v = (\mathbf{D}\nabla v)\cdot\mathbf{n} & \Rightarrow & \text{Neumann} \\ \mathcal{B}v = (\mathbf{D}\nabla v)\cdot\mathbf{n} + \varphi v & \Rightarrow & \text{Robin} \end{array}$$

- The balance law in the previous slide models diffusion because

  if $b = 0$ and $g = 0$ and for any of the choices for $\mathcal{B}$

  we have that, for u not a constant function,

$$\frac{d}{dt}\int_\Omega u^2\,dx = -2\int_\Omega (\mathbf{D}\nabla u)\cdot\nabla u\,dx < 0$$

Steady-state local diffusion

- Steady-state diffusion occurs when $u_t = 0$

- We then have that the initial-boundary value problem reduces to the elliptic boundary-value problem

- The variational analysis for steady-state diffusion starts by considering the solution of

$$\min_{u \in H^1(\Omega)} E(u) \qquad \text{subject to} \quad u = g_1 \quad \text{on} \quad \partial\Omega_d$$

- The energy functional is given by

$$E(u) = \frac{1}{2}\int_{\Omega} \mathbf{D}\nabla u \cdot \nabla u \, d\mathbf{x} + \frac{1}{2}\int_{\partial\Omega_r} \varphi u^2 \, dA - \int_{\Omega} ub \, d\mathbf{x} - \int_{\partial\Omega_n \cap \partial\Omega_r} u g_2 \, dA$$

where

$\partial\Omega_d =$ Dirichlet part of the boundary

$\partial\Omega_n =$ Neumann part of the boundary

$\partial\Omega_r =$ Robin part of the boundary

– for economy of exposition, we will consider only the homogeneous "pure" Dirichlet and Neumann boundary conditions

- For the Dirichlet problem
  - define the constrained subspace $H_0^1(\Omega) = \{u \in H^1(\Omega) \mid v = 0 \text{ on } \partial\Omega\}$
  - then, for $b \in H^{-1}(\Omega)$, solutions $u \in H_0^1(\Omega)$ of the minimization problem equivalently satisfy the Euler-Lagrange equations

$$\int_\Omega \mathbf{D}\nabla v \cdot \nabla u \, d\mathbf{x} = \int_\Omega vb \, d\mathbf{x} \qquad \forall\, v \in H_0^1(\Omega) \tag{1}$$

  - for sufficiently smooth u, this is equivalent to the second-order elliptic Dirichlet boundary-value problem

$$\begin{cases} -\nabla \cdot (\mathbf{D}\nabla u) = b & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

    - this is easily seen by using the classical Green's first identity and recalling that $v = 0$ on $\partial\Omega$
  - the Dirichlet boundary condition $u = 0$ is essential
    - it must be imposed on candidate minimizers

- For the Neumann problem
  - define the constrained subspace $H^1_c(\Omega) := \{u \in H^1(\Omega) \mid \int_\Omega u \, d\mathbf{x} = 0\}$
  - then, for $b \in (H^1_c(\Omega))'$ such that $\int_\Omega b \, d\mathbf{x} = 0$, where $(H^1_c(\Omega))'$ denotes the dual space of $H^1_c(\Omega)$, solutions $u \in H^1_c(\Omega)$ of the minimization problem equivalently satisfy the Euler-Lagrange equation

$$\int_\Omega \mathbf{D}\nabla v \cdot \nabla u \, d\mathbf{x} = \int_\Omega v b \, d\mathbf{x} \qquad \forall\, v \in H^1_c(\Omega)$$

  - for sufficiently smooth u, this is equivalent to the second-order elliptic Neumann boundary-value problem

$$\begin{cases} -\nabla \cdot (\mathbf{D}\nabla u) = b & \text{in } \Omega \\ \displaystyle\int_\Omega u = 0 & \\ (\mathbf{D}\nabla u) \cdot \mathbf{n} = 0 & \text{on } \partial\Omega \end{cases}$$

    - this is easily seen by using the classical Green's first identity and recalling that $\int_{\partial\Omega} v \, dA = 0$

- the constraint $\int_{\partial\Omega} u\, dA = 0$ is essential
  - it must be imposed on candidate minimizers
- the Neumann boundary condition $(\mathbf{D}\nabla u) \cdot \mathbf{n} = 0$ is natural
  - it does not have to be imposed on candidate minimizers

- Everything anyone wants to know about classical steady-state diffusion is known, e.g.,
  - well posedness
  - convergence of finite element approximations

NONLOCAL DIFFUSION

- The key to understanding the connection between the operator $\mathcal{L}$ and models for diffusion is identifying a nonlocal flux

- $\Omega_1, \Omega_2 =$ two disjoint regions, both having nonzero volume

  $f(\mathbf{x},\mathbf{y}) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ an anti-symmetric function

  $$\Rightarrow f(\mathbf{x},\mathbf{y}) = -f(\mathbf{y},\mathbf{x})$$

  nonlocal flux from Ω_1 into $\Omega_2 \Rightarrow$ $$\int_{\Omega_1}\int_{\Omega_2} f(\mathbf{x},\mathbf{y})\, d\mathbf{y}\, d\mathbf{x}$$

  – the flux is nonlocal because

  the flux may be nonzero even when Ω_1 and Ω_2 are disjoint

  - this is in stark contrast to the classical case for which there is flux between two regions only when they are in contact

- the antisymmetry of f is equivalent to the action-reaction principle

$$\int_{\Omega_1}\int_{\Omega_2} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x} + \int_{\Omega_2}\int_{\Omega_1} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x} = 0 \qquad \forall\,\Omega_1,\Omega_2 \subset \mathbb{R}^d$$

  - in words,

    the flux from Ω_1 into Ω_2 is equal and opposite
    to the flux from Ω_2 to Ω_1

- the antisymmetry of f further implies that

$$\int_{\Omega_1}\int_{\Omega_2} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x} + \int_{\Omega_2}\int_{\Omega_1\cup\Omega_2} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x} = 0 \qquad \forall\,\Omega_1,\Omega_2 \subset \mathbb{R}^d$$

Nonlocal diffusion

- Ω = open set in $\mathbb{R}^3$

- Nonlocal balance laws have the form

$$\frac{d}{dt}\int_{\widehat{\Omega}} u(\mathbf{x},t)\,dx = \int_{\widehat{\Omega}} b\,d\mathbf{x} - \int_{\widehat{\Omega}}\int_{\Omega\setminus\widehat{\Omega}} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x} \qquad \forall\,\widehat{\Omega}\subseteq\Omega$$

b = source density for u in $\widehat{\Omega}$

$\int_{\Omega\setminus\widehat{\Omega}} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}$ = the flux density corresponding to u

  - in words,

    the temporal rate of change of the quantity $\int_{\widehat{\Omega}} u(\mathbf{x},t)\,dx$

    is given by

    the amount of u created within $\widehat{\Omega}$ by the source b

    minus

    the flux of u out of $\widehat{\Omega}$ into $\Omega\setminus\widehat{\Omega}$

- Nonlocal diffusion flux arises when

$$\int_{\widehat{\Omega}} f(\mathbf{x},\mathbf{y})\,d\mathbf{y} = \int_{\widehat{\Omega}} \Big(\boldsymbol{\Theta}\mathcal{D}^*(u) + \big(\boldsymbol{\Theta}\mathcal{D}^*(u)\big)' \Big) \cdot \boldsymbol{\alpha}\,d\mathbf{y}$$

  - it is then easy to show that

$$\int_{\widehat{\Omega}} \int_{\Omega\setminus\widehat{\Omega}} f(\mathbf{x},\mathbf{y})\,d\mathbf{y} = \int_{\Omega\setminus\widehat{\Omega}} \mathcal{N}(\boldsymbol{\Theta}\mathcal{D}^* u)\,d\mathbf{x}$$

- Then, the balance law governing nonlocal diffusion is given by

$$\frac{d}{dt}\int_{\widehat{\Omega}} u(\mathbf{x},t)\,dx = \int_{\widehat{\Omega}} b\,d\mathbf{x} - \int_{\Omega\setminus\widehat{\Omega}} \mathcal{N}(\boldsymbol{\Theta}\mathcal{D}^* u)\,d\mathbf{x} \qquad \forall\,\widehat{\Omega} \subseteq \Omega$$

- Then, using the nonlocal Gauss' theorem, for $\widetilde{\Omega} \subset \Omega$, we have the nonlocal diffusion equation

$$u_t + \mathcal{D}(\mathbf{\Theta}\mathcal{D}^* u) = b \qquad \forall\, \mathbf{x} \in \widetilde{\Omega} \subset \Omega,\ t > 0$$

- We have that

$$\mathcal{D}(\mathbf{\Theta}\mathcal{D}^* u) = 2\int_\Omega \big(u(\mathbf{x}) - u(\mathbf{y})\big)\gamma(\mathbf{x},\mathbf{y})\,d\mathbf{x} \qquad \text{with} \qquad \gamma(\mathbf{x},\mathbf{y}) = \boldsymbol{\alpha}\cdot(\mathbf{\Theta}\boldsymbol{\alpha})$$

so that

$$\mathcal{D}(\mathbf{\Theta}\mathcal{D}^* u) = -\mathcal{L}u$$

so that the nonlocal diffusion equation is given by

$$u_t - \mathcal{L}u = b \qquad \forall\, \mathbf{x} \in \widetilde{\Omega} \subset \Omega,\ t > 0$$

- As we did for the local diffusion case, we now consider steady-state nolocal diffusion problems

VOLUME-CONSTRAINED STEADY-STATE NONLOCAL DIFFUSION PROBLEMS

VARIATIONAL FORMULATION

- For $\widetilde{\Omega} \subset \Omega$, define the energy functional

$$\boxed{E(u) = E_f(u) + E_b(u)}$$

$$\begin{cases} E_f(u) := \dfrac{1}{2}\displaystyle\int_\Omega \int_\Omega \mathcal{D}^*(u)(\mathbf{x},\mathbf{y}) \cdot \boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\, \mathcal{D}^*(u)(\mathbf{x},\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} \\ \qquad\qquad = \dfrac{1}{2}\displaystyle\int_\Omega \int_\Omega \big(u(\mathbf{y}) - u(\mathbf{x})\big)^2 \gamma(\mathbf{x},\mathbf{y})\, d\mathbf{y}\, d\mathbf{x}, \\ E_b(u) := -\displaystyle\int_{\widetilde{\Omega}} b(\mathbf{x}) u(\mathbf{x})\, d\mathbf{x}. \end{cases}$$

where

$$\gamma(\mathbf{x},\mathbf{y}) = \boldsymbol{\alpha} \cdot \boldsymbol{\Theta}\boldsymbol{\alpha}$$

$\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})$ = a second-order, symmetric (in the matrix and function sense), positive definite tensor

- Consider the constrained minimization problem

$$\text{minimize} \quad E(u) \quad \text{subject to} \quad E_c(u) = 0$$

where

$E_c(u)$ denotes a constraint functional

- The first-order necessary condition corresponding to the minimization problem is given by

$$\int_\Omega \int_\Omega \mathcal{D}^*(u)(\mathbf{x},\mathbf{y}) \cdot \boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\, \mathcal{D}^*(v)(\mathbf{x},\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} = \int_{\widetilde{\Omega}} b(\mathbf{x}) v(\mathbf{x})\, d\mathbf{x}$$

where the test functions $v(\mathbf{x})$ satisfy the constraint $E_c(v) = 0$

- For example, first let

$$E_c(u) = E_c^d(u) = \int_{\Omega\setminus\widetilde{\Omega}} u^2 \, d\mathbf{x}$$

where $\qquad \Omega \setminus \widetilde{\Omega} =$ a subset of Ω having nonzero measure

  – note that $E_c^d(u) = 0$ implies that $u(\mathbf{x}) = 0$ a.e. in $\Omega \setminus \widetilde{\Omega}$

  – then, using the nonlocal Green's first identity of the nonlocal vector calculus, we obtain, using $E_c^d(v) = 0$, that

$$\int_{\widetilde{\Omega}} v\mathcal{D}(\boldsymbol{\Theta}\mathcal{D}^* u) \, d\mathbf{x} - \int_{\Omega\setminus\widetilde{\Omega}} v\mathcal{N}(\boldsymbol{\Theta}\mathcal{D}^* u) \, d\mathbf{x} = \int_{\Omega\setminus\widetilde{\Omega}} bv \, d\mathbf{x}, \qquad \mathbf{x} \in \widetilde{\Omega}$$

  – because $v(\mathbf{x})$ is arbitrary in $\widetilde{\Omega}$ and $v(\mathbf{x}) = 0$ a.e. in $\Omega \setminus \widetilde{\Omega}$

$\Rightarrow$ solution of the minimization problem satisfies

$$\begin{cases} -\mathcal{L}(u) = \mathcal{D}\big(\boldsymbol{\Theta}\mathcal{D}^*(u)\big) = b & \text{on } \widetilde{\Omega} \\ u = 0 & \text{on } \Omega \setminus \widetilde{\Omega} \end{cases}$$

- On the other hand, let

$$E_c(u) = E_c^n(u) = \Big(\int_\Omega u \, d\mathbf{x} \Big)^2$$

and assume that

$$\int_{\widetilde{\Omega}} b \, d\mathbf{x} = 0$$

  – then, solutions of the minimization problem satisfy

$$\begin{cases} -\mathcal{L}(u) = \mathcal{D}\big(\boldsymbol{\Theta}\mathcal{D}^*(u)\big) = b & \text{on } \widetilde{\Omega} \\ \mathcal{N}(\boldsymbol{\Theta}\mathcal{D}^* u) = 0 & \text{on } \Omega \setminus \widetilde{\Omega} \\ \displaystyle\int_\Omega u \, d\mathbf{x} = 0 & \end{cases}$$

- Both choices discussed for the constraint operator $E_c(u)$ in the variational principle, or, equivalently, in the nonlocal volume-constrained problems, are essential to the variational principle
  - they must be imposed on candidate minimizers as conditions that ensure that solutions are unique

- However, the constraints $E_c^d(\cdot)$ and $E_c^n(\cdot)$ are very different
  - $E_c^d(\cdot)$ involves the selection of a subdomain $\widetilde{\Omega} \subset \Omega$ and the integral of the square of u over $\Omega \setminus \widetilde{\Omega}$
  - $E_c^n(\cdot)$ does not require the selection of a subdomain and involves the square of the integral of u over the domain Ω

- This leads to distinct forms for the constraints appearing in the nonlocal volume-constrained problems
  - $E_c^d(\cdot)$ holds pointwise almost everywhere in the subdomain $\Omega \setminus \widetilde{\Omega}$
  - $E_c^n(\cdot)$ is a single integral constraint

– with some justification one can view $E_c^n(\cdot)$ as a "Neumann" constraint

– again with justification, $E_c^d(\cdot)$ can be viewed as a "Dirichlet" constraint

- In general,

  – we assume that $E_c(\cdot)$ denotes a bounded, quadratic functional on a suitable Hilbert space, e.g., if that space is $L^2(\Omega)$, we have

$$E_c(u) \leq \widehat{c}\|u\|_{L^2}^2 \qquad \forall\, u \in L^2(\Omega)$$

  – moreover, we assume that the intersection of the set of constant-valued functions with the set of functions satisfying $E_c(u) = 0$ is $u \equiv 0$

  – clearly, both $E_c^d(\cdot)$ and $E_c^n(\cdot)$ satisfy these assumptions

THE KERNEL

- Assume that the domain Ω is bounded with piecewise smooth boundary and satisfies the interior cone condition
  - for simplicity, we also assume that both $\widetilde{\Omega}$ and $\Omega \setminus \widetilde{\Omega}$ have the same properties

- The smoothing effected by solving volume-constrained problems involving the operator $\mathcal{L} = -\mathcal{D}\big(\boldsymbol{\Theta}\,\mathcal{D}^*(\cdot)\big)$ depends on the regularity associated with the kernel $\gamma = \boldsymbol{\alpha} \cdot \boldsymbol{\Theta}\boldsymbol{\alpha}$

- Given positive constants γ_0 and ε, we first assume that γ satisfies

$$\begin{array}{ll} \gamma(\mathbf{x},\mathbf{y}) \geq \gamma_0 > 0 & \forall\, \mathbf{y} \in B_\varepsilon^{\mathbf{x}} \\ \gamma(\mathbf{x},\mathbf{y}) = 0 & \forall\, \mathbf{y} \in \Omega \setminus B_\varepsilon^{\mathbf{x}} \end{array}$$

  where

$$B_\varepsilon^{\mathbf{x}} := \{\mathbf{y} \in \Omega \colon |\mathbf{y} - \mathbf{x}| \leq \varepsilon\}$$

- Recall that γ is symmetric $\Rightarrow \gamma(\mathbf{x},\mathbf{y}) = \gamma(\mathbf{y},\mathbf{x})$

- We consider the following two cases

Case 1. There exist positive constants $s \in (0,1)$, γ_*, and γ^* such that

$$\frac{\gamma_*}{|\mathbf{y}-\mathbf{x}|^{d+2s}} \leq \gamma(\mathbf{x},\mathbf{y}) \leq \frac{\gamma^*}{|\mathbf{y}-\mathbf{x}|^{d+2s}}, \qquad |\mathbf{y}-\mathbf{x}| \leq \varepsilon$$

Case 2. The function γ is non-degenerate in the sense that there exist positive constants γ_1 and γ_2 such that

$$\gamma_1 \leq \int_\Omega \gamma^2(\mathbf{x},\mathbf{y})\, d\mathbf{y} \leq \gamma_2 \quad \forall \mathbf{x} \in \widetilde{\Omega} \subseteq \Omega$$

and γ is a Hilbert-Schmidt kernel, e.g., satisfies

$$\int_\Omega \int_{B_\delta^{\mathbf{x}}} \gamma^2(\mathbf{x},\mathbf{y})\, d\mathbf{x}\, d\mathbf{y} < \infty$$

- We remark that a complete classification of kernels is not our goal, rather we want to consider a sufficiently broad class that includes the applications of interest to us
  - the two cases meet our requirement

EQUIVALENCE OF SPACES

- We define the energy norm

$$|||u||| := \big(E_f(u)\big)^{1/2}$$

the nonlocal energy space

$$V(\Omega) := \big\{u \in L^2(\Omega) \colon |||u||| < \infty\big\}$$

and the volume-constrained nonlocal energy space

$$V_c(\Omega) := \{u \in V(\Omega) \colon E_c(u) = 0\}$$

- We also define $|||u|||_{V_c^*(\Omega)}$ to be the norm for the dual space $V_c^*(\Omega)$ of $V_c(\Omega)$ with respect to the standard $L^2(\Omega)$ duality pairing

- We want to characterize the nonlocal energy space in terms of known Sobolev spaces

- For $s \in (0,1)$, the standard fractional-order Sobolev space is defined as

$$H^s(\Omega) := \Big\{ u \in L^2(\Omega) : \|u\|_{L^2(\Omega)} + |u|_{H^s(\Omega)} < \infty \Big\}$$

where

$$|u|^2_{H^s(\Omega)} := \int_\Omega \int_\Omega \frac{\big(u(\mathbf{y}) - u(\mathbf{x})\big)^2}{|\mathbf{y} - \mathbf{x}|^{d+2s}} \, d\mathbf{y} d\mathbf{x}$$

  – moreover, define the subspace

$$H^s_c(\Omega) := \{ u \in H^s(\Omega) : E_c(u) = 0 \}$$

  and recall that $|\cdot|_{H^s(\Omega)}$ is an equivalent norm on the quotient space $H^s_c(\Omega)$

  – similarly, we define the subspace

$$L^2_c(\Omega) := \Big\{ u \in L^2(\Omega) : E_c(u) = 0 \Big\}$$

Case 1

- We have the following results that are used to demonstrate that the spaces $V_c(\Omega)$ and $H^s_c(\Omega)$ are continuously embedded within each other

$$|u|^2_{H^s(\Omega)} \le \gamma_*^{-1} |||u|||^2 + 4|\Omega|\varepsilon^{-(d+2s)} \|u\|^2_{L^2(\Omega)}$$

$$|||u|||^2 \le \gamma^* |u|^2_{H^s(\Omega)}$$

- We also have the following nonlocal Poincaré-type inequality

$$\|u\|^2_{L^2(\Omega)} \le C |||u|||^2 \qquad \forall\, u \in V_c(\Omega)$$

- Together, these three results imply the equivalence of the spaces $H^s(\Omega)$ and $V(\Omega)$

$$C_*\|u\|_{H^s} \le |||u||| \le C^*\|u\|_{H^s} \quad \forall\, u \in V(\Omega)$$

where C_* is a positive constants satisfying $C_*^{-2} = \max\left(\gamma_*^{-1}, C(1+4|\Omega|\varepsilon^{-(d+2s)})\right)$ and $C^* = \gamma^*$

- We then immediately obtain the equivalence of the constrained spaces $H_c^s(\Omega)$ and $V_c(\Omega)$

$$C_*\|u\|_{H_c^s} \le |||u||| \le C^*\|u\|_{H_c^s} \quad \forall u \in V_c(\Omega)$$

- These results imply that in Case 1, $V(\Omega)$ and its constrained subspace $V_c(\Omega)$ are compactly embedded in $L^2(\Omega)$ and $L_c^2(\Omega)$, respectively

- We note that the equivalence of spaces holds with no restrictions on the exponent $s \in (0, 1)$ because of our consideration of volume constraints rather than constraints on the boundary of the domain or other lower dimensional manifolds
  - this is an important point, particularly for the case corresponding to $s \leq 1/2$
  - indeed, for $s \leq 1/2$, there is no well-defined trace spaces in the standard manner for functions in the Sobolev space $H^s(\Omega)$ which is why conventional local boundary-value problems have not been discussed for such cases in the literature
  - volume-constrained problems for nonlocal operators can however be well-defined for any $s \in (0, 1)$ as is shown later
  - of particular interest is the fact that for $s \leq 1/2$, nonlocal volume-constrained problems admit solutions containing jump discontinuities

Case 2

- We now demonstrate that the constrained space $V_c(\Omega) = L^2_c(\Omega)$

- We have
$$|||u||| \leq C_2 \|u\|_{L^2(\Omega)} \quad \forall\, u \in V_c(\Omega)$$
for some positive constant C_2. and the second Poincaré-like inequality
$$C_1 \|u\|_{L^2(\Omega)} \leq |||u||| \quad \forall\, u \in V_c(\Omega)$$

- We immediately have that
$$\boxed{V_c(\Omega) = L^2_c(\Omega)}$$

- Of course, $L^2(\Omega)$ function do not posses well-defined traces

WEll POSEDNESS OF VOLUME-CONSTRAINED PROBLEMS

- One easily obtains that
  - the nonlocal variational problem of minimizing $E(u) = E_f(u) + E_b(u)$ over $V_c(\Omega)$ has a unique solution u for any $b \in V_c^*(\Omega)$
  - moreover, the Euler-Lagrange equation is given by nonlocal "mixed Dirichlet-Neumann" problem for $E_c = E_c^d$ and the nonlocal "Neumann" problem for $E_c = E_c^n$
  - furthermore, there exists a constant $C > 0$, independent of b, such that

$$|||u||| \le C\|b\|_{V_c^*(\Omega)}$$

- Note that

Case 1: $\|u\|_{H^s(\Omega)} \le C\|b\|_{H^{-s}(\Omega)}, \quad 0 < s < 1$

Case 2: $\|u\|_{L^2(\Omega)} \le C\|b\|_{L^2(\Omega)}$

  - on the other hand, for second-order elliptic PDEs we have

$$\|u\|_{H^1(\Omega)} \le C\|b\|_{H^{-1}(\Omega)}$$

- We see that that the nonlocal volume-constrained problems result in a lessened gain in regularity
  - for second-order elliptic PDEs, there is gain of regularity of 2
  - for the nonlocal volume-constrained problem in Case 1, there is gain of regularity of $2s$, $0 < s < 1$
  - for the nonlocal volume-constrained problem in Case 2, there is no gain of regularity

FINITE ELEMENT APPROXIMATIONS

- A discretization method can be defined by
  - choosing a finite-dimensional space of functions V^h
  - then setting $V_c^h = \{v \in V^h \ : \ E_c(v) = 0\}$
  - then the requiring $u^h(\mathbf{x}) \in V_c^h$ to satisfy, for all $v^h(\mathbf{x}) \in V_c^h$,

$$\boxed{\int_\Omega \int_\Omega \mathcal{D}^*(u^h)(\mathbf{x},\mathbf{y}) \cdot \mathbf{\Theta}(\mathbf{x},\mathbf{y})\, \mathcal{D}^*(v^h)(\mathbf{x},\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} = \int_\Omega b(\mathbf{x}) v^h(\mathbf{x})\, d\mathbf{x}}$$

    and also satisfy

$$\boxed{E_c(u^h) = 0}$$

- Note that this is equivalent to minimizing the energy $E(u)$ over V_c^h

- Such a discretization method is said to be conforming if

$$\boxed{V_c^h \subset V_c}$$

  that is, the approximating space is a subspace of the function space for which the variational problem is well posed

– for example, for second-order elliptic PDEs, we usually have that $V^h \subset H^1\Omega)$

- Finite element methods are defined by choosing V^h to consist of piecewise polynomial functions with respect to a "triangulation" of the domain Ω

  – the standard approach for second-order elliptic PDEs is to also require that the functions in V^h be continuous on Ω

    - in this case, V^h is conforming

  – for discontinuous Galerkin (DG) methods, one chooses V^h to consist of functions that are discontinuous across element faces

    - for second-order elliptic PDEs, DG methods are nonconforming

- For the nonlocal volume-constrained problems, DG methods are conforming when $s \leq 1/2$

Error estimates

- We assume that both Ω and $\widetilde{\Omega}$ are polyhedral domains

- For a given triangulation of Ω that simultaneously triangulates $\widetilde{\Omega}$, we let V_c^h consist of those functions in $V_c(\Omega)$ that are piecewise polynomials of degree no more than m defined with respect to the triangulation

- We assume that the triangulation is shape-regular as the diameter of the largest element $h \to 0$

- We let u denote the exact solution and u^h its finite element approximation

- We then have for both Case 1 and Case 2 that, for any $b \in V_c^*(\Omega)$,

$$|||u - u^h||| \leq \min_{h_n \in V_c^n} |||u - v^h||| \to 0 \quad \text{as} \quad h \to 0$$

- If the exact solution u is sufficiently smooth, we have that, if m be a non-negative integer,

  Case 1: if $u \in V_c(\Omega) \cap H^{m+t}(\Omega)$, where $0 \leq r \leq s$ and $s \leq t \leq 1$, there exists a constant C such that for sufficiently small h,

$$\|u - u^h\|_{H^r(\Omega)} \leq Ch^{m+t-r}\|u\|_{H^{m+t}(\Omega)}$$

  Case 2: if $u \in V_c(\Omega) \cap H^{m+t}(\Omega)$ where $0 \leq t \leq 1$. Then there exists a constant C such that for sufficiently small h,

$$\|u - u^h\|_{L^2(\Omega)} \leq ch^{m+t}\|u\|_{H^{m+t}(\Omega)}$$

- In particular, if $m = 1$, then second-order convergence with respect to the $L^2(\Omega)$ norm can be expected for linear elements by setting $r = 0$, $t = 1$ for Case 1 and $t = 1$ for Case 2

Condition numbers

- If $\mathbf{K}$ denotes the stiffness matrix associated with the finite element approximation, we have that there exists a constant c such that

$$\text{Case 1:} \qquad \mathrm{cond}(\mathbf{K}) \leq ch^{-2s}, \qquad 0 < s < 1$$

$$\text{Case 2:} \qquad \mathrm{cond}(\mathbf{K}) \leq c$$

  - this should be contrasted with the second-order elliptic PDE case for which

$$\mathrm{cond}(\mathbf{K}) \leq ch^{-2}$$

COMPUTATIONAL RESULTS

- We have implemented finite element methods for nonlocal volume-constrained problems in 1D, using
  - continuous piecewise linear finite element spaces
  - (discontinuous) piecewise constant finite element spaces
  - discontinuous piecewise linear finite element spaces
    - this turns out to be the most robust choice

- We have tested the implementation on problems with
  - smooth exact solutions
  - exact solutions containing a jump discontinuity
    - this is an interesting case because such solutions are not admissible for second-order elliptic problems

- For the smooth solution case, the two piecewise linear finite element spaces do fine but the piecewise constant space has some trouble

- For the solution with a jump discontinuity, the discontinuous piecewise linear finite element space is best
  - the piecewise constant space has (mild) trouble in regions where the solution is smooth
  - the continuous piecewise linear space has big trouble near the jump discontinuity in the exact solution

- Discontinuous linear approximations also have trouble for solutions containing jump discontinuities
  - for example, if one uses a uniform grid of size h, the best accuracy one can achieve with respect to L^2 norm of the error, is $O(h^{1/2})$

- However, unlike the other choices, discontinuous linear approximations can be saved by abrupt mesh refinement near points where the exact solution is discontinuous
  - such neighborhoods can be detected from the approximate solution
  - then the mesh in such neighborhoods can be abruptly refined
  - then, one obtains the full $O(h^2)$ accuracy, where h refers to grid size of the unrefined part of the mesh

- Nonlocality has its price

  e.g., many more nonzero entries in matrices encountered,

  so that naive implementations of nonlocal models may be costly

  – however, in regions where solutions behave well, most nonlocal models can be implemented in a way that costs no more than local PDE models

    e.g., by reducing the extents of interactions

  – then, using adaptive strategies

    with respect to grids, model parameters, and model forms,

    one can reduce the cost almost to that of local models