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AN INVITATION TO NONLOCAL MODELING, ANALYSIS AND COMPUTATION

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Abstract

This lecture serves as an invitation to further studies on nonlocal models, their mathematics, computation, and applications. We sample our recent attempts in the development of a systematic mathematical framework for nonlocal models, including basic elements of nonlocal vector calculus, well-posedness of nonlocal variational problems, coupling to local models, convergence and compatibility of numerical approximations, and applications to nonlocal mechanics and diffusion. We also draw connections with traditional models and other relevant mathematical subjects.

1 Introduction

Nonlocal phenomena are ubiquitous in nature but their effective modeling and simulations can be difficult. In early mathematical and scientific inquiries, making local approximations has been a dominant strategy. Over centuries, popular continuum models are presented as partial differential equations (PDEs) that are expressed by local information in an infinitesimal neighborhood and are derived, in their origins, for smooth quantities. Entering into the digital age, there have been growing interests and capabilities in the modeling of complex processes that exhibit singularities/anomalies and involve nonlocal interactions. Nonlocal continuum models, fueled by the advent in computing technology, have the potential to be alternatives to local PDE models in many applications, although there are many new challenges for mathematicians and computational scientists to tackle.

While mathematical analysis and numerical solution of local PDEs are well established branches of mathematics, the development of rigorous theoretical and computational framework for nonlocal models, relatively speaking, is still a nascent field. This

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lecture serves as an invitation to further studies on this emerging subject. We refer to Du [n.d.], an NSF-CBMS monograph, for a review on the historical development, recent progress and connections with other mathematical subjects such as multiscale analysis, calculus of variations, functional analysis, fractional PDEs, differential geometry, graph, data and image analysis, deep learning, as well as various applications. Instead of a brief survey, we present here samples of our recent attempts to develop a systematic mathematical framework for nonlocal models, including some basic building blocks, algorithms and applications. In particular, our discussions are centered around nonlocal models with a finite range of interactions typically characterized by a horizon parameter δ. Their local ($\delta \to 0$) and global ($\delta \to \infty$) limits offer natural links to local and fractional PDEs and their discretization are also tied with graph operators, point clouds and discrete networks. A few questions on nonlocal modeling, analysis and computation are addressed here: how do nonlocal models compare with local and discrete models and how are they connected with each other? what are the ingredients of nonlocal vector calculus? how to develop robust discretization of nonlocal models that are asymptotically compatible with their local limit? how to get well defined trace maps in larger nonlocal function spaces to couple nonlocal and local models? and, how to explain the crossover of diffusion regimes using nonlocal in time dynamics? It is our intention to demonstrate that studies on nonlocal modeling not only provoke the discovery of new mathematics to guide practical modeling efforts, but also provide new perspectives to understand traditional models and new insight into their connections.

2 Modeling choices and emergence of nonlocal modeling

Mathematical models have various types, e.g., discrete or continuum, and deterministic or stochastic. Historically, influenced by the great minds like Newton, Leibniz, Maxwell and others, most popular continuum models are those given by PDEs whose simple close-form or approximate solutions have often been utilized. As more recent human endeavors, nevertheless, computer simulations have made discrete models equally prominent.

We consider some simple continuum and discrete equations as illustrations. Let $u = u(x)$ be a function to be determined on a domain (an interval) $\Omega \subset \mathbb{R}$. The differential equation

$$-\mathfrak{L}_0 u(x) = -\frac{d^2u}{dx^2}(x) = f(x, u(x)), \quad \forall\, x \in \Omega$$

with a prescribed function $f = f(x, u)$, represents a local continuum model: it only involves the value and a few derivatives of the solution at any single point x. By introducing a set of grid points $\{x_j\}$ in Ω, equally spaced with a grid spacing h and the standard 2nd order center difference operator $\mathfrak{L}_h = D_h^2$ on the grid. We then have a discrete difference model

$$-\mathfrak{L}_h u(x_j) = -D_h^2 u(x_j) = -\frac{u(x_j+h) - 2u(x_j) + u(x_j-h)}{h^2} = f(x_j, u(x_j))\ \forall x_j$$

that, as $h \to 0$, approximates the local continuum model. In comparison, we consider

$$-\mathfrak{L}_\delta u(x) = f(x, u(x)), \quad x \in \Omega, \tag{1}$$

which is a nonlocal model Du [2015, 2017b] and Du and X. Tian [2015] with a nonlocal operator $\mathfrak{L}_\delta$ defined, for a prescribed nonlocal interaction kernel $\underline{\omega}_\delta$ associated with a given horizon parameter $\delta > 0$, by

$$\mathfrak{L}_\delta u\,(x) = \int_0^\delta \frac{u(x+s) - 2u(x) + u(x-s)}{s^2} \underline{\omega}_\delta(s) ds. \tag{2}$$

The model (1) is generically nonlocal, particularly if the support of $\underline{\omega}_\delta$ extends beyond the origin. It, at any x, involves function values of u at not only x but possibly its δ-neighborhood. With $\underline{\omega}_\delta = \underline{\omega}_\delta(s)$ a probability density function, $\mathfrak{L}_\delta$ can be interpreted as a continuum average (integral) of the difference operator D_s^2 over a continuum of scales $s \in [0, \delta]$. This interpretation has various implications as discussed below.

First, differential and discrete equations are special cases of nonlocal equations: let $\underline{\omega}_\delta(s)$ be the Dirac-delta measure at either $s = 0$ or h, we get $\mathfrak{L}_0 = \frac{d^2}{dx^2}$ or $\mathfrak{L}_h = D_h^2$ respectively, showing the generality of nonlocal continuum models. A better illustration is via a limiting process, e.g., for smooth u, small δ, and $\underline{\omega}_\delta$ going to the Dirac-delta at $s = 0$, we have

$$\mathfrak{L}_\delta u\,(x) = \frac{d^2 u}{dx^2}(x) \int_0^\delta \underline{\omega}_\delta(s) ds + c_2 \delta^2 \frac{d^4 u}{dx^4}(x) + \cdots \approx \frac{d^2 u}{dx^2} = \mathfrak{L}_0 u(x)$$

showing that nonlocal models may resemble their local continuum limit for smooth quantities of interests (QoI), while encoding richer information for QoIs with singularity.

In addition, with a special class of fractional power-law kernel $\underline{\omega}_\delta(s) = c_{\alpha,1}|s|^{1-2\alpha}$ for $0 < \alpha < 1$ and $\delta = \infty$, $\mathfrak{L}_\delta$ leads to a fractional differential operator Bucur and Valdinoci [2016], Caffarelli and Silvestre [2007], Nochetto, Otárola, and Salgado [2016], Vázquez [2017], and West [2016]:

$$\mathfrak{L}_\infty u\,(x) = c_{\alpha,1} \int_0^\infty D_s^2 u(x) |s|^{1-2\alpha} ds = \left(-\frac{d^2}{dx^2}\right)^\alpha u(x).$$

One may draw further connections from the Fourier symbols of these operators Du [n.d.] and Du and K. Zhou [2011].

Nonlocal models and operators have many variations and extensions. For example, one may define a nonlocal jump (diffusion) operator for a particle density $u = u(x)$,

$$\mathfrak{L}_\delta u\,(x) = \int (\beta(x,y)u(y) - \beta'(y,x)u(x))\,dy\,,$$

with $\beta = \beta(x,y)$ and $\beta' = \beta'(y,x)$ the jumping rates. We can recover (2) if $\beta(x,y) = \beta'(y,x) = |x-y|^{-2}\underline{\omega_\delta}(|x-y|)$, and make connections with stochastic processes Du, Huang, and Lehoucq [2014].

Other extensions include systems for vector and tensor fields such as nonlocal models of mechanics. A representative example is the peridynamic theory Silling [2000] which attempts to offer a unified treatment of balance laws on and off materials discontinuities, see Bobaru, Foster, Geubelle, and Silling [2017] for reviews on various aspects of peridynamics. We briefly describe a simple linear small strain state-based peridynamic model here. Let Ω be either $\mathbb{R}^d$ or a bounded domain in $\mathbb{R}^d$ with Lipshitz boundary, and $\Omega^* = \Omega \cup \Omega_I$ where Ω_I is an interaction domain. Let $\mathbf{u} = \mathbf{u}(\mathbf{x},t) = \mathbf{y}(\mathbf{x},t) - \mathbf{x}$ denote the displacement field at the point $\mathbf{x} \in \Omega^*$ and time t so that $\mathbf{y} = \mathbf{x} + \mathbf{u}$ gives the deformed position, the peridynamic equation of motion can be expressed by

$$\rho \mathbf{u}_{tt}(\mathbf{x},t) = \mathfrak{L}_\delta \mathbf{u}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t), \quad \forall \mathbf{x} \in \Omega,\ t > 0,$$

where ρ is the constant density, $\mathbf{b} = \mathbf{b}(\mathbf{x},t)$ the body force, and $\mathfrak{L}_\delta \mathbf{u}$ the interaction force derived from the variation of the nonlocal strain energy. Under a small strain assumption, for any $\mathbf{x}, \mathbf{x}' = \mathbf{x} + \boldsymbol{\xi}$, the linearized total strain and dilatational strain are given by

$$s(\mathbf{u})(\mathbf{x}',\mathbf{x}) := \mathbf{e}(\boldsymbol{\xi}) \cdot \frac{\boldsymbol{\eta}}{|\boldsymbol{\xi}|} \quad \text{and} \quad \mathfrak{d}_\delta(\mathbf{u})(\mathbf{x}) := \int \omega_\delta(\mathbf{x}',\mathbf{x}) s(\mathbf{u})(\mathbf{x}',\mathbf{x})\, d\mathbf{x}'\,. \tag{3}$$

where $\mathbf{e}(\boldsymbol{\xi}) = \boldsymbol{\xi}/|\boldsymbol{\xi}|$, $\boldsymbol{\eta} = \mathbf{u}(\mathbf{x}+\boldsymbol{\xi}) - \mathbf{u}(\mathbf{x})$ and the kernel ω_δ has its support over a spherical neighborhood $|\mathbf{x}' - \mathbf{x}| < \delta$ (with δ being the horizon parameter) and is normalized by

$$\int \omega_\delta(\mathbf{x}',\mathbf{x})\, d\mathbf{x}' = 1.$$

The linearized deviatoric strain is denoted by $\mathfrak{S}_\delta(\mathbf{u})(\mathbf{x}',\mathbf{x}) := s(\mathbf{u})(\mathbf{x}',\mathbf{x}) - \mathfrak{d}_\delta(\mathbf{u})(\mathbf{x})$. Then, the small strain quadratic last energy density functional is given by

$$\mathfrak{W}_\delta(\mathbf{x}, \{\boldsymbol{\xi}, \boldsymbol{\eta}\}) = \kappa |\mathfrak{d}_\delta(\mathbf{u})(\mathbf{x})|^2 + \mu \int_{\Omega^*} \omega_\delta(\mathbf{x}+\boldsymbol{\xi}, \mathbf{x})\, |s(\mathbf{u})(\mathbf{x}+\boldsymbol{\xi}, \mathbf{x}) - \mathfrak{d}_\delta(\mathbf{u})(\mathbf{x})|^2\, d\boldsymbol{\xi} \tag{4}$$

where κ represents the peridynamic *bulk modulus* and μ the peridynamic *shear modulus*.

For $\kappa = \mu$, we get a nondimensionalized bond-based peridynamic energy density Mengesha and Du [2014] and Silling [2000]

$$\mathfrak{W}_\delta(\mathbf{x}, \{\boldsymbol{\xi}, \boldsymbol{\eta}\}) = \int \omega_\delta(\mathbf{x}+\boldsymbol{\xi}, \mathbf{x}) \left| \frac{\boldsymbol{\xi}}{|\boldsymbol{\xi}|} \cdot \frac{\mathbf{u}(\mathbf{x}+\boldsymbol{\xi}) - \mathbf{u}(\mathbf{x})}{|\boldsymbol{\xi}|} \right|^2 d\boldsymbol{\xi}\,, \tag{5}$$

For a scalar function $u = u(x)$, we get a simple one dimensional energy density

$$\mathcal{W}_\delta(x,\{u\}) = \int \underline{\omega}_\delta(|y-x|)\frac{|u(y)-u(x)|^2}{|y-x|^2}dy\,,$$

associated with the nonlocal operator in (1), if a translation invariant and even kernel $\underline{\omega}_\delta$ is adopted. This special case has often served as a benchmark problem for peridynamics, even though in most practical applications, peridynamic models do take on nonlinear vector forms to account for complex interactions Du, Tao, and X. Tian [2017].

3 Nonlocal vector calculus and nonlocal variational problems

We introduce the theory through an example, accompanied by some general discussions.

A model equation. The systematic development of the nonlocal vector calculus was originated from the study of peridynamics Du, Gunzburger, Lehoucq, and K. Zhou [2013]. Let us consider a time-independent linear bond-based peridynamic model associated with the strain energy (5) given by

(6)
$$-\mathcal{L}_\delta \mathbf{u}(\mathbf{x}) = -2\int_{\Omega^*}\omega_\delta(\mathbf{x}+\boldsymbol{\xi},\mathbf{x})\left[\frac{\mathbf{u}(\mathbf{x}+\boldsymbol{\xi})-\mathbf{u}(\mathbf{x})}{|\boldsymbol{\xi}|^2}\cdot\mathbf{e}(\boldsymbol{\xi})\right]\mathbf{e}(\boldsymbol{\xi})d\boldsymbol{\xi} = \mathbf{b}(\mathbf{x})\,,\quad \forall\ \mathbf{x}\in\Omega,$$

where $\mathbf{u}$ is a displacement field and $\mathbf{b}$ is a body force. Intuitively, (6) describes the force balance in a continuum body of linear springs, with the spring force aligned with the undeformed bond direction between any pair of points $\mathbf{x}$ and $\mathbf{x}' = \mathbf{x}+\boldsymbol{\xi}$. This gives a nonlocal analog of classical linear elasticity model with a particular Poisson ratio, yet it does not, at the first sight, share the same elegant form of linear elasticity. Nonlocal vector calculus can make the connections between local and nonlocal models more transparent.

Examples of nonlocal operators. Let us introduce some nonlocal operators as illustrative examples. First, we define a nonlocal two-point gradient operator $\mathcal{G}$ for any $\mathbf{v}\colon \mathbb{R}^d \to \mathbb{R}^m$ such that $\mathcal{G}\mathbf{v}\colon \Omega^*\times\Omega^*\to\mathbb{R}^{d\times n}$ is a two-point second-order tensor field given by,

$$(7)\quad (\mathcal{G}\mathbf{v})(\mathbf{x}',\mathbf{x}) = \mathbf{e}(\mathbf{x}'-\mathbf{x})\otimes\frac{\mathbf{v}(\mathbf{x}')-\mathbf{v}(\mathbf{x})}{|\mathbf{x}'-\mathbf{x}|}\quad\text{where}\quad \mathbf{e}(\mathbf{x}'-\mathbf{x}) = \frac{\mathbf{x}'-\mathbf{x}}{|\mathbf{x}'-\mathbf{x}|},\quad \forall\ \mathbf{x}',\mathbf{x}\in\Omega^*.$$

There are two cases of particular interests, namely, $n = 1$ and $n = d$. In the latter case, we also define a nonlocal two-point divergence operator $\mathcal{D}$ by

$$(8)\qquad (\mathcal{D}\mathbf{v})(\mathbf{x}',\mathbf{x}) = \mathbf{e}(\mathbf{x}'-\mathbf{x})\cdot\frac{\mathbf{v}(\mathbf{x}')-\mathbf{v}(\mathbf{x})}{|\mathbf{x}'-\mathbf{x}|} = \mathrm{Tr}(\mathcal{G}\mathbf{v})(\mathbf{x},\mathbf{x}')\,,\qquad \text{for}\ \ n=d.$$

For peridynamics, $(\mathcal{D}\mathbf{v})(\mathbf{x}',\mathbf{x})$ corresponds to the linearized strain described in (3).

Next, we define a nonlocal two-point dual divergence operator $\mathcal{D}^*$ acting on any two-point scalar field $\boldsymbol{\Psi}\colon \Omega^* \times \Omega^* \to \mathbb{R}$ such that $\mathcal{D}^*\boldsymbol{\Psi}$ becomes a vector field given by,

$$(\mathcal{D}^*\boldsymbol{\Psi})(\mathbf{x}) = \int_{\Omega^*} \big(\boldsymbol{\Psi}(\mathbf{x},\mathbf{x}') + \boldsymbol{\Psi}(\mathbf{x}',\mathbf{x})\big)\frac{\mathbf{e}(\mathbf{x}'-\mathbf{x})}{|\mathbf{x}'-\mathbf{x}|}d\mathbf{x}', \quad \forall\, \mathbf{x}\in\Omega^*. \tag{9}$$

We may interpret $\mathcal{D}^*$ and $\mathcal{D}$ as adjoint operators to each other in the sense that

$$\int_{\Omega^*} \mathbf{v}(\mathbf{x})\cdot(\mathcal{D}^*\boldsymbol{\Psi})(\mathbf{x})d\mathbf{x} = -\int_{\Omega^*}\int_{\Omega^*}(\mathcal{D}\mathbf{v})(\mathbf{x}',\mathbf{x})\boldsymbol{\Psi}(\mathbf{x}',\mathbf{x})d\mathbf{x}'d\mathbf{x} \tag{10}$$

for all $\mathbf{v}$ and $\boldsymbol{\Psi}$ that make integrals in (10) well defined. The duality may also be written more canonically as $(\mathbf{v}, \mathcal{D}^*\boldsymbol{\Psi})_{\Omega^*} = -(\mathcal{D}\mathbf{v}, \boldsymbol{\Psi})_{\Omega^*\times\Omega^*}$ where $(\cdot,\cdot)_{\Omega^*}$ and $(\cdot,\cdot)_{\Omega^*\times\Omega^*}$ denote L^2 inner products for vector and scalar fields in their respective domains of definition. Similarly, we can define a nonlocal two-point dual gradient operator $\mathcal{G}^*$ acting on any two-point vector field $\boldsymbol{\Psi}\colon \Omega^*\times\Omega^* \to \mathbb{R}^d$ by the duality that $(v, \mathcal{G}^*\boldsymbol{\Psi})_{\Omega^*} = -(\mathcal{G}v, \boldsymbol{\Psi})_{\Omega^*\times\Omega^*}$ for $\mathcal{G}$ given by (7).

Some basic elements of nonlocal vector calculus are listed in Table 2 in comparison with the local counterpart. Discussions on concepts like the nonlocal flux and further justifications on labeling $\mathcal{G}$ and $\mathcal{D}$ as two-point gradient and divergence can be found in Du [n.d.] and Du, Gunzburger, Lehoucq, and K. Zhou [2013].

Newton's vector calculus	$\Leftrightarrow$	Nonlocal vector calculus
Differential operators, local flux	$\Leftrightarrow$	Nonlocal operators, nonlocal flux
Green's identity, integration by parts		Nonlocal Green's identity (duality)
$\int_\Omega \mathbf{u}\cdot\Delta\mathbf{v} - \mathbf{v}\cdot\Delta\mathbf{u} = \int_{\partial\Omega}\mathbf{u}\cdot\partial_n\mathbf{v} - \mathbf{v}\cdot\partial_n\mathbf{u}$	$\Leftrightarrow$	$\iint_{\Omega^*\times\Omega^*}\mathbf{u}\cdot\mathcal{D}^*(\mathcal{D}\mathbf{v}) - \mathbf{v}\cdot\mathcal{D}^*(\mathcal{D}\mathbf{u}) = 0$

Table 1: Elements of vector calculus: local versus nonlocal.

Reformulation of nonlocal models. Let the kernel in (6) $\omega_\delta = \omega_\delta(\mathbf{x}',\mathbf{x}) = \omega_\delta(\mathbf{x},\mathbf{x}')$ be symmetric. We consider $\mathcal{D}^*\boldsymbol{\Psi}$ with $\boldsymbol{\Psi}(\mathbf{x}',\mathbf{x}) = \omega_\delta(\mathbf{x}',\mathbf{x})(\mathcal{D}\mathbf{u})(\mathbf{x}',\mathbf{x})$. This leads to

$$-\mathcal{L}_\delta\mathbf{u} = -\mathcal{D}^*(\omega_\delta\mathcal{D}\mathbf{u}) = \mathbf{b}$$

a concise reformation of (6) that starts to resemble, in appearance, the PDE form of classical elasticity, with local differential (gradient and divergent) operators replaced by their nonlocal counterparts. Analogously, a scalar nonlocal diffusion equation for a translation invariant ω_δ, i.e., $\omega_\delta(\mathbf{x}',\mathbf{x}) = \underline{\omega}_\delta(\mathbf{x}'-\mathbf{x}) = \underline{\omega}_\delta(\mathbf{x}-\mathbf{x}')$, and its reformulation can be given by

(11)
$$-\mathcal{L}_\delta v(\mathbf{x}) = -\int_{\Omega^*} \underline{\omega}_\delta(\boldsymbol{\xi}) \frac{v(\mathbf{x}+\boldsymbol{\xi}) - 2v(\mathbf{x}) + v(\mathbf{x}-\boldsymbol{\xi})}{|\boldsymbol{\xi}|^2} d\boldsymbol{\xi} = f(\mathbf{x}) \quad \Leftrightarrow \quad -\mathcal{G}^*(\underline{\omega}_\delta \mathcal{G} v) = f.$$

similar to the one-dimensional version (2). Moreover, not only nonlocal models can be nicely reformulated like classical PDEs, their mathematical theory may also be developed in a similar fashion along with interesting new twists Du, Gunzburger, Lehoucq, and K. Zhou [2013, 2012] and Mengesha and Du [2014, 2015].

Variational problems. Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with Lipshitz boundary and Ω_I be where constraints on the solution are imposed. We consider an energy functional

$$(12)\quad E_\delta(\mathbf{u}) := \frac{1}{2}|\mathbf{u}|^2_{\mathcal{S}_2^\delta} - (\mathbf{b},\mathbf{u})_{\Omega^*} \text{ with } |\mathbf{u}|^2_{\mathcal{S}_2^\delta} := \iint_{\Omega^*\times\Omega^*} \underline{\omega}_\delta(\mathbf{x}'-\mathbf{x})\,(\mathcal{D}\mathbf{u}(\mathbf{x}',\mathbf{x}))^2 d\mathbf{x}' d\mathbf{x}$$

for a prescribed body force $\mathbf{b} = \mathbf{b}(\mathbf{x}) \in L^2(\Omega^*_\delta)^d$ and a kernel $\underline{\omega}_\delta = \underline{\omega}_\delta(\boldsymbol{\xi})$ satisfying

$$(13)\qquad \begin{cases} \underline{\omega}_\delta(\boldsymbol{\xi}) \geq 0 \text{ is radially symmetric, } B_{\sigma\delta}(\mathbf{0}) \subset \operatorname{supp}(\underline{\omega}_\delta) \subset B_\delta(\mathbf{0}) \subset \mathbb{R}^d \\ \text{for } 0 < \sigma < 1, \text{ and } \displaystyle\int_{B_\delta(0)} \underline{\omega}_\delta(\boldsymbol{\xi})\, d\boldsymbol{\xi} = 1\,. \end{cases}$$

Let $\mathcal{S}_2^\delta$ be the set of $\mathbf{u} \in L^2(\Omega^*)^d$ with $\|\mathbf{u}\|^2_{\mathcal{S}_2^\delta} = \|\mathbf{u}\|^2_{L^2(\Omega^*)^d} + |\mathbf{u}|^2_{\mathcal{S}_2^\delta}$ finite, which is a separable Hilbert space with an inner product induced by the norm $\|\cdot\|_{\mathcal{S}_2^\delta}$ Mengesha and Du [2014]. For a weakly closed subspace $V \subset L^2(\Omega^*)^d$ that has no nontrivial affine maps with skew-symmetric gradients, we let $V_{c,\delta} = \mathcal{S}_2^\delta \cap V$. One can establish a compactness result on $V_{c,\delta}$ Mengesha and Du [2014] and Mengesha [2012]:

Lemma 3.1. *For a bounded sequence* $\{\mathbf{u}_n\} \in V_{c,\delta}$, $\lim_{n\to\infty} |\mathbf{u}_n|_{\mathcal{S}_2^\delta} = 0$ *gives* $\|\mathbf{u}_n\|_{L^2(\Omega^*)} \to 0$.

This leads to a nonlocal Poincaré inequality and the coercivity of the energy functional.

Proposition 3.2 (Nonlocal Poincaré). *There exists a positive constant C such that*

$$\|\mathbf{u}\|_{L^2(\Omega^*)^d} \leq C|\mathbf{u}|_{\mathcal{S}_2^\delta}, \quad \forall\ \mathbf{u} \in V_{c,\delta}.$$

The well-posedness of the variational problem then follows Mengesha and Du [2014]. Moreover, one can get a uniform Poincaré constant, independent of δ as $\delta \to 0$, if the nonlocal interaction kernels behave like a Diract-delta sequence. More specifically, they satisfy that

$$(14)\qquad \lim_{\delta\to 0} \int_{|\boldsymbol{\xi}|>\epsilon} \underline{\omega}_\delta(\boldsymbol{\xi}) d\boldsymbol{\xi} = 0, \quad \forall\, \epsilon > 0.$$

The assumption is particularly true for a rescaled kernel $\underline{\omega}_\delta(\boldsymbol{\xi}) = \delta^{-d}\underline{\omega}(\boldsymbol{\xi}/\delta)$ Du [n.d.] and Mengesha and Du [2014].

Note that the above line of analysis can be carried out by extending similar results for the scalar function spaces originated from the celebrated work Bourgain, Brezis, and Mironescu [2001] and further studied in Ponce [2004]. One complication for vector fields is that the energy seminorm only uses a projected difference $\mathcal{D}\mathbf{u}$ instead of the total difference, see Mengesha [2012] and Mengesha and Du [2014, 2015, 2016] for detailed discussions.

The nonlocal Poincaré inequality and energy coercivity then imply a well-posed variational formulation of the nonlocal model through minimizing $E_\delta(\mathbf{u})$ over $\mathbf{u} \in V_{c,\delta}$. The weak form of the Euler–Lagrange equation is given by

$$B_\delta(\mathbf{u},\mathbf{v}) := (\underline{\omega}_\delta \mathcal{D}\mathbf{u}, \mathcal{D}\mathbf{v})_{\Omega^*\times\Omega^*} = (\mathbf{u},\mathbf{b})_{\Omega^*}, \quad \forall\, \mathbf{v} \in V_{c,\delta}.$$

We note a special case with $V_{c,\delta} = \mathcal{S}_{0,\delta}$, the closure of $C_0^\infty(\Omega)^d$ in $\mathcal{S}_2^\delta$ with all of its elements satisfying $\mathbf{u}(\mathbf{x}) = \mathbf{0}$ on $\Omega_I = \Omega_\delta = \{\mathbf{x} \in \mathbb{R}^d \setminus \Omega \mid \operatorname{dist}(\mathbf{x},\Omega) < \delta\}$, corresponding to a problem with a homogeneous nonlocal Dirichlet constraint on a δ-layer around Ω, see Figure 1.

$$\begin{aligned} -\mathcal{L}_\delta \mathbf{u} = -\mathcal{D}^*(\underline{\omega}_\delta \mathcal{D})\mathbf{u} = \mathbf{b}, &\quad \text{in } \Omega, \\ \mathbf{u} = \mathbf{0}, &\quad \text{in } \Omega_I = \Omega_\delta. \end{aligned} \tag{15}$$

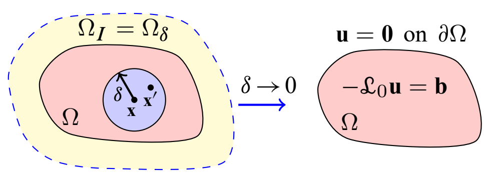

Figure 1: A nonlocal constrained value problem and its local PDE limit

Furthermore, under the assumption (14), we can show that as $\delta \to 0$, the solution of (15), denoted by $\mathbf{u}_\delta$, converges in $L^2(\Omega)$ to the solution $\mathbf{u}_0 \in H_0^1(\Omega)$ of the equation $-\mathcal{L}_0\mathbf{u} = -(d+2)^{-1}(\Delta\mathbf{u} + 2\nabla(\nabla\cdot\mathbf{u})) = \mathbf{b}$ in Ω Mengesha and Du [2014], thus compatible with linear elasticity.

Elements of mathematical foundation of nonlocal models. Without going into details, we summarize some basic elements in Table 2. For brevity, the illustration is devoted to the case of nonlocal diffusion model and its local limit, with $\underline{K}$ denoting a generic 2nd order positive definite coefficient tensor, and the same notation $(\cdot,\cdot)$ for L^2 inner products of scalar, vector and tensor fields over their respective domains.

Local variational problems	$\Leftrightarrow$	Nonlocal variational problems
Local energy: $(\nabla u, \nabla u)$	$\Leftrightarrow$	Nonlocal energy: $(\underline{\omega}_\delta \mathcal{G} u, \mathcal{G} u)$
Sobolev space $H^1(\Omega)$	$\Leftrightarrow$	Nonlocal function space $\mathcal{S}_2^\delta$
Local balance (PDE): $-\nabla \cdot (\underline{K} \nabla u) = f$	$\Leftrightarrow$	Nonlocal balance: $-\mathcal{G}^*(\underline{\omega}_\delta \mathcal{G} u) = f$
Boundary conditions on $\partial\Omega$	$\Leftrightarrow$	Volumetric constraints on Ω_I
Local weak forms: $(\underline{K} \nabla u, \nabla u) = (f, v), \ \forall\, v$	$\Leftrightarrow$	Nonlocal weak forms: $(\underline{\omega}_\delta \mathcal{G} u, \mathcal{G} v) = (f, v), \ \forall\, v$
Classical Poincaré: $\lVert u \rVert_{L^2} \le c \lVert \nabla u \rVert_{L^2}$	$\Leftrightarrow$	Nonlocal Poincaré: $\lVert u \rVert_{L^2} \le c \lvert u \rvert_{\mathcal{S}_2^\delta}$

Table 2: Elements of variational problems: local versus nonlocal.

Other variants of nonlocal operators and nonlocal calculus. As part of the nonlocal vector calculus, there are other on possible variants to the nonlocal operators introduced here, e.g., the one-point nonlocal divergence and nonlocal dual gradient given by

$$\mathfrak{D}_\rho \mathbf{v}(\mathbf{x}) = \int_\Omega \rho_\delta(\mathbf{x}' - \mathbf{x})(\mathcal{D}\mathbf{v})(\mathbf{x}', \mathbf{x}) d\mathbf{x}', \quad \mathcal{G}_\rho^* \mathbf{v}(\mathbf{x}) = \int_\Omega \rho_\delta(\mathbf{x}' - \mathbf{x}) \mathbf{e}(\mathbf{x}' - \mathbf{x}) \otimes \frac{\mathbf{v}(\mathbf{x}') + \mathbf{v}(\mathbf{x})}{|\mathbf{x}' - \mathbf{x}|} d\mathbf{x}'$$

for an averaging kernel ρ_δ. With ρ_δ approaching a Dirac-delta measure at the origin as $\delta \to 0$, $\mathfrak{D}_\rho$ and $\mathcal{G}_\rho^*$ recover the conventional local divergence and gradient opertors Du, Gunzburger, Lehoucq, and K. Zhou [2013] and Mengesha and Du [2016]. They also form a duality pair and have been used for robust nonlocal gradient recovery Du, Tao, X. Tian, and J. Yang [2016]. Their use in the so-called correspondence peridynamic materials models could be problematic but more clarifications have been given recently Du and X. Tian [n.d.]. Moreover, these one-point operators are needed to reformulate more general state-based peridynamics Du, Gunzburger, Lehoucq, and K. Zhou [2013] and Mengesha and Du [2015, 2016] where the equation of motion is often expressed by Silling [2010], Silling, Epton, Weckner, Xu, and Askari [2007], and Silling and Lehoucq [2010]

$$\rho \mathbf{u}_{tt} = \int \{\underline{\mathrm{T}}[\mathbf{x}, \mathbf{u}]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathrm{T}}[\mathbf{x}', \mathbf{u}]\langle \mathbf{x} - \mathbf{x}' \rangle\} d\mathbf{x}'$$

with $\underline{\mathrm{T}}[\mathbf{x}, \mathbf{u}]\langle \mathbf{x}' - \mathbf{x} \rangle$ and $\underline{\mathrm{T}}[\mathbf{x}', \mathbf{u}]\langle \mathbf{x} - \mathbf{x}' \rangle$ denoting the peridynamic force states. In fact, $\mathfrak{D}_\rho \mathbf{u}$ can be used to represent the linear dilational strain in (3). Thus, we once again see that the study of nonlocal models of mechanics further enriches the mathematical theory of nonlocal operators and makes nonlocal vector calculus highly relevant to applications.

4 Numerical discretization of nonlocal models

There are many ways to discretizef nonlocal models Du [2017a], such as mesh-free Bessa, Foster, Belytschko, and Liu [2014], Parks, Seleson, Plimpton, Silling, and Lehoucq [2011], and Parks, Littlewood, Mitchell, and Silling [2012], quadrature based difference or collocation Seleson, Du, and Parks [2016], H. Tian, H. Wang, and W. Wang [2013], and X. Zhang, Gunzburger, and Ju [2016a,b], finite element Tao, X. Tian, and Du [2017], H. Tian, Ju, and Du [2017], and K. Zhou and Du [2010] and spectral methods Du and J. Yang [2017]. In particular, finite difference, finite element and collocation schemes in one dimension were considered in X. Tian and Du [2013], including comparisons and analysis of the differences and similarities. Discontinuous Galerkin approximations have also been discussed, including conforming DG Chen and Gunzburger [2011] and Ren, C. Wu, and Askari [2017] nonconforming DG X. Tian and Du [2015] and local DG Du, Ju, and Lu [2018].

Since nonlocal models are developed as alternatives when conventional continuum PDEs can neither capture the underlying physics nor have meaningful mathematical solutions, we need to place greater emphasis on verification and validation of results from the more tortuous simulations. A common practice for code verification is to consider the case where the nonlocal models can lead to a physically valid and mathematically well-defined local limit on the continuum level and to check if one can numerically reproduce solutions of the local limit by solving nonlocal models with the same given data. Such popular benchmark tests may produce surprising results as discussed here.

Asymptotical compatibility. Addressing the consistency on both continuum and discrete levels and ensuring algorithmic robustness have been crucial issues for modeling and code development efforts, especially for a theory like peridynamics that is developed to capture highly complex physical phenomena. In the context of nonlocal models and their local limits, the issues on various convergent paths are illustrated in the diagram shown in Figure 2 X. Tian and Du [2014] (with smaller discretization parameter h representing finer resolution).

The paths along the diagram edges are for taking limit in one of the parameters while keeping the other fixed: ♠ shows the convergence of solutions of nonlocal continuum models to their local limit as $\delta \to 0$, which has been established for various linear and nonlinear problems; ♣ is a subject of numerical PDE; ♢ assures a convergent discretization to nonlocal problem by design; ♡ is more intriguing, as it is not clear whether the local limit of numerical schemes for nonlocal problems would remain an effective scheme for the local limit of the continuum model. An affirmative answer would lead to a nice *commutative diagram*, or *asymptotic compatibility* (AC) X. Tian and Du [ibid.], one can follow

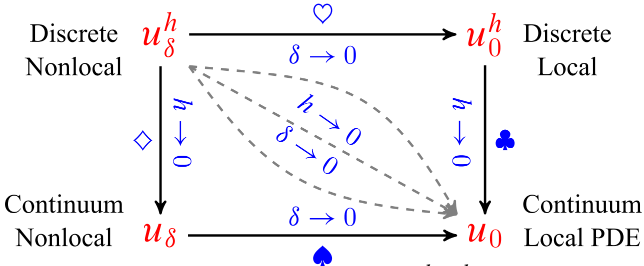

Figure 2: A diagram of possible paths between u_δ, u_δ^h, u_0^h and u_0 via various limits.

either the paths through those marked with $\diamondsuit$ and $\spadesuit$ or ones marked with $\heartsuit$ and $\clubsuit$ to get the convergence of u_δ^h to u_0.

AC schemes offer robust and convergent discrete approximations to parameterized problems and preserve the correct limiting behavior. While the variational characterization and framework are distinctive, they are reminicent in spirit to other studies of convergent approximations in the limiting regimes, see for example Arnold and Brezzi [1997], Guermond and Kanschat [2010], and Jin [1999].

Getting wrong solution from a convergent numerical scheme. To motivate the AC schemes, we consider a 1d linear nonlocal problem $-\mathfrak{L}_\delta u_\delta(x) = b(x)$ for $x \in (0,1)$, where $\mathfrak{L}_\delta$ is given by (2) with a special kernel, i.e.,

$$\mathfrak{L}_\delta u\,(x) = \frac{3}{\delta^3}\int_0^\delta \big(u(x+s) - 2u(x) + u(x-s)\big)ds = \frac{3}{\delta^3}\int_0^\delta h^2 D_h^2 u(x) dh\,, \tag{16}$$

We impose the contraint that $u_\delta(x) = u_0(x)$ for $x \in (-\delta, 0) \cup (1, 1+\delta)$ where u_0 solves the local limiting problem $-u_0''(x) = b(x)$ in $\mathbb{R}$. On the continuum level, we have $u_\delta \to u_0$ as $\delta \to 0$ in the appropriate function spaces, as desired. For (16), we may obtain a discrete system if we replace the *continuum difference* $\mathfrak{L}_\delta$ by discrete finite differences through suitable quadrature approximations (leading to the *quadrature based finite difference* discretization as named in X. Tian and Du [2013]). For example, following Du and X. Tian [2015] and X. Tian and Du [2013], we consider a scheme for (16) obtained from a Riemann sum quadrature: for $1 \le i \le N = 1/h$, $\delta = rh$,

$$-\mathfrak{L}_\delta^h u_i = -\frac{3h}{\delta^3}\sum_{m=1}^{r} (D_{mh}^2 u)_i = b(x_i)\,, \tag{17}$$

where $\{u_i\}$ are approximations of $\{u(x_i)\}$ at nodal points $\{x_i = ih\}_{i=-r}^{N+r}$. For any given $\delta > 0$, we can show the convergence of the discretization as $h \to 0$ for any given δ by combining both stability with consistency estimates X. Tian and Du [2013]. However, by considering a special case with $r = 1$ in (17), we end up with a scheme $-3(D_h^2 u)_i = b_i$, which converges to the differential equation $-3u''(x) = b(x)$ as $h = \delta \to 0$, but not to the correct local limit. In other words, if we set h and δ to zero proportionally, the numerical solution of the discrete scheme for the nonlocal problem yields a convergent approximation to a *wrong* local limit associated with, unfortunately, a consistently over-estimated elastic constant!

The possibility of numerical approximations converging to a wrong solution is alarming; if without prior knowledge, such convergence might be mistakenly used to verify or disapprove numerical simulation, and we see the risks involved due to the wrong local limits produced by discrete solutions to nonlocal models. Although illustrated via a simple example here, it has been shown to be a generic feature of discretizations represented by (17) and other schemes such as the piecewise constant Galerkin finite element approximations, for scalar nonlocal diffusion models and general state-based peridynamic systems Du and X. Tian [2015] and X. Tian and Du [2013, 2014].

Robust discretization via AC schemes. On a positive note, the complications due to the use of discrete schemes like (17) can be resolved through other means. For example, it is proposed in X. Tian and Du [2013] that an alternative formulation works much more robustly by suitably adjusting the weights for the second order differences $\{D_{mh}^2 u\}$ so that the elastic constant always maintain its correct constant value 1, independently of r! Hence, as shown in X. Tian and Du [ibid.], we have a scheme that is convergent to the nonlocal model for any fixed δ as $h \to 0$ and to the correct local limit whenever $\delta \to 0$ and $h \to 0$ simultaneously, regardless how the two parameters are coupled. Moreover, for a fixed h, it recovers the standard different scheme for the correct local limit models as $\delta \to 0$. Thus, we have a robust numerical approximation that is free from the risk of going to the wrong continuum solution. Naturally, it is interesting to characterize how such schemes can be constructed in general.

Quadrature based finite difference AC scheme. Approximations for multidimensional scalar nonlocal diffusion equations have been developed Du, Tao, X. Tian, and J. Yang [n.d.], which are not only AC but also preserve the discrete maximum principle. We consider a set of nodes (grid points) $\{\mathbf{x_j}\}$ of a uniform Cartesian mesh with a mesh size h and a multi-index $\mathbf{j}$ corresponding to $\mathbf{x_j} = h\mathbf{j}$. It is natural to approximate the nonlocal operator in (11) by

$$\mathcal{L}_\delta u(\mathbf{x_i}) \approx \int \mathcal{I}_h \left(\frac{u(\mathbf{x_i}+\mathbf{z}) - 2u(\mathbf{x_i}) + u(\mathbf{x_i}-\mathbf{z})}{|\mathbf{z}|^2 W(\mathbf{z})} \right) W(\mathbf{z}) \underline{\omega}_\delta(\mathbf{z}) d\mathbf{z}, \tag{18}$$

where $\mathcal{I}_h$ represents the piecewise d-multi-linear interpolation operator in $\mathbf{z}$ associated with the uniform Cartesian mesh $\{\mathbf{x_j} = h\mathbf{j}\}$, but the key that is crucial for the AC property and the discrete maximum principle is to choose a properly defined nonnegative weight $W = W(\mathbf{z})$. The choice adopted in Du, Tao, X. Tian, and J. Yang [ibid.] corresponds to $W(\mathbf{z}) = 1/|\mathbf{z}|_1$ where $|\mathbf{z}|_1$ denotes the ℓ_1 norm in $\mathbb{R}^d$. This particular weight makes the quadrature exact for all quadratic functions. One can then show, through a series of technical calculations, that the resulting numerical solution converges to the solution of the nonlocal model on the order of $O(h^2)$ for a fixed $\delta > 0$, and converges to that of the local limit model on the order of $O(\delta^2 + h^2)$ as both $h, \delta \to 0$ simultaneously, thus demonstrating the AC property.

AC finite element approximations. For multidimensional systems, one can extend, as in X. Tian and Du [2014], to more general abstract settings using conforming Galerkin finite element (FE) methods on unstructured meshes. In particular, the concept and theory of asymptotically compatible schemes are introduced for general parametrized variational problems. A special application is to pave a way for identifying robust approximations to linear nonlocal models that are guaranteed to be consistent in the local limit. Specifically, we have the following theorem that agrees with numerical experiments reported in the literature Bobaru, M. Yang, Alves, Silling, Askari, and Xu [2009] and X. Tian and Du [2013].

Theorem 4.1. *Let $\mathbf{u}_\delta$ be the solution of (15) and $\mathbf{u}_{\delta,h}$ be the conforming Galerkin FE approximation on a regular quasi-uniform mesh with meshing parameter h. If the FE space $V_{\delta,h}$ contains all continuous piecewise linear elements, then $\|\mathbf{u}_{\delta,h} - \mathbf{u}_0\|_{L^2(\Omega)} \to 0$ as $\delta \to 0$ and $h \to 0$. If in addition, the FE subspace is given by a conforming FE space of the local limit PDE model with zero extension outside Ω with $u_{0,h}$ being the FE solution, then on each fixed mesh, $\|u_{\delta,h} - u_{0,h}\|_{L^2} \to 0$ as $\delta \to 0$. On the other hand, if $V_{\delta,h}$ is the piecewise constant space and conforming for (15), then $\|u_{\delta,h} - u_0\|_{L^2} \to 0$ if $h = o(\delta)$ as $\delta \to 0$.*

The above theorem, proved under minimal solution regularity, remains valid for nonlocal diffusion and state-based peridynamic models. The same framework of AC schemes can establish the convergence of numerical approximation to linear fractional diffusion equations (that correspond to $\delta = \infty$) via the approximation of a nonlocal diffusion model with a finite horizon X. Tian, Du, and Gunzburger [2016]. For example, consider a scalar fractional diffusion model, for $\alpha \in (0, 1)$,

$$(-\Delta)^\alpha u = f, \text{ on } \Omega, \; u = 0, \text{ on } \mathbb{R}^d \backslash \Omega, \; (-\Delta)^\alpha u(\mathbf{x}) = C_{d,\alpha} \int_{\mathbb{R}^d} \frac{u(\mathbf{x}) - u(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|^{d+2\alpha}} d\mathbf{x}',$$

and $C_{d,\alpha}$ is a positive constant dependent on d and α. We have that X. Tian, Du, and Gunzburger [ibid.],

Theorem 4.2. *Let u_δ be the solution of the above fractional diffusion model with the integral truncated to a spherical neighborhood of radius $\delta > 0$. Let u_δ^h be a conforming Galerkin FE approximation with the discretization parameter h, then $\|u_\delta^h - u_\delta\|_{H^\alpha} \to 0$ as $h \to 0$ for any given δ and $\|u_\delta^h - u_\infty\|_{H^\alpha} \to 0$ as $\delta \to \infty$ and $h \to 0$.*

We note that studies of AC schemes have been extended to nonconforming DG FE X. Tian and Du [2015], local DG FE Du, Ju, and Lu [2018], spectral approximation Du and J. Yang [2016] and nonlocal gradient recoveries Du, Tao, X. Tian, and J. Yang [2016]. There were also extensions to nonlinear nonlocal models Du and Huang [2017] and Du and J. Yang [2016].

5 Nonlocal and local coupling

Nonlocal models can be effective alternatives to local models by accommodating singular solutions, which makes nonlocal models particularly useful to subjects like fracture mechanics. Yet treating nonlocality in simulations may incur more computation. Thus, exploring localization and effective coupling of nonlocal and local models can be helpful in practice. Nevertheless, nonlocal models, unlike local PDEs, generically do not employ local boundary or interface conditions imposed on a co-dimension-1 surface, hence motivating the development of different approaches for local-nonlocal coupling Li and Lu [2017] and Du, Tao, and X. Tian [2018].

Heterogeneous localization. A particular mathematical quest for a coupled local and nonlocal model is through heterogeneous localization, as initiated in X. Tian and Du [2017].

The aim is to characterize subspaces of $L^2(\Omega)$, denoted by $\mathcal{S}(\Omega)$, that are significantly larger than $H^1(\Omega)$ and have a continuous trace map into $H^{1/2}(\partial\Omega)$. One such example is defined as the completion of $C^1(\Omega)$ with respect to the nonlocal norm for a kernel γ_δ,

$$\|u\|_{\mathcal{S}(\Omega)} = \left(\|u\|^2_{L^2(\Omega)} + |u|^2_{\mathcal{S}(\Omega)}\right)^{\frac{1}{2}}, \text{ with}$$
$$|u|^2_{\mathcal{S}(\Omega)} = \int_\Omega \int_{\Omega\cap B_\delta(\mathbf{x})} \gamma_\delta(\mathbf{x},\mathbf{y}) \frac{(u(\mathbf{y}) - u(\mathbf{x}))^2}{|\mathbf{y}-\mathbf{x}|^2} d\mathbf{y} d\mathbf{x}.$$

The main findings of X. Tian and Du [ibid.] are that the trace map exists and is continuous on a nonlocal function space $\mathcal{S}(\Omega)$ if the radius of the support of γ_δ, i.e., the horizon, is heterogeneously localized as $\mathbf{x} \to \partial\Omega$. By considering such a class of kernels, the study departs from many existing works, such as Bourgain, Brezis, and Mironescu [2001], corresponding to typical translate-invariant kernels. In X. Tian and Du [2017], the class of kernels under consideration is given by

$$\gamma(\mathbf{x},\mathbf{y}) = \frac{1}{|\delta(\mathbf{x})|^d}\hat{\gamma}\left(\frac{|\mathbf{y}-\mathbf{x}|}{\delta(\mathbf{x})}\right) \tag{19}$$

where $\hat{\gamma} = \hat{\gamma}(s)$ is a non-increasing nonnegative function defined for $s \in (0,1)$ with a finite $d-1$ moment. The heterogeneously defined horizon $\delta = \delta(\mathbf{x})$ approaches zero when $\mathbf{x} \to \Gamma \subset \partial\Omega$. A simple choice taken in X. Tian and Du [ibid.] is $\delta(\mathbf{x}) = \sigma\,\mathrm{dist}(\mathbf{x},\Gamma)$ for $\sigma \in (0,1]$.

The following proposition has been established in X. Tian and Du [ibid.], which is of independent interests by showing the continuous imbedding of classical Sobolev space $H^1(\Omega)$ in the new heterogeneously localized nonlocal space $\mathcal{S}(\Omega)$. The result generalizes a well-known result of Bourgain, Brezis, and Mironescu [2001] for the case with a constant horizon and translation invariant kernel.

Proposition 5.1. *For the kernel in (19) and the horizon $\delta(\mathbf{x}) = \sigma\mathrm{dist}(x,\Gamma)$ with $\sigma \in (0,1)$, $H^1(\Omega)$ is continuously imbedded in $\mathcal{S}(\Omega)$ and for any $u \in H^1(\Omega)$, $\|u\|_{\mathcal{S}(\Omega)} \le C\|u\|_{H^1(\Omega)}$ where the constant $C = C(\Omega)$ is independent of σ for σ small.*

New trace theorems. A key observation proved in X. Tian and Du [2017] is that, with heterogeneously vanishing interaction neighborhood when $\mathbf{x} \to \partial\Omega$, we expect a well defined continuous trace map from the nonlocal space $\mathcal{S}(\Omega)$, which is larger than $H^1(\Omega)$, to $H^{1/2}(\partial\Omega)$.

Theorem 5.2 (General trace theorem). *Assume that Ω is a bounded simply connected Lipschitz domain in $\mathbb{R}^d$ ($d \ge 2$) and $\Gamma = \partial\Omega$, for a kernel in (19) and the heterogeneously defined horizon given by $\delta(\mathbf{x}) = \sigma$ dist$(\mathbf{x},\Gamma)$ for $\sigma \in (0,1]$. there exists a constant C depending only on Ω such that the trace map T for Γ satisfies $\|Tu\|_{H^{\frac{1}{2}}(\Gamma)} \le C\|u\|_{\mathcal{S}(\Omega)}$, for any $u \in \mathcal{S}(\Omega)$.*

By Proposition 5.1, we see that the above trace theorem is indeed a refinement of the classical trace theorem in the space $H^1(\Omega)$, with the latter being a simple consequence.

An illustrative example with a simple kernel on a stripe domain. A complete proof of the trace Theorem 5.2 is presented in X. Tian and Du [ibid.]. To help understanding what the result conveys and how it compares with other relevant works, it is suggestive to consider a special case.

For Ω and Γ, we take a special stripe domain $\Omega = (0,r)\times\mathbb{R}^{d-1}$ and a portion of its boundary $\Gamma = \{0\}\times\mathbb{R}^{d-1}$ for a constant $r > 0$, see equation (20) and Figure 3.

(20)
$$\begin{cases} \gamma(\mathbf{x},\mathbf{y}) = \dfrac{\chi_{(0,1)}(|\mathbf{y}-\mathbf{x}|)|\mathbf{y}-\mathbf{x}|^2}{|\delta(\mathbf{x})|^{d+2}}, \\ \text{where } \delta(\mathbf{x}) = \operatorname{dist}(\mathbf{x},\Gamma) = x_1, \\ \ \forall\ \mathbf{x} = (x_1, \tilde{\mathbf{x}}),\ \tilde{\mathbf{x}} \in \mathbb{R}^{d-1}. \end{cases}$$

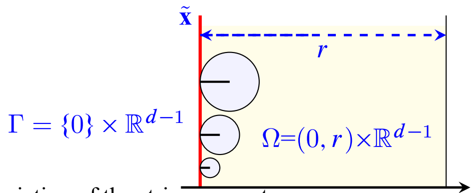

Figure 3: Nonlocal kernel and depiction of the stripe geometry.

This case serves as not only a helpful step towards proving the more general trace Theorem 5.2 but also an illustrative example on its own. Indeed, this special nonlocal (semi)-norm is

$$|u|^2_{\mathcal{S}(\Omega)} = \int_\Omega \int_{\Omega\cap\{|\mathbf{y}-\mathbf{x}|<|x_1|\}} \frac{(u(\mathbf{y})-u(\mathbf{x}))^2}{|x_1|^{2+d}} d\mathbf{y} d\mathbf{x}. \tag{21}$$

Clearly, the denominator x_1 penalizes the spatial variation only at $x_1 = 0$, thus $\mathcal{S}(\Omega)$ contains all functions in $L^2(\tilde{\Omega})$ (and possibly discontinuous) for any domain $\tilde{\Omega}$ with its closure being a compact subset of Ω. Hence, functions in $\mathcal{S}(\Omega)$ are generally not expected to have regularity better than $L^2(\Omega')$ over any strict subdomain Ω'. Yet, as elucidated in X. Tian and Du [2017], due to the horizon localization at the boundary, the penalization of spatial variations provides enough regularity for the functions in $\mathcal{S}(\Omega)$ to have well-defined traces just on the boundary itself. Intuitively, this is a natural consequence of the localization of nonlocal interactions on the boundary. In contrast, a standard norm associated with fractional Sobolev space is defined by

$$|u|^2_{H^\alpha(\Omega)} = \int_\Omega \int_\Omega \frac{(u(\mathbf{y})-u(\mathbf{x}))^2}{|\mathbf{y}-\mathbf{x}|^{2\alpha+d}} d\mathbf{y} d\mathbf{x}.$$

The regularity of the functions is effected by the denominator which vanishes at $\mathbf{x} = \mathbf{y}$.

We now state the special trace theorem, see X. Tian and Du [ibid.] for a complete proof.

Theorem 5.3 (Special trace theorem). *For $\Omega = (0,r)\times\mathbb{R}^{d-1}$ and $\Gamma = \{0\}\times\mathbb{R}^{d-1}$, there exists a constant C depends only on d such that for any $u \in C^1(\bar{\Omega}) \cap \mathcal{S}(\Omega)$,*

$$\|u\|_{L^2(\Gamma)} \le C\left(r^{-1/2}\|u\|_{L^2(\Omega)} + r^{1/2}|u|_{\mathcal{S}(\Omega)}\right), \quad \textit{for } d \ge 1,$$
$$|u|_{H^{1/2}(\Gamma)} \le C\left(r^{-1}\|u\|_{L^2(\Omega)} + |u|_{\mathcal{S}(\Omega)}\right), \quad \textit{for } d \ge 2.$$

where the nonlocal semi-norm of $\mathcal{S}(\Omega)$ is as given in (20).

Coupled local and nonlocal models. We use Ω_- and Ω_+ to denote two open domains in $\mathbb{R}^d$ that satisfy $\overline{\Omega_-}\cap\overline{\Omega_+} = \Gamma$, a co-dimension-1 interface, and Ω to denote their union. We consider the coupling of a local model on Ω_- with a nonlocal model on Ω_+, see Figure 4. Let $\mathcal{S}(\Omega_+)$ be the nonlocal space with heterogeneous localization on the boundary. By the trace theorem, we define the energy (solution) space and the test function space as

$$\mathcal{W}(\Omega) = \{u \in H^1(\Omega_-) \cap \mathcal{S}(\Omega_+) \,|\, u_- = u_+ \text{ on } \Gamma\}$$

$$\mathcal{W}_0(\Omega) = \{u \in \mathcal{W}(\Omega) \,|\, u = 0 \text{ on } \partial\Omega\},$$

where $\{u_\pm(x)\}$ denotes the traces of u defined from $\Omega_\pm$ respectively. From Proposition 5.1, we have the space $H^1(\Omega)$ continuously imbedded in $\mathcal{W}(\Omega)$ and $H_0^1(\Omega)$ also continuously imbedded in $\mathcal{W}_0(\Omega)$. For $u \in \mathcal{W}(\Omega)$, its norm is defined as $\|u\|_{\mathcal{W}(\Omega)} = \|u\|_{H^1(\Omega_-)} + \|u\|_{\mathcal{S}(\Omega_+)}$. For $g \in H^{1/2}(\partial\Omega)$ and $f \in L^2(\Omega)$, we have a coupled nonlocal-to-local model (22).

(22)
$$\min \left\{ \tfrac{1}{2}|u|^2_{H^1(\Omega_-)} + \tfrac{1}{2}|u|^2_{\mathcal{S}(\Omega_+)} - (f, u)_\Omega \right\},$$
$$\text{subject to } \; u \in \mathcal{W}(\Omega) \; \text{ and } \; u|_{\partial\Omega} = g.$$

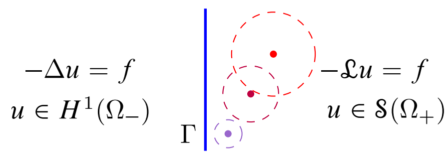

Figure 4: Variational formulation of a coupled local-nonlocal model.

Well-posedness of the coupled model. For (22) to be well-posed, the coercivity of the energy functional is the key, which is consequence of a Poincaré inequality on $\mathcal{W}_0(\Omega)$. The latter can be established in a similar fashion as that on the nonlocal space with the constant horizon (and the local Sobolev space $H_0^1(\Omega)$ as well). We thus have

Proposition 5.4. *The coupled variational problem* (22) *has a unique minimizer* $u \in \mathcal{W}_0(\Omega)$.

The seamless coupling of the nonlocal and local model means that one could use the same numerical discretization to solve the coupled problems if the heterogenous localization of horizon can be handled effectively. Indeed, this is where we can circle back to utilize the concept of robust asymptotically compatible schemes X. Tian [2017], Du, Tao, and X. Tian [2018], and X. Tian and Du [2014].

6 Nonlocal in time dynamics

Spatial nonlocality is often accompanied by temporal correlations and memory effects. The latter involves nonlocality in time. Let us note first that a major difference in time and space nonlocality is perhaps the generic time irreversibility. While a local time derivative may be defined by an infinitesimal change either backward to the history or forward to the future, it is more natural to view nonlocal time derivative as only dependent on past history. Thus, it is of much interests to reconsider the basic operators of the nonlocal vector calculus to accommodate the nonlocal interactions that are not symmetric. Of course, the issue of symmetry does not only pertain to changes in time. In earlier works, nonlocal gradients of the *upwind type*, variants of the operators given in Section 3, have been utilized in the modeling of convective effects H. Tian, Ju, and Du [2017] and in the nonlocal formulation of conservation laws Du and Huang [2017] and Du, Huang, and LeFloch [2017]. They have also been used to perform nonlocal gradient recovery Du, Tao, X. Tian, and J. Yang [2016]. The first rigorous treatment of a nonlocal in time dynamics with a finite memory span, in the spirit of nonlocal vector calculus, was given in Du, J. Yang, and Z. Zhou [2017], which we follow here.

Nonlocal time derivative and nonlocal-in-time dynamics. We take the operator

$$(\mathcal{G}_\delta u)(t) = \lim_{\epsilon\to 0}\int_\epsilon^\delta \frac{u(t)-u(t-s)}{s}\rho_\delta(s)\,ds, \qquad \text{for} \quad t>0,$$

as the nonlocal time derivative for a nonnegative density kernel ρ_δ that is supported in the interval $[0,\delta)$. This leads to the study of an abstract nonlocal-in-time dynamics:

$$\text{(23)}\quad \mathcal{G}_\delta u + \mathcal{A} u = f, \quad \forall\, t\in\Omega_T=(0,T)\subset\mathbb{R}_+, \quad u(t)=g(t), \quad \forall\, t\in(-\delta,0)\subset\mathbb{R}_-.$$

for a linear operator $\mathcal{A}$ in an abstract space, together with some nonlocal initial (historical) data $g=g(t)$. We recall a well-posedness result for (23) corresponding to $\mathcal{A}=-\Delta$ on a bounded spatial domain Ω with a homogeneous Dirichlet boundary condition Du, J. Yang, and Z. Zhou [ibid.].

Theorem 6.1. *For $f\in L^2(0,T;H^{-1}(\Omega))$, the problem (23) for $\mathcal{A}=-\Delta$ on Ω with the homogeneous Dirichlet boundary condition and $g(x,t)\equiv 0$ has a unique weak solution $u\in L^2(0,T;H^1_0(\Omega))$. Moreover, there is a constant c, independent of δ, f and u, such that.* $\|u\|_{L^2(0,T;H^1_0(\Omega))} + \|\mathcal{G}_\delta u\|_{L^2(0,T;H^{-1}(\Omega))} \le c\|f\|_{L^2(0,T;H^{-1}(\Omega))}$.

The nonlocal-in-time diffusion equation may be related to fractional in time sub-diffusion equations like $\partial_t^\alpha u - \Delta u = 0$ for $\alpha\in(0,1)$ Du, J. Yang, and Z. Zhou [2017], Metzler and Klafter [2004], and Sokolov [2012] by taking some special memory kernels Allen, Caffarelli, and Vasseur [2016]. Such equations have often been used to describe the continuous time random walk (CTRW) of particles in heterogeneous media, where trapping events occur. In particular, particles get repeatedly immobilized in the environment for a trapping time drawn from the waiting time PDF that has a heavy tail Metzler and Klafter

[2004]. In general though, (23) provides a new class of models, due to the finite memory span, that serves to bridge anomalous and normal diffusion, with the latter being the limit as $\delta \to 0$. Indeed, the model (23) can also be related to a trapping model, see Du [n.d.], Du, J. Yang, and Z. Zhou [2017], and Du and Z. Zhou [2018] for more detailed studies.

Crossover of diffusion regimes. Diffusions in heterogeneous media have important implications in many applications. Using single particle tracking, recent studies have revealed many examples of anomalous diffusion, such as sub-diffusion with a slower spreading process in more constricted environment Berkowitz, Klafter, Metzler, and Scher [2002], He, Song, Su, Geng, Ackerson, Peng, and Tong [2016], and Jeon, Monne, Javanainen, and Metzler [2012]. Meanwhile, the origins and models of anomalous diffusion might differ significantly Korabel and Barkai [2010], McKinley, Yao, and Forest [2009], and Sokolov [2012]. On one hand, new experimental standards have been called for Saxton [2012]. On the other hand, there are needs for in-depth studies of mathematical models, many of which are non-conventional and non-local Du, Huang, and Lehoucq [2014], Du, Gunzburger, Lehoucq, and K. Zhou [2012], and Sokolov [2012].

Motivated by recent experimental reports on the crossover between initial transient sub-diffusion and long time normal diffusion in various settings He, Song, Su, Geng, Ackerson, Peng, and Tong [2016], the simple dynamic equation (23) with $\mathcal{A} = -\Delta$ provides an effective description of the diffusion process encompassing these regimes Du and Z. Zhou [2018]. For model (23), the memory effect dominates initially, but as time goes on, the fixed memory span becomes less significant over the long life history. As a result, the transition from sub-diffusion to normal diffusion occurs naturally. This phenomenon can be illustrated by considering the mean square displacement (MSD) $m(t)$ which can be explicitly computed Du and Z. Zhou [ibid.]. In Figure 5, we plot a solution of $\mathcal{G}_\delta m(t) = 2$, i.e., the mean square displacement of the nonlocal solution for $f \equiv 0$ and $\rho_\delta(s) = (1-\alpha)\delta^{\alpha-1}s^{-\alpha}$ with $\alpha = 0.2$ and $\delta = 0.5$. The result again illustrates the analytically suggested transition from the early fractional anomalous diffusion regime to the later standard diffusion regime. This "transition" or "crossover" behavior have been seen in many applications, e.g. diffusions in lipid bilayer systems of varying chemical compositions Jeon, Monne, Javanainen, and Metzler [2012, Fig.2], and lateral motion of the acetylcholine receptors on live muscle cell membranes He, Song, Su, Geng, Ackerson, Peng, and Tong [2016, Figs.3, 4].

7 Discussion and conclusion

Nonlocal models, arguably more general than their local or discrete analogs, are designed to account for nonlocal interactions explicitly and to remain valid for complex

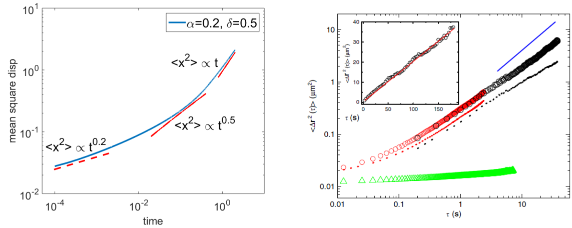

Figure 5: The MSD plot for (23) and the MSD curve He, Song, Su, Geng, Ackerson, Peng, and Tong [2016, Fig. 3] showing the crossover from sub-diffusion to normal diffusion for immobile AChRs.

systems involving possibly singular solutions. They have the potential to be alternatives and bridges to existing local continuum and discrete models. Their increasing popularity in applications makes the development of a systematic/axiomatic mathematical framework for nonlocal models necessary and timely. This work attempts to answer a few questions on nonlocal modeling, analysis and computation, particularly for models involving a finite-range nonlocal interactions and vector fields, To invite further studies on the subject, it might be more enticing to identify some issues worthy further investigation and to explore connections with other relevant topics. This is the purpose here, but before we proceed, we note that there are already many texts and online resources devoted to nonlocal models (scalar fractional equations in particular, see for example more recent books Bucur and Valdinoci [2016], Vázquez [2017], and West [2016] and `http://www.ma.utexas.edu/mediawiki/index.php/Starting_page`). We also refer to Du [n.d.] for more details and references on topics discussed below.

Nonlocal exterior calculus and geometry. While an analogy has been drawn between traditional local calculus and the nonlocal vector calculus involving nonlocal operators and fluxes, nonlocal integration by parts and nonlocal conservation laws, the nonlocal framework still needs to be updated or revamped. For example, a geometrically intrinsic framework for nonlocal exterior calculus and nonlocal forms on manifolds is not yet available. It would be of interests to develop nonlocal geometric structures that are more general than both discrete complexes and smooth Riemannian manifolds. In connection with such investigations, there are relevant studies on metric spaces Burago, Ivanov, and Kurylev [2014] and Fefferman, Ivanov, Kurylev, Lassas, and Narayanan [2015], Laplace-Beltrami Belkin and Niyogi [2008] and Lévy [2006], and combinatorial Hodge theory with scalar nonlocal forms Bartholdi, Schick, N. Smale, and S. Smale [2012]. We also made attempts like Le [2012] to introduce nonlocal vector forms, though more coherent constructions are desired. Given the close relations between local continuum models of mechanics and differential geometry, one expects to find deep and intrinsic connections between nonlocal mechanics and geometry.

Nonlocal models, kernel methods, graph and data. Discrete, graph, network models and various kernel based methods in statistics often exhibit nonlocality. Exploring their continuum limits and localization can offer fundamental insights. In this direction, we mention some works related to graph Laplacians, diffusion maps, spectral clustering and so on Coifman and Lafon [2006], Singer and H.-T. Wu [2017], Spielman [2010], Trillos and Slepčev [2016], and van Gennip and A. L. Bertozzi [2012]. These subjects are also connected with the geometric analysis already mentioned and applications such as image and data analysis and learning Buades, Coll, and Morel [2010], Gilboa and Osher [2008], and Lou, X. Zhang, Osher, and A. Bertozzi [2010]. For instance, one can find, for applications to image analysis, the notion of nonlocal means Buades, Coll, and Morel [2010] and nonlocal (NL) gradient operator Gilboa and Osher [2008] together with a graph divergence all defined for scalar fields. Indeed, there have been much works on nonlocal calculus for scalar quantities, see Du [n.d.] for more detailed comparisons.

Nonlocal function spaces, variational problems and dynamic systems. While there have been a vast amount of studies on nonlocal functional spaces, related variational problems and dynamic systems, such as Ambrosio, De Philippis, and Martinazzi [2011], Bourgain, Brezis, and Mironescu [2001], Bucur and Valdinoci [2016], Caffarelli and Silvestre [2007], Silvestre [2014], and West [2016], the majority of them have focused on scalar quantities of interests and are often associated with fractional differential operators, fractional calculus, fractional Sobolev spaces and fractional PDEs having global interactions. On the other hand, motivated by applications in mechanics, our recent works can serve as a starting point of further investigations on nonlocal functional analysis of vector and tensor fields and systems of nonlocal models. For example, one may consider nonlocal extensions to the variational theory of nonlinear elasticity Ball [2010] and use them to develop better connections with atomistic modeling. One may further consider nonlocal spaces that can account for anisotropies and heterogeneities in both state and configuration variables. Extensions of the new trace theorems on heterogeneously localized nonlocal spaces to various vector field forms are also topics of more subsequent research. For instance, one may investigate possible nonlocal generalization of the trace theorems on the normal component of vector fields in the $H(\mathrm{div})$ space Buffa and Ciarlet [2001]. Moreover, there are also interesting questions related to nonlocal models of fluid mechanics, including the nonlocal Navier-Stokes equations involving fractional order derivatives Constantin and Vicol [2012] and more recently analyzed nonlocal analogs of the linear incompressible Stokes equation as presented in the following forms, together with a comparison with their classical form in the local limit:

$$
(24) \quad \begin{cases} -\mathfrak{L}_\delta \mathbf{u} + \mathfrak{G}_\delta p = \mathbf{b}, \\ -\mathfrak{D}_\delta \mathbf{u} \qquad\quad = 0, \end{cases} \quad \text{or} \quad \begin{cases} -\mathfrak{L}_\delta \mathbf{u} + \mathfrak{G}_\delta p \quad = \mathbf{b}, \\ -\mathfrak{D}_\delta \mathbf{u} - \delta^2 \hat{\mathfrak{L}}_\delta p = 0, \end{cases} \quad \text{and} \quad \begin{cases} -\Delta \mathbf{u} + \nabla p = \mathbf{b}, \\ \nabla \cdot \mathbf{u} \qquad\quad = 0, \end{cases}
$$

where $\mathfrak{L}_\delta$ and $\hat{\mathfrak{L}}_\delta$ are nonlocal diffusion operators, $\mathfrak{G}_\delta$ and $\mathfrak{D}_\delta$ are one-point nonlocal gradient and divergence operators, similar to ones described in Section 3. There are surely more questions about the extensions to time-dependent and nonlinear systems.

Nonlocal, multiscale and stochastic modeling. Nonlocality arises naturally from model reductions and has appeared (either knowingly or implicitly) in many early works (such as the Mori-Zwanzig formalism Chorin, Hald, and Kupferman [2002]). Nonlocal modeling could play more prominent roles in multiscale and stochastic modeling, ranging from bridging atomistic and continuum models, to data-driver model reductions of dynamic systems. There are also strong connections of nonlocal models with hydrodynamic descriptions of collective behavior and flocking hydrodynamics Motsch and Tadmor [2014] and Shvydkoy and Tadmor [2017]. Exploring nonlocal models in diffusion and dispersal processes has also received much attention Fuentes, Kuperman, and Kenkre [2003], Kao, Lou, and Shen [2010], and Massaccesi and Valdinoci [2017], with the resulting nonlocal models having strong ties with stochastic processes, particularly, non-Gaussian and non-Markovian behaviors Kumagai [2014] and Zaburdaev, Denisov, and Klafter [2015]. Stochastic nonlocal modeling is certainly an interesting subject on its own. In addition, inverse problems related to nonlocal models are also essential research subjects of both theoretical and practical interests and they can also be connected with various design and control problems.

Nonlocal modeling, numerical analysis and simulation. Numerical simulations of nonlocal models bring new computational challenges, from discretization to efficient solvers. To elevate the added cost associated with nonlocal interactions, it is of interests to explore a whole host of strategies, including local and nonlocal coupling Li and Lu [2017] and Du, Tao, and X. Tian [2018], adaptive grids Du, L. Tian, and Zhao [2013], multigrid and fast solvers Du and Z. Zhou [2017] and H. Wang and H. Tian [2012], some of them are less examined than others and most of topics remain to be further studied. The subject is naturally linked to sparse and low rank approximations that would allow one to explore the nonlocal structure to achieve efficient evaluation of nonlocal interactions as well as the solution of associated algebraic systems. Scalable algorithms via domain decomposition or other strategies that can particularly handle the information exchange (communications between processors) involving nonlocal interactions are interesting and important research questions. Let us also mention that nonlocal models can also become effective tools to analyze numerical schemes that were initially developed to solve local PDEs. For example, to understand the interplay between the smoothing length and the particle spacing in the context of smoothed particle hydrodynamics Gingold and Monaghan [1977] and Monaghan [2005], nonlocal continuum systems (24) can help providing a rigorous mathematical foundation for improving the stability and robustness of the discretization Du and X. Tian [2017]. Another example is concerned with discretization schemes for multidimensional local diffusion equations through the nonlocal integral formulation Du, Tao, X. Tian, and J. Yang [n.d.] and Nochetto and W. Zhang [2017], a topic linked with approximations of fully nonlinear elliptic equations such as the Monge-Ampére. An open question there is whether or not there are discretization schemes on unstructured meshes which can preserve the discrete maximum principles and are asymptotically compatible for general anisotropic and heterogeneous diffusion equations.

Thinking nonlocally, acting locally. The pushes for nonlocal modeling come from several fronts. Foremost, the development of nonlocal models is driven by the interests in studying singular/anomalous/stochastic/multiscale behavior of complex systems where nonlocal models can potentially unify and bridge different models. Nowadays, the imminent growth of nonlocal modeling may also be attributed to the inescapable presence of nonlocality in the daily human experience. The emergence of augmented reality, information technology and data science as well as intelligent computing has been fueling the popularity of nonlocal modeling as the world is getting more than ever remotely and nonlocally networked together. With extreme computing capabilities beyond doing simple analytical approximations, we could be ready to tackle nonlocal interactions directly. Yet, despite the huge lift in computing power, exploring simple representations and closure relations via local, sparse, low rank or low dimensional approximations is still of great theoretical interest and practical significance. We thus conclude by saying that promoting the role of nonlocal modeling is to not only argue for the need to think nonlocally and to retain nonlocal features wherever necessary, but also point out the importance in utilize local models wherever feasible, hence to act locally, as our goal is to have the efficiency and robustness of mathematical modeling and numerical simulations while maintaining their generality and predicability.

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