An invitation to nonlocal and fractional models, part one: nonlocal models

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Recent Progress in Nonlocal Modeling, Analysis, and Computation

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Outline

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Local vs. Nonlocal operators

- A differential operator can be performed locally by taking infinitesimal changes of functions.

(Laplacian) $\Delta u = \sum_{i=1}^{n} u_{x_i x_i}$

- In contrast, nonlocal operators can mean all operators that are not local.

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Lévy-Khintchine formula (1930s)
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Beurling-Deny formula (1958)
for characterizing generalized Dirichlet forms

Some illustrative examples (one)

One: A numerical analysis point of view

- Differential operator $u''(x)$
- Difference operator $D_h^2 u(x) = \dfrac{u(x+h) - 2u(x) + u(x-h)}{h^2}$
- Nonlocal integral operator $L_\delta u(x) = \int_{-\delta}^{\delta} \dfrac{u(x+s) - 2u(x) + u(x-s)}{s^2} \omega_\delta(s) ds$
- $L_\delta u(x)$ can be viewed as a combination of finite differences, with $u''(x)$ and $D_h^2 u(x)$ being its two special cases:

  - if $\omega_\delta(s)$ is a Dirac delta measure at $s = 0$, then $L_\delta u = u''$;

  - if $\omega_\delta(s)$ is a Dirac delta measure at $s = h$, then $L_\delta u = D_h^2 u$.

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- $-L_\delta u(x) = f(x)$ gives a spatially nonlocal continuum model that

  - bridges PDE models and nonlocal discrete models;

  - allows more singular solutions than those of PDE models;

  - when the quantity of interest is smooth enough, differential equations can be seen as approximation of the nonlocal equation since

$$L_\delta u(x) = u''(x) \int_{-\delta}^{\delta} \omega_\delta(s) ds + c_1 \delta^2 \frac{d^4}{dx^4} u(x) + \cdots$$

Some illustrative examples (one)

- In concern of solving PDEs, it is actually quite common to introduce nonlocal integral relaxations of the PDEs along with numerical discretizations. This has been seen in the SPH methods[1] and the vortex method[2] for simulating fluids, the regularization techniques[3] for solving PDEs with singularities, and the point integral method[4] for solving PDEs on manifolds.
- Some of the above-mentioned methods, however, do not differentiate the nonlocal length parameter δ with the discretization parameter h.
- We will see in the next that by separating the nonlocal length scale δ and discretization parameter h and analyzing the properties of the continumm models first, we can have a more systematic way of studying numerical methods and their limits as $\delta \to 0$ and $h \to 0$.

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[1] [Gingold-Monaghan, 1977]
[2] [Beale-Majda, 1985]
[3] [Tornberg-Engquist, 2003]
[4] [Li-Shi-Sun, 2017]

Some illustrative examples (two)

Two: Infinitely divisible distributions and Lévy processes

It is of great interest in probability theory and its applications to look for the collective behaviors of large-scale repetition of random phenomena.

- The renowned central limit theorem says

$$\frac{X_1}{\sqrt{n}} + \frac{X_2}{\sqrt{n}} + \cdots \frac{X_n}{\sqrt{n}} \rightsquigarrow \text{normal distribution}$$

for a sequence $(X_1, X_2, \dots, X_n)$ of *i.i.d.* random variables with $\mathbb{E}(X_k) = 0$.

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[5] That is to say, intuitively, that no single $Y_{n,k}$ is going to play the dominant role.

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- More generally, one could consider a sequence $(Y_{n,1}, Y_{n,2}, \ldots, Y_{n,r_n})$ of independent random variables, with each random variable being asymptotically negligible[5], then

$$Y_{n,1} + Y_{n,2} + \cdots + Y_{n,r_n} \rightsquigarrow \text{ infinitely divisible distribution}^6$$

An infinitely divisible distribution μ is described through its characteristic function by the Lévy-Khintchine formula,

$$\hat{\mu}(\theta) = \exp\left[ia\theta - \frac{1}{2}\sigma^2\theta^2 + \int_{\mathbb{R}} (e^{i\theta x} - 1 - i\theta x 1_{|x|<1})\nu(dx)\right].$$

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Some illustrative examples (two)

- A Lévy process $(X_t)_{t\geq 0}$ is a right-continuous process with stationary and independent increments. From the definition X_t has an infinitely divisible law, and

$$\mathbb{E}[e^{i\theta X_t}] = \exp\left[t\left(ia\theta - \frac{1}{2}\sigma^2\theta^2 + \int (e^{i\theta x} - 1 - i\theta x 1_{|x|<1})\nu(dx)\right)\right],$$

where the Lévy measure ν satisfies $\nu(\{0\}) = 0$ and $\int_{\mathbb{R}}(1 \wedge x^2)\nu(dx) < \infty$.

- The infinitesimal generator [7] of the pure Lévy jump process is given by

$$Lu(x) = \int_{\mathbb{R}} (u(x+s) - u(x) - su'(x)1_{|s|<1})\nu(ds)$$

[7] The infinitesimal generator $\mathscr{A}$ of a continuous-time Markov process $\{X_t\}$ is defined by $\mathscr{A}u(x) := \lim_{t\to 0}(\mathbb{E}(u(X_t)|X_0 = x) - u(x))/t$.

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Some illustrative examples (three)

Three: Model reductions – spatial and temporal nonlocality

- Schur complement from linear algebra

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$$

$\rightsquigarrow$ $$(A - BD^{-1}C)\,x = f - BD^{-1}g$$

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- Caffarelli-Silvestre extension/reduction

Let $u : \mathbb{R}^d \times [0, \infty) \to \mathbb{R}$ solve the following PDE,

$$\begin{cases} \nabla \cdot (y^\beta \nabla u(x,y)) = 0 & (x,y) \in \mathbb{R}^d \times [0,\infty)\,, \\ -\lim\limits_{y \to 0^+} y^\beta \dfrac{\partial u(x,y)}{\partial y} = c f(x) & x \in \mathbb{R}^d\,. \end{cases}$$

Then $u|_{\mathbb{R}^d \times \{0\}}$ solves a fractional Possion equation on $\mathbb{R}^d$.

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- Reduction of ODE

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- Reduction of variables usually results in a nonlocal in time memory effect, unless y is a fast variable that goes to equilibrium very quickly.

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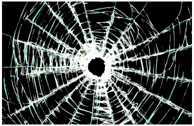
- The previous examples suggest that both spatial and temporal nonlocal interactions are common in coarse graining and multiscale modeling.

Some illustrative examples (four)



Four: Peridynamics – a nonlocal mechanics model

Peridynamics (PD) proposed in 2000 by Silling is a spatially nonlocal continuum mechanics model that replaces spatial derivatives in Newton's law by nonlocal/integral operators.

Classical elasticity model

$$\rho \ddot{u} = \nabla \cdot \sigma + b$$

- Local, certain smoothness of displacement field.
- Additional equations need to be included when fracture is involved.

The bond-based PD model

$$\rho \ddot{u} = \int_{B_\delta(x)} \mathrm{f}(u(y) - \mathrm{u}(x), y - x)\, dy + b$$

- Nonlocal, no spatial regularity required.
- Models continuous media and cracks within a single framework.

Linearized PD model

- $f(u(y)-u(x), y-x) \sim$ relative change (Hooke's law)

$(\eta = u(y)-u(x), \xi = y-x)$ $$f(\eta,\xi) = c_\delta(|\xi|)\frac{|\eta+\xi|-|\xi|}{|\xi|}\frac{\eta+\xi}{|\eta+\xi|}$$

- Linearized force density function

$$f(\eta,\xi) = c_\delta(\xi)\frac{\xi\otimes\xi}{|\xi|^3}\eta \implies \rho\,\ddot{u}(x,t) = L_\delta^{\mathrm{PD}} u(x,t) + b(x,t)\,,$$

where $L_\delta^{\mathrm{PD}} u(x) = \int_{B_\delta(x)} c_\delta(|y-x|)\frac{(y-x)\otimes(y-x)}{|y-x|^3}(u(y)-u(x))\,dy.$ [8]

- Localization. $\delta \to 0$ to linear elasticity equation with certain Poisson's ratio 1/4 in 3d and 1/3 in 2d. [9]

- For scalar functions $u : \mathbb{R}^d \to \mathbb{R}$ and let $K_\delta(|s|) = c_\delta(|s|)/|s|$

$$L_\delta u = \int_{B_\delta(x)} K_\delta(|y-x|)(u(y)-u(x))\,dy$$

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Summary of nonlocal modeling

We have seen four examples that are related to

- Numerical analysis
- Probability theory and stochastic processes
- Model reduction and coarse graining
- Fracture mechanics

There are still many other applications that uses nonlocal models, such as fluid mechanics [10], image processing and data analysis [11], ecology [12], biophysics [13], etc.

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[10] [Constantin, 2006]

[11] [Lou-Zhang-Osher-Bertozzi, 2010], [Coifman-Lafon, 2006]

[12] [Humphries et al., 2010]

[13] [Kou-Xie, 2004]

Outline

Nonlocal problems on bounded domains

- We consider the nonlocal boundary value problem on a bounded domain $\Omega \subset \mathbb{R}^d$,

$$\begin{cases} -L_\delta u(x) = f(x), & \forall\, x \in \Omega\,, \\ \mathscr{B}_\delta u(x) = g_\delta(x), & \forall\, x \in \Omega_\delta \; := \{x \in \mathbb{R}^d \backslash \Omega \,:\, \mathrm{dist}(x, \partial\Omega) < \delta\}\,. \end{cases}$$

$x \in \Omega$, $L_\delta u(x) = \int_{B_\delta(x)} K_\delta(|y-x|)(u(y)-u(x))\,dy = \int_{\Omega\cup\Omega_\delta} K_\delta(|y-x|)(u(y)-u(x))\,dy.$

- The nonlocal boundary condition is given as volume constraints

$$\mathscr{B}_\delta u(x) = \begin{cases} u(x) = g_\delta^D(x) & x \in \Omega_\delta^D \text{ (Dirichlet)}, \\ \mathscr{N}_\delta u(x) = g_\delta^N(x) & x \in \Omega_\delta^N \text{ (Neumann)}. \quad (\Omega_\delta^D \cup \Omega_\delta^N = \Omega_\delta) \end{cases}$$

- The kernel function $K_\delta(s)$ is non-negative and supported in the ball $B_\delta(0)$, and $\int (1 \wedge |s|^2) K_\delta(|s|) ds < \infty$. The two different scalings in regard to the two limiting cases $\delta \to 0$ and $\delta \to \infty$ are
  - (K1) $0 < \delta \ll \mathrm{diam}(\Omega)$: $K_\delta(s) = \frac{1}{\delta^{d+2}} K_1\left(\frac{s}{\delta}\right)$, where $\int |s|^2 K_1(|s|) ds = 2d$;
  - (K2) $\delta \gg \mathrm{diam}(\Omega)$: $K_\delta(s) = C_{d,s} \frac{1}{|s|^{d+2\alpha}} 1_{|s|<\delta}$.

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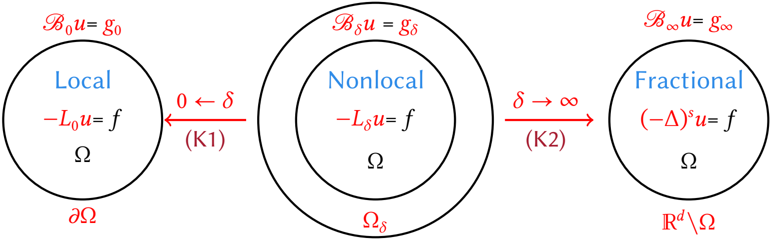

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Variational formulations

- The week formulation is found by integrating the strong form with a test function v

$$\int_\Omega f(x)v(x)dx = -\int_\Omega L_\delta u(x)v(x)dx = -\int_\Omega \int_{\Omega\cup\Omega_\delta} K_\delta(|y-x|)(u(y)-u(x))v(x)dydx$$
$$= -\iint_{(\Omega\cup\Omega_\delta)^2\setminus\Omega_\delta^2} K_\delta(|y-x|)(u(y)-u(x))v(x)dydx$$
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$(\mathcal{N}_\delta u(x) := \int_\Omega K_\delta(|y-x|)(u(y)-u(x))dy)$

$(b_\delta[u,v] := \frac{1}{2}\iint_{(\Omega\cup\Omega_\delta)^2\setminus\Omega_\delta^2} K_\delta(|y-x|)(u(y)-u(x))(v(y)-v(x))dydx)$

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$(\mathcal{N}_\delta u(x) := \int_\Omega K_\delta(|y-x|)(u(y)-u(x))dy)$ (nonlocal Green's first identity)

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$(\mathcal{N}_\delta u(x) := \int_\Omega K_\delta(|y-x|)(u(y)-u(x))dy)$ (nonlocal Green's first identity)

$(b_\delta[u,v] := \frac{1}{2}\iint_{(\Omega\cup\Omega_\delta)^2\setminus\Omega_\delta^2} K_\delta(|y-x|)(u(y)-u(x))(v(y)-v(x))dydx)$

- Define an *energy space* $S_\delta := \{v \in L^2(\Omega\cup\Omega_\delta) \,|\, b_\delta[v,v] < \infty\}$ endowed with norm $\|v\|_{S_\delta} := (\|v\|^2_{L^2(\Omega\cup\Omega_\delta)} + b_\delta[v,v])^{1/2}$. The corresponding *constrained energy space* is $S_{c,\delta} := \{v \in S_\delta \,|\, v(x) = 0 \text{ for } x \in \Omega_\delta^D\}$.
- The week formulation of the problem is given by: find $u \in S_\delta$ with $u|_{\Omega_\delta^D} = g_\delta^D$ such that $b_\delta[u,v] = (f,v)_{L^2(\Omega)} + (g_\delta^N, v)_{L^2(\Omega_\delta^N)}$ for all $v \in S_{c,\delta}$.

Properties of energy spaces

- The energy space S_δ is a Hilbert space. [14]
- Continuous embedding: $\|u\|_{L^2(\Omega\cup\Omega_\delta)} \le \|u\|_{S_\delta} \le C\|u\|_{H^1(\Omega\cup\Omega_\delta)}$. [15]
- Poincare inequality: let $|u|_{S_\delta} = (b_\delta[v,v])^{1/2}$, then

$$\|u\|_{L^2(\Omega\cup\Omega_\delta)} \le C|u|_{S_\delta} \qquad \forall u \in S_{c,\delta} .$$ [16]

This shows that the semi-norm $|\cdot|_{S_\delta}$ is a norm on the constrained energy space $S_{c,\delta}$. And by the Lax–Milgram theorem, this shows the well-posedness of week formulation.

- Asymptotic limit:
  - assume that K_δ satisfies (K1), then $|u|_{S_\delta} \xrightarrow{\delta\to 0} |u|_{H^1(\Omega)}$; [17]
  - assume that K_δ satisfies (K2), then $|u|_{S_\delta} \xrightarrow{\delta\to\infty} |u|_{H^\alpha(\Omega|\mathbb{R}^d)}$. [18]

[14] [Mengesha-Du, 2013]
[15] [Bourgain-Brezis-Mironescu, 2001]
[16] [Du-Gunzburger-Lehoucq-Zhou, 2012], [Mengesha-Du, 2013, 2014]
[17] [Bourgain-Brezis-Mironescu, 2001]
[18] defined as $\iint_{\mathbb{R}^{2d}\setminus\Omega^2} K_\infty(|y-x|)(u(y)-u(x))^2 dydx$. See [Dipierro-Ros-Oton-Valdinoci, 2017], [Dyda-Kassmann,2019]

Compactness

- (Bourgain-Brezis-Mironescu) Assume K_δ satisfies (K1) and let $\delta_n \to 0$ as $n \to \infty$. For any sequence $\{v_n \in S_{\delta_n}\}$ with uniform bound,

$$\sup_n \|v_n\|_{S_{\delta_n}} \leq C\,,$$

$\{v_n\}$ is relatively compact in $L^2(\Omega)$ and any limit v is in $H^1(\Omega)$ with $\|v\|_{H^1} \leq C$.

- (A variant of BBM)[19] Let δ be fixed and assume K_δ satisfies (K2) with $\alpha \in (1/2, 1)$. Let $\{K_\delta^n\}_n$ be a sequence of kernels converging to K_δ as $n \to \infty$ (*e.g.* $K_\delta^n = \min(n, K_\delta)$). Let S_δ^n be the energy space corresponding to the kernel K_δ^n. Then for any sequence $\{v_n \in S_\delta^n\}$ with uniform bound,

$$\sup_n \|v_n\|_{S_\delta^n} \leq C\,,$$

$\{v_n\}$ is relatively compact in $L^2(\Omega \cup \Omega_\delta)$ and any limit v is in S_δ with $\|v\|_{S_\delta} \leq C$.

[19] [Tian-Du, 2015]

Limits of nonlocal equations

Using the compactness theorem, one can show the convergence of weak solutions as $\delta \to 0$. [20]

Theorem Convergence of solution as $\delta \to 0$

Let u_δ and u_0 be the weak solutions to nonlocal and local boundary value problems respectively. Assume that K_δ satisfies (K1), then

$$\|u_\delta - u_0\|_{L^2(\Omega)} \to 0\,.$$

The $\delta \to \infty$ limit can also be shown. [21]

Theorem Convergence of solution as $\delta \to \infty$

Let u_δ and u_∞ be the weak solutions to nonlocal and fractional boundary value problems respectively. Assume that K_δ satisfies (K2), then,

$$\|u_\delta - u_\infty\|_{H^\alpha} \to 0\,.$$

---

[20] [Mengesha-Du, 2014]

[21] [D'Elia-Gunzburger, 2013], [Tian-Du-Gunzburger, 2016]

Reformulation of the problem using nonlocal calculus

L_δ can be reformulated by the *nonlocal vector calculus* [22].

- The *nonlocal divergence operator* $\mathscr{D}$ acting on a two-point function $v(x,y) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ is defined as

$$(\mathscr{D}v)(x) := \int_{\mathbb{R}^d} (v(x,y) + v(y,x)) \cdot e(x,y)dy \text{ for } e(x,y) = \frac{y-x}{|y-x|}.$$

- The *nonlocal gradient operator* $\mathscr{D}^*$ acting on a one-point function $u(x) : \mathbb{R}^d \to \mathbb{R}$ is defined as

$$(\mathscr{D}^*u)(x,y) := -(u(y) - u(x))e(x,y).$$

- Integration by parts: $\int_{\mathbb{R}^d} (\mathscr{D}v)u(x)dx = \iint_{\mathbb{R}^d\times\mathbb{R}^d} v(x,y)(\mathscr{D}^*u)(x,y)dydx$.
- L_δ is reformulated as $L_\delta u(x) = -\frac{1}{2}\mathscr{D}(K_\delta \mathscr{D}^* u)(x)$,
- The energy norm can be rewritten as

$$|u|^2_{S_\delta(\widehat{\Omega})} = \frac{1}{2} \iint_{(\Omega\cup\Omega_\delta)^2\setminus\Omega_\delta^2} K_\delta(|y-x|)|(\mathscr{D}^*u)(x,y)|^2 dydx.$$

---

[22] [Du-Gunzburger-Lehoucq-Zhou , 2013]

More on nonlocal vector calculus

The peridynamics model can also be reformulated using *nonlocal vector calculus*. Here we give the reformulation of the bond-based PD model.[23]

- Given the tensor two-point function $\Psi : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^{d\times d}$ and the one-point function $u : \mathbb{R}^d \to \mathbb{R}^d$, we can similarly define the nonlocal divergence operator $\mathscr{D}\Psi$ for tensors and its adjoint $\mathscr{D}^* u$ by

$$(\mathscr{D}\Psi)(x) = \int_{\mathbb{R}^d} (\Psi(y,x) + \Psi(x,y)) \cdot e(x,y) dy \,,$$
$$(\mathscr{D}^* u)(x,y) = -(u(y) - u(x)) \otimes e(x,y) \,,$$

- The linear bond-based peridynamic operator is reformulated as $L_\delta^{\mathrm{PD}}(x) = -\frac{1}{2}\mathscr{D}(K_\delta(\mathscr{D}^* u)^T)(x)$, where $K_\delta = K_\delta(|y-x|) = c_\delta(|y-x|)/|y-x|$.

- The PD equation has also a variational formulation with corresponding energy norm

$$\frac{1}{2}\iint K_\delta(|y-x|)(\mathrm{Tr}(\mathscr{D}^* u)(x,y))^2 dydx$$

[23] [Mengesha-Du, 2014]

Summary of nonlocal calculus

The nonlocal vector calculus is a systematic framework that mimics the classical local calculus for PDEs. [24]

Differential operators	$\Leftrightarrow$	Nonlocal operators
Local flux	$\Leftrightarrow$	Nonlocal flux
Green's identity and integration by parts $\int_\Omega u\Delta v - v\Delta u = \int_{\partial\Omega} u\partial_n v - v\partial_n u$	$\Leftrightarrow$	Nonlocal Green's identity and changing integration order $\iint u\mathscr{D}(\mathscr{D}^* v) - v\mathscr{D}(\mathscr{D}^* u) = 0$
Local balance (PDE) $-\nabla \cdot (K\nabla u) = f$	$\Leftrightarrow$	Nonlocal balance $-\mathscr{D} \cdot (K_\delta \mathscr{D}^* u) = f$
Local energy $\int (\nabla u)^{\mathrm{T}} K \nabla u$	$\Leftrightarrow$	Nonlocal energy $\iint K_\delta \lvert\mathscr{D}^* u\rvert^2$
Boundary conditions on $\partial\Omega$	$\Leftrightarrow$	Volume constraints on Ω_δ

[24] [Qiang Du, *Nonlocal Modeling, Analysis, and Computation*, SIAM, 2019.]

Outline

I. Introduction of nonlocal models

II. Nonlocal calculus

III. Numerical methods for nonlocal models

Summary

Overview of numerical methods

- Finite difference methods: methods based on directly approximating the operators by difference quotients.

$$\text{Find } u_\delta^h : \{x_i\}_{i=1}^N \to \mathbb{R} \text{ such that } -L_{\delta,h} u_\delta^h(x_i) = f(x_i).$$ [25]

- Finite element methods: methods based on variational principles and approximating infinite-dimensional spaces by finite-dimensional spaces.

$$\text{Find } u_\delta^h \in W_{\delta,h} \subset S_{c,\delta} \text{ such that } b_\delta[u_\delta^h, v] = (f, v)\ \forall v \in W_{\delta,h}.$$

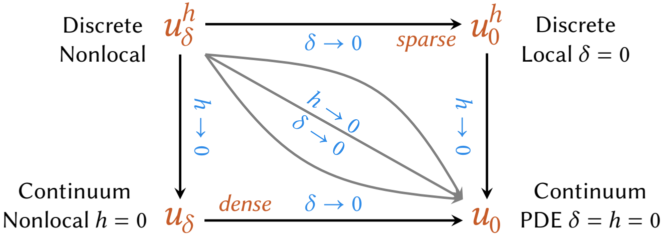
- Collocation/meshless methods: methods based on finite basis expansions and approximating the equations at sampling points.

$$\text{Find } u_\delta^h(x) = \sum_{i=1}^N a_i \Phi_i(x) \text{ such that } -L_\delta u_\delta^h(x_i) = f(x_i).$$

- Others ...

[25] We will focus on the homogeneous pure Dirichlet boundary condition (volume constraint) from now on for simplicity.

Asymptotically compatible (AC) schemes



Q: Why AC? They are robust, useful for validation and verification, and suitable for multiscale simulations.

Q: What schemes are AC?

An illustrative example

For $u : \mathbb{R} \to \mathbb{R}$,

$$L_\delta u(x) = \int_{-\delta}^{\delta} (u(x+s) - u(x)) K_\delta(|s|) ds = \int_0^{\delta} D^2 u(x,s) K_\delta(|s|) ds$$

where $D^2 u(x,s) = u(x+s) + u(x-s) - 2u(x)$.

Direct Riemann sum: $L_{\delta,h} u(x_i) = h \sum_{j=1}^{r} (u(x_i - jh) + u(x_i + jh) - 2u(x_i)) K_\delta(jh)$

It is convergent with fixed δ, but not convergent with a fixed ratio $r = \delta/h$.

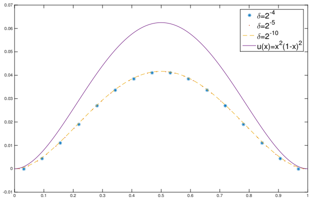


Figure: $\delta = 3h$

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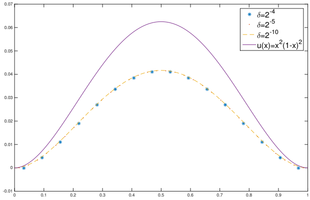

Figure: $\delta = 3h$

Take the example $u(x) = x^2/2$.

- $D^2 u(x,s) = s^2$
- $L_\delta u(x) = \int_0^{\delta} |s|^2 K_\delta(|s|) ds = 1, \forall \delta.$
- $L_{\delta,h} u(x_i) = h \sum_{j=1}^{r} (jh)^2 K_\delta(jh)$

$= h \sum_{j=1}^{r} (jh)^2/\delta^3 K(jh/\delta)$

$= 1/r^3 \sum_{j=1}^{r} j^2 K(j/r) = C(r) \neq 1.$

An illustrative example

For $u : \mathbb{R} \to \mathbb{R}$,

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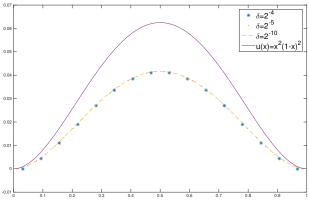

Figure: $\delta = 3h$

- (good) simple and convergent for fixed δ
- (bad) small δ deteriorates convergence rates as $O(h/\delta)$
- (bad) inconsistent for $\delta \to 0$ when we fix $r = \delta/h$

An illustrative example

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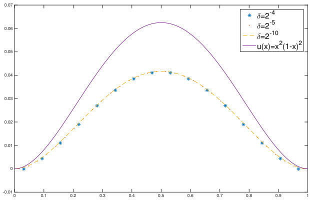

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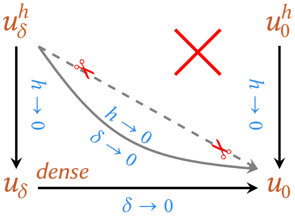

An improved quadrature-based finite difference scheme

- An improved finite difference scheme is given by

$$L_{\delta,h}u(x_i) = \int_0^\delta I_h^1 \left[\frac{u(x_i+s)+u(x_i-s)-2u(x_i)}{s} \right] sK_\delta(s)ds\,,$$

where I_h^1 is the piecewise linear interpolation of function, namely $I_h^1 v(s) = \sum_j v(jh)\varphi_j(s)$, where $\varphi_j(s)$ is the piecewise linear (hat) function centered at jh. The finite difference operator is then written as

$$L_{\delta,h}u(x_i) = \sum_j a_j(u(x_i - jh) + u(x_i + jh) - 2u(x_i))\,,$$

where $a_j = 1/(jh)\int_0^\delta \varphi_j(s)sK_\delta(s)ds$.

- The improved scheme is *quadratically exact*, namely if $u = x^2/2$,

$$L_{\delta,h}u(x_i) = \sum_j a_j(jh)^2 = \sum_j (jh)\int_0^\delta \varphi_j(s)sK_\delta(s)ds$$

- The extension of the scheme to multi-dimensions on uniform grid is given by [26] $L_{\delta,h}u(x_i) = \int_{B_\delta(0)} I_h^1 \left[\frac{u(x_i+s)-u(x_i)}{W_1(s)} \right] W_1(s)K_\delta(s)ds$ with $W_1(s) = |s|^2/|s|_1$.

[26] [Du-Tao-Tian-Yang, 2018]

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- The improved scheme is *quadratically exact*, namely if $u = x^2/2$,

$$L_{\delta,h}u(x_i) = \textstyle\sum_j a_j(jh)^2 = \int_0^\delta |s|^2K_\delta(|s|)ds = 1 = L_\delta u$$

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[26] [Du-Tao-Tian-Yang, 2018]

Consistency and stability

Lemma Uniform truncation error

Assume that $u \in C^4$, then

$$\left|L_{\delta,h}u(x_i) - L_\delta u(x_i)\right| \le C \left(\int |s|^2 K_\delta(|s|)ds\right) |u^{(4)}|_\infty h^2$$

where C is a constant independent of δ and h.

Lemma Discrete maximum principle (DMP)

The finite difference scheme $-L_{\delta,h}u_\delta^h(x_i) = f(x_i)$ satisfies the DMP:

$$f \le 0 \Rightarrow u_\delta^h(x_i) \le \max_{x_j \in \Omega_\delta} u_\delta^h(x_j) \quad \forall x_i \in \Omega;$$

$$f \ge 0 \Rightarrow u_\delta^h(x_i) \ge \min_{x_j \in \Omega_\delta} u_\delta^h(x_j) \quad \forall x_i \in \Omega.$$

This further implies the stability of the scheme, namely that $\|(-L_{\delta,h})\|_\infty^{-1} \le C$ for C independent of δ and h.

Note: the DMP is obvious since $a_j = 1/(jh)\int_0^\delta \varphi_j(s)sK_\delta(s)ds \ge 0$.

Convergence theorems

Let $u_\delta^h : \{x_i\} \to \mathbb{R}$ be the solutions of the finite difference scheme $-L_{\delta,h} u_\delta^h(x_i) = f(x_i)$. u_δ and u_0 are the nonlocal and local continuous solutions respectively.

Theorem Uniform Convergence

For a fixed δ,

$$\left|u_\delta^h - u_\delta\right|_\infty \leq C \left|u_\delta^{(4)}\right|_\infty h^2 ,$$

where C is a constant independent of δ and h.

Theorem Convergence as $\delta \to 0$ and $h \to 0$

For $\delta < \delta_0$

$$\left|u_\delta^h - u_0\right|_\infty \leq C \left|u_0^{(4)}\right|_\infty (h^2 + \delta^2) ,$$

where C is a constant independent of δ and h.

Proof: consistency + stability $\Rightarrow$ convergence.

The variational Galerkin approximation

- Galerkin approximation. Let $W_{\delta,h} \subset S_{c,\delta}$ be a finite dimensional approximation of the energy space $S_{c,\delta}$. The finite element scheme is given by finding $u_\delta^h \in W_{\delta,h}$ such that

$$b_\delta[u_\delta^h, v] = (f, v)_{L^2(\Omega)} \quad \forall v \in W_{\delta,h}$$

- Best approximation property. Let u_δ be the weak solution of the nonlocal problem. Standard arguments shows that

$$\|u_\delta - u_\delta^h\|_{S_\delta} \le C \inf_{v \in W_{\delta,h}} \|u_\delta - v\|_{S_\delta} .$$

For a fixed δ, we have $\inf_{v \in W_{\delta,h}} \|u - v\|_{S_\delta} \to 0$ as $h \to 0$ for any $u \in S_{c,\delta}$.

- However, it was found [27] that in the case of $\delta \to 0$ and $h \to 0$, piecewise constant FEM does not converge if $\delta/h \le C$, and piecewise linear FEM converges independent of the relation of δ and h. Why?

[27] [Chen-Gunzburger, 2011], [Tian-Du, 2013]

A variational framework of AC schemes

A) About the spaces $\{S_{c,\delta}\}_{\delta<\delta_0}$

- Ai) Uniform embedding: $C_1\|u\|_{L^2} \le \|u\|_{S_\delta} \le C_2\|u\|_{H^1}$
- Aii) Asymptotically compact embedding: Let $u_n \in S_{c,\delta_n}$ and $\delta_n \to 0$. If $\{\|u_n\|_{S_{\delta_n}}\}_{\delta<\delta_0}$ is uniformly bounded, then $\{u_n\}$ is relatively compact in L^2 and each limit point is in H_0^1.

B) About the bilinear forms $\{b_\delta[u,v]\}_{\delta<\delta_0}$

- $B_\delta[u,v]$ is uniformly bounded & coercive. (Nonlocal Poincaré inequality)

C) Consistency in a dense subspace

- Ci) ∃ dense subspace $C_0^\infty \subset H_0^1$ such that $L_\delta u \in L^2$, $\quad \forall u \in C_0^\infty$
- Cii) Δ is the limit of L_δ in C_0^∞, $\lim_{\delta\to 0}\|L_\delta u - \Delta u\|_{L^2} = 0 \quad \forall u \in C_0^\infty$

D) Approximation properties $\{W_{\delta,h}\}_{\delta<\delta_0,h<h_0}$

- Di) Given $\delta > 0$, $\forall v \in S_\delta$, $\inf_{v^h \in W_{\delta,h}}\{\|v - v^h\|_{S_\delta}\} \to 0$ as $h \to 0$,
- Dii) $\{W_{\delta,h}, \delta \in (0,\delta_0), h \in (0,h_0)\}$ is asymptotically dense in H_0^1,i.e., $\forall v \in H_0^1$, $\exists\{v_k \in W_{\delta_k,h_k}\}_{\delta_k\to 0}^{h_k\to 0}$, such that $\|v - v_k\|_{H^1} \to 0$.

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- Ci) $\exists$ dense subspace $C_0^\infty \subset H_0^1$ such that $L_\delta u \in L^2$, $\forall u \in C_0^\infty$
- Cii) Δ is the limit of L_δ in C_0^∞, $\lim_{\delta\to 0}\|L_\delta u - \Delta u\|_{L^2} = 0 \quad \forall u \in C_0^\infty$

D) Approximation properties $\{W_{\delta,h}\}_{\delta<\delta_0,h<h_0}$

- Di) Given $\delta > 0$, $\forall v \in S_\delta$, $\inf_{v^h\in W_{\delta,h}}\{\|v - v^h\|_{S_\delta}\} \to 0$ as $h \to 0$,
- Dii) $\{W_{\delta,h}, \delta \in (0,\delta_0), h \in (0,h_0)\}$ is asymptotically dense in H_0^1,i.e., $\forall v \in H_0^1$, $\exists\{v_k \in W_{\delta_k,h_k}\}_{\delta_k\to 0}^{h_k\to 0}$, such that $\|v - v_k\|_{H^1} \to 0$.

Convergence theorems [28]

Assume A) - D), we can show

Theorem Asymptotically compatible schemes

Any continuous or discontinuous Galerkin approximation containing all continuous linear elements (so that Dii) is satisfied) is AC, thus is good for both nonlocal and local regimes.

Without assumption Dii), we can show

Theorem Conditional convergence

Galerkin approximation containing only piecewise constant elements (where Dii) is violated) is convergent if $h/\delta \to 0$.

[28] [Tian-Du, 2014], [Tian-Du, 2020]

Sketch of Proof

1. Take any sequence $\delta_n \rightarrow, h_n \rightarrow 0$, we have the uniform boundedness of $\{u_n = u_{\delta_n}^{h_n}\}$ in the energy norms.
2. From the compactness result, there is a L^2-limit $u^* \in H_0^1$
3. The limit point u^* satisfies for any $v \in C_c^\infty$

$$
\begin{aligned}
b_0(u^*, v) - (f, v) = & [b_0(u^*, v) - b_0(u_n, v)] + [b_0(u_n, v) - b_n(u_n, v)] \\
& + [b_n(u_n, v) - b_n(u_n, v_n)] + [(f, v_n) - (f, v)] \\
& = \text{I} + \text{II} + \text{III} + \text{IV} \,,
\end{aligned}
$$

   for $v_n \in W_{\delta_n, h_n}$.
4. Take $n \rightarrow \infty$, we can show I, II, III, IV $\rightarrow 0$, which implies u^* is the solution to the local equation.

Sketch of Proof

In particular, for III , we have

$$\text{III} = [b_n(u_n, v) - b_n(u_n, v_n)] \le C\|u_n\|_{S_{\delta_n}} \|v - v_n\|_{S_{\delta_n}}$$
$$\le \tilde{C}\|v - v_n\|_{S_{\delta_n}} .$$

- If $W_{\delta,h}$ contains p.w. linear functions (AC schemes), then we could choose v_n such that $v_n \in H^1$,

$$\|v - v_n\|_{S_{\delta_n}} \le \|v - v_n\|_{H^1} \to 0 .$$

- Otherwise $W_{\delta,h}$ has only p.w. constant functions, then

$$\|v - v_n\|_{S_{\delta_n}} \le C\delta_n^{\alpha-1}\|v - v_n\|_{H^\alpha} ,$$

for $0 \le \alpha < \frac{1}{2}$, which converges to 0 only if $h_n/\delta_n \to 0$, since [29]

$$\|v - v_n\|_{H^\alpha} \le Ch_n^{1-\alpha}\|v\|_{H^1} .$$

[29] [Belgacem-Brenner, 2001]

Numerical experiments

Table: L^2 errors and convergence rates using discontinuous p.w. linear FEM. From left to right: $\delta = \sqrt{h}, \delta = 3h, \delta = h^2$.

h	$\|e\|_0$	h	$\|e\|_0$	$\|e\|_0$
2^{-2}	$2.35 \times 10^{-1}(-)$	2^{-3}	$1.15 \times 10^{-1}(-)$	$1.67 \times 10^{-2}(-)$
2^{-4}	$4.31 \times 10^{-2}(1.2)$	2^{-4}	$2.25 \times 10^{-2}(2.4)$	$4.62 \times 10^{-3}(1.9)$
2^{-6}	$9.54 \times 10^{-3}(1.1)$	2^{-5}	$5.26 \times 10^{-3}(2.1)$	$1.21 \times 10^{-3}(1.9)$
2^{-8}	$2.31 \times 10^{-3}(1.0)$	2^{-6}	$1.29 \times 10^{-3}(2.0)$	$3.08 \times 10^{-4}(2.0)$

More applications of the variational framework

- The variational framework can be applied for the finite element discretization of the peridynamics model and its local limit of linear elasticity equation.[30]
- Let $K_\delta(s) = C\frac{1}{|s|^{d+2\alpha}}1_{|s|<\delta}$ for $\alpha \in (1/2, 1)$ and a fixed number δ. In this case, the energy space is equivalent to H^α that excludes discontinuous functions, so discontinuous basis functions cannot be used directly.
- A non-conforming DG scheme can be designed.[31] Let $K_\delta^n = \min(n, K_\delta)$ and $S_{c,\delta}^n$ be the energy space corresponding to the kernel K_δ^n. Then since K_δ^n is integrable, $S_{c,\delta}^n$ contains discontinuous p.w. polynomials as a subspace. Then one can use discontinuous p.w. polynomials FEM for the nonlocal problem corresponding to kernel K_δ^n, and it serves as a non-conforming DG scheme for the original problem corresponding to K_δ. The convergence of the scheme relies on the variational framework that shows how the numerical scheme converges as both $n \to \infty$ and $h \to 0$.

---

[30] [Tian-Du, 2014]

[31] [Tian-Du, 2015]

More applications of the variational framework

- The variational framework can also be applied to the fractional limit as $\delta \to \infty$ in replace of the $\delta \to 0$ limit. Assume that the kernel K_δ satisfies (K2), then it is shown [32] that any conforming Galerkin approximation of the nonlocal is AC, namely that u_δ^h converges (in H^α) to u_∞ as $\delta \to \infty$ and $h \to 0$ independent of the relation of δ and h.

[32] [Tian-Du-Gunzburger, 2016]

More applications of the variational framework

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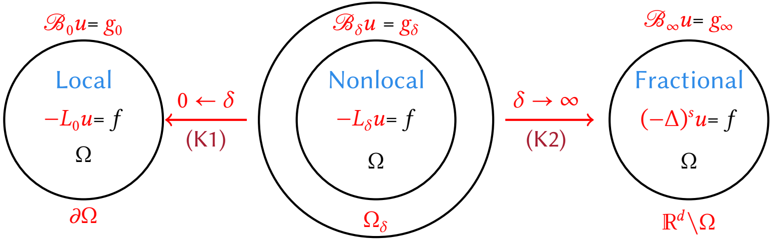

[32] [Tian-Du-Gunzburger, 2016]

Summary of numerical methods

- We have introduced finite difference methods (for nonlocal diffusion on uniform grid, based on truncation error analysis + DMP) and finite element methods (a much more general theory, based on the variational framework) for solving nonlocal equations. The key concept is the asymptotically compatible (AC) schemes that are insensitive to the change of model parameters.

- There are also discussions on other methods of AC type such as spectral methods [33] and collocation/meshless methods [34].

- For numerical discretization of the strong form (finite difference, collocation/meshless), it is difficult to show stability of the numerical schemes while trying to keep the AC property. In fact, for finite difference methods, DMP will be lost in more general situations, *e.g.* higher orders discretizations, non-uniform grids (even rectangular ones), or anisotropic diffusion. [Leng-Tian-Trask-Foster, 2019, 2020] has made an attempt to show stability of collocation methods without relying on DMP, but the analysis only applies to rectangular grids. There are much more to be done in the future.

[33] [Du-Yang, 2016]

[34] [Trask-You-Yu-Parks, 2019], [Leng-Tian-Trask-Foster, 2019, 2020]

Outline

Summary

- Nonlocal connections are ubiquitous in nature. We have introduced nonlocal models with a finite range of nonlocal interactions, which serve as bridges connecting the classical PDEs, nonlocal discrete models and the fractional differential equations.
- Nonlocal vector calculus and nonlocal calculus of variations have provided a systematic framework for analyzing nonlocal models and their local/fractional limits. They are also indispensable tools for the design and analysis of numerical methods for nonlocal models.
- Developments of numerical methods for nonlocal model include finite difference, finite element, collocation/meshless, and spectral methods. A particular attention is paid to the asymptotically compatible schemes, which are robust numerical schemes under parameter changing and are desirable in a problem with multiple scales.

Thank you!

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