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On Neumann-type Boundary Conditions for Nonlocal Models

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Michael Parks
Center for Computing Research
Sandia National Laboratories

Petronela Radu
Dept. of Mathematics
University of Nebraska, Lincoln

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Outline

Peridynamics Review

Motivating Neumann Boundary Conditions

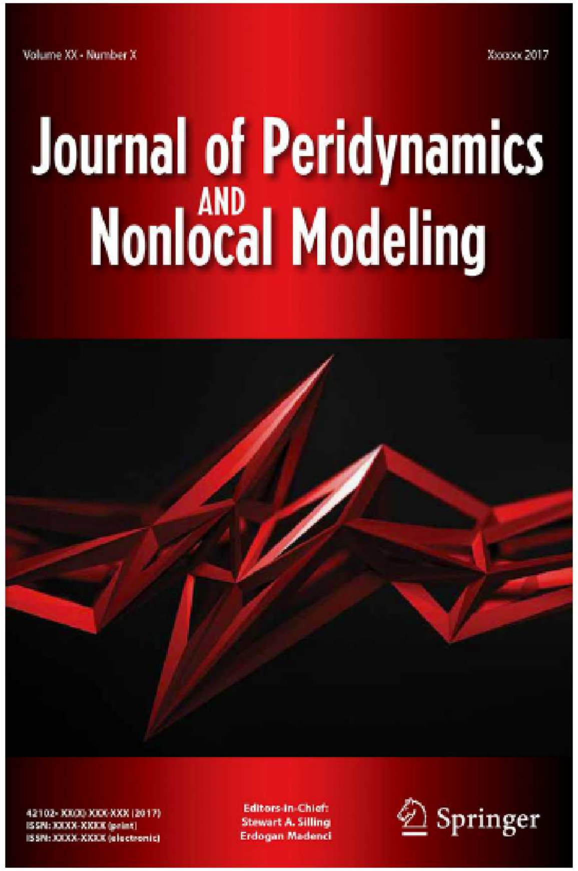
Review of Local Neumann

Nonlocal Neumann
- Theory
- Numerical Results

Conclusions

New Journal

- ❑ Peridynamics is growing rapidly
- ❑ PD needed its own journal. Co-Editor-in-Chief: S. Silling; E. Madenci.
- ❑ Now accepting submissions.



Journal of Peridynamics and Nonlocal Modeling

Co-Editor-in-Chief: S. Silling; E. Madenci

- ► Explores the development of peridynamics
- ► Analyzes modeling and simulation applications of peridynamics
- ► Connects peridynamics with high performance computing research

This journal explores theoretical development of peridynamics and nonlocal modeling and simulation applications across different disciplines such as aerospace, electronics, marine, defense, and composites.

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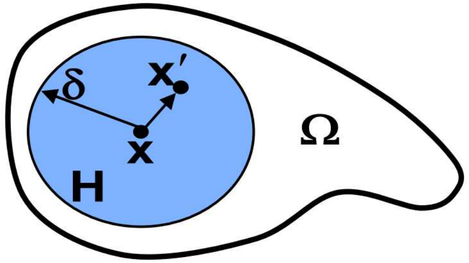
What is Peridynamics?

- Peridynamics is a nonlocal extension of classical solid mechanics

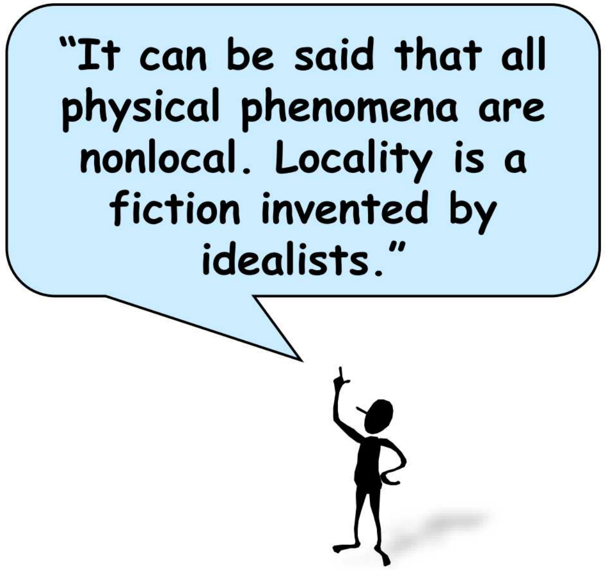
- Peridynamic equation of motion (integral, nonlocal)

$$\rho\ddot{u}(x,t) = \int_{H_x} f(u(x') - u(x), x'-x)dV' + b(x,t)$$

  - Replace PDEs with integral equations
  - Utilize same equation everywhere; nothing “special” about cracks
  - No assumption of differentiable fields (admits fracture)
  - No obstacle to integrating nonsmooth functions
  - $f(\cdot,\cdot)$ is “force” function; contains constitutive model
  - f = 0 for points x,x’ more than δ apart (like cutoff radius in MD!)
  - Peridynamics is “continuum form of molecular dynamics”
- Impact
  - Nonlocality
  - Larger solution space (fracture)
  - Account for material behavior at small & large length scales (multiscale material model)
- Ancestors
  - Kröner, Eringen, Edelen, Kunin, Rogula, etc.



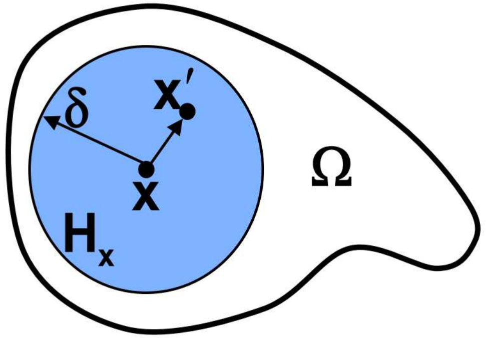
Point x interacts directly with all points x’ within H



A. Cemal Eringen

Peridynamics: The Basics

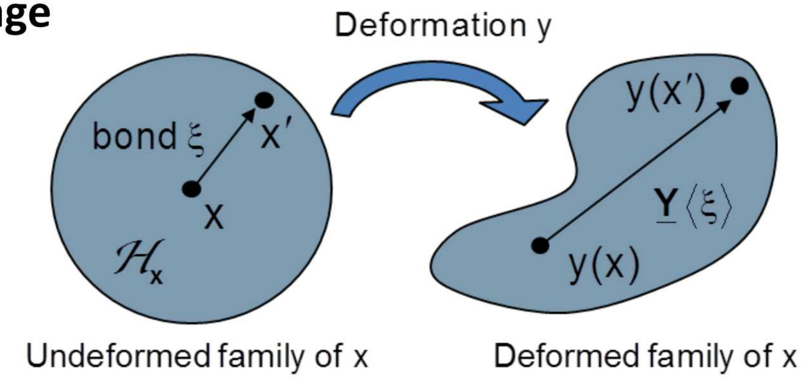
- **Horizon and family**
  - **Point x interacts directly with all points with distance δ (horizon)**
  - **Material within distance δ of x is denoted H_x (family of x)**



- **Bonds and bond forces**
  - **Vector between x and any point in its family is called a bond: ξ = x' – x**
  - **Each bond has pairwise force density vector applied at both points: f(x', x, t)**
  - **This vector is determined jointly by collective deformation of H_x and collective deformation of $H_{x'}$**
  - **Bond forces are antisymmetric: f(x', x, t) = - f(x, x', t)**
  - **Bond degrade and fail, admitting damage, failure, and fracture**

- **Deformation state**
  - **Deformation state operator $\underline{Y}$ maps each bond ξ into its deformed image**

$$\underline{\mathbf{Y}}\langle\xi\rangle = \mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x})$$



Peridynamics: The Basics

- **Bonds and states**
  - f(x′, x) has contributions from material models at both x and x′

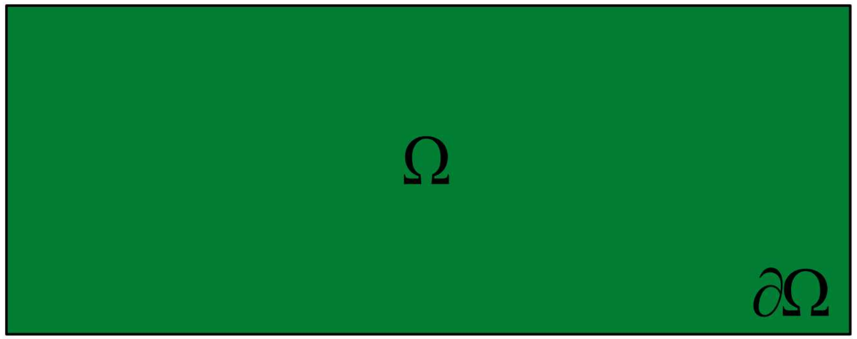
$$\mathbf{f}(\mathbf{x}',\mathbf{x}) = \underline{\mathbf{T}}[\mathbf{x},t]\langle \mathbf{x}'-\mathbf{x}\rangle - \underline{\mathbf{T}}[\mathbf{x}',t]\langle \mathbf{x}-\mathbf{x}'\rangle$$

  - T[x] is the force state – it maps bonds onto bond force densities
- **Mechanical Properties of Peridynamics**
  - Conserves energy (in absence of fracture, plastic deformation, etc.)
  - Conserves linear & angular momentum (always)
  - Obeys the laws of thermodynamics (restrictions on constitutive models)
- **Peridynamics vs. standard equations**
  - Peridynamic operators and relationships are nonlocal analogues of standard theory

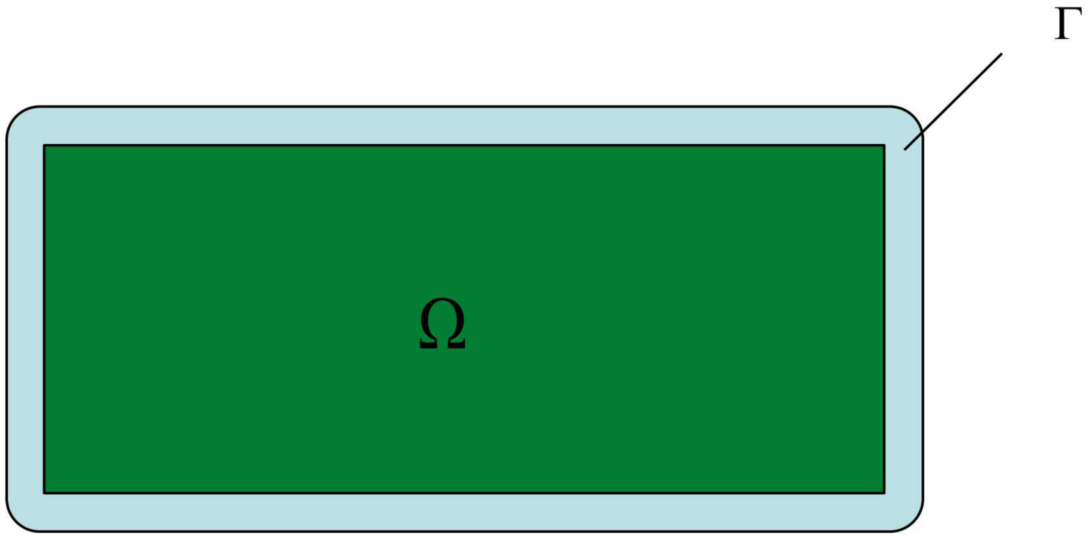
Relation	Peridynamic theory	Standard theory
Kinematics	$\underline{\mathbf{Y}}\langle \mathbf{x}'-\mathbf{x}\rangle = \mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x})$	$\mathbf{F}(\mathbf{x}) = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}(\mathbf{x})$
Linear momentum balance	$\rho\ddot{\mathbf{u}}(\mathbf{x}) = \int_{H_x} \left(\underline{\mathbf{T}}[\mathbf{x}]\langle \mathbf{x}'-\mathbf{x}\rangle - \underline{\mathbf{T}}[\mathbf{x}']\langle \mathbf{x}-\mathbf{x}'\rangle\right) dV_{x'} + \mathbf{b}(\mathbf{x})$	$\rho\ddot{\mathbf{y}}(\mathbf{x},t) = \nabla\cdot\sigma(\mathbf{x}) + \mathbf{b}(\mathbf{x})$
Constitutive model	$\underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}})$	$\sigma = \hat{\sigma}(\mathbf{F})$
Angular momentum balance	$\int_{H_x} \underline{\mathbf{Y}}\langle \mathbf{x}'-\mathbf{x}\rangle \times \underline{\mathbf{T}}\langle \mathbf{x}'-\mathbf{x}\rangle dV_{x'} = 0$	$\sigma = \sigma^T$
Elasticity	$\underline{\mathbf{T}} = W_{\underline{Y}}$ (Frechet derivative)	$\sigma = W_F$ (tensor gradient)
First law of thermodynamics	$\dot{\varepsilon} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} + h + r$	$\dot{\varepsilon} = \sigma\cdot\dot{\mathbf{F}} + h + r$

Nonlocal Boundary Conditions

- For local models (for example, PDE-based models), we apply boundary conditions on boundary of domain (hence the name)



- A Peridynamic "boundary" becomes a volumetric region, sometimes called a "nonlocal boundary", "collar", etc.
- Boundary conditions for these models are called "nonlocal boundary conditions", "volume constraints", etc.



* M. Fender, F. Lechenault, and K. Daniels, Universal Shapes Formed by Two Interacting Cracks, Phys. Rev. Lett. 105, 125505 (2010) .

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- Theory
- Numerical Results

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Motivation for Neumann Boundary Conditions

- Neumann (or second-type) boundary condition specifies value of derivative of solution at boundary
- Example: Poisson Equation

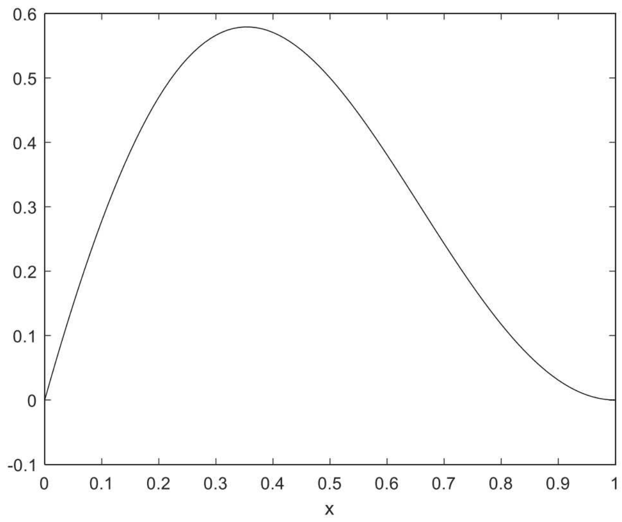
$$-k\frac{d^2u}{dx^2}(x) = f(x) \qquad x \in (0,1)$$

$$u = 0 \qquad x = 0$$

$$\frac{du}{dx} = 0 \qquad x = 1$$

Physical Problem:
Temperature distribution in bar
u = temperature
q = heat flux

$$\frac{dq}{dx} = f(x) \qquad q = -k\frac{du}{dx}$$



- **Physical interpretation of Neumann Boundary**: Heat flux across boundary
- **Mathematical interpretation of Neumann Boundary**: Slope of temperature field at boundary

- Locally (i.e., for differential equations) these concepts are the same. *For nonlocal models, they are not*.

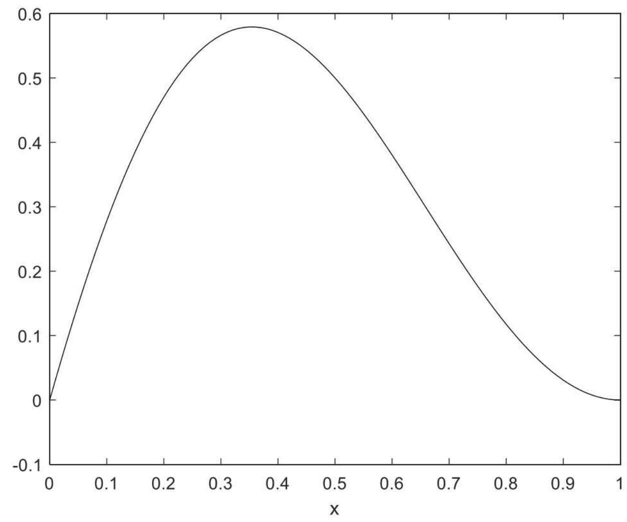
Motivation for Neumann Boundary Conditions

- Neumann (or second-type) boundary condition specifies value of derivative of solution at boundary
- Example: Poisson Equation

$$-k\frac{d^2u}{dx^2}(x) = f(x) \qquad x \in (0,1)$$
$$u = 0 \qquad x = 0$$
$$\frac{du}{dx} = 0 \qquad x = 1$$

Physical Problem:
Displacement of bar
u = displacement
σ = stress, ε = strain

$$\frac{d\sigma}{dx} + f(x) = 0 \qquad \sigma = E\varepsilon \qquad \varepsilon = \frac{du}{dx}$$



- **Physical interpretation of Neumann Boundary**: Stress at boundary
- **Mathematical interpretation of Neumann Boundary**: Slope of displacement field at boundary

- Locally (i.e., for differential equations) these concepts are the same. *For nonlocal models, they are not*.

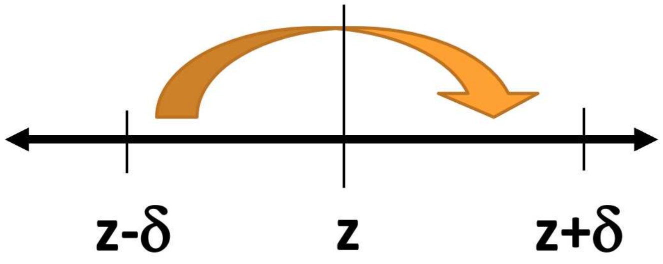
Motivation for Neumann Boundary Conditions

- ❑ Neumann-type boundary conditions for nonlocal models must describe flux into / out of domain
  - ❑ Slope of the solution field at boundary in nonlocal model has no physical meaning

- ❑ So what is nonlocal flux? In 1D, let's consider stress as a physical guide.
- ❑ Weckner & Abeyarante*: "By adapting Cauchy's notion of stress in a crystal …"

PD EOM

$$\int_{x-\delta}^{x+\delta} \big(u(y) - u(x)\big)\,\kappa(y,x)\,dy + b(x,t) = 0$$



PD Stress*

$$\sigma(z) = \int_0^{\delta}\int_0^{\delta} \big(u(z+r) - u(z-s)\big)\;\kappa(z+r, z-s)\;dr\,ds$$

- ❑ Physical interpretation*: total force that all material to right of z exerts on all material to left of z

- ❑ Note that nonlocal stress necessarily takes form of double integral

*O. Weckner and R. Abeyaratne, The effect of long-range forces on the dynamics of a bar, Journal of the Mechanics and Physics of Solids, 53, pp. 705-728, 2005.

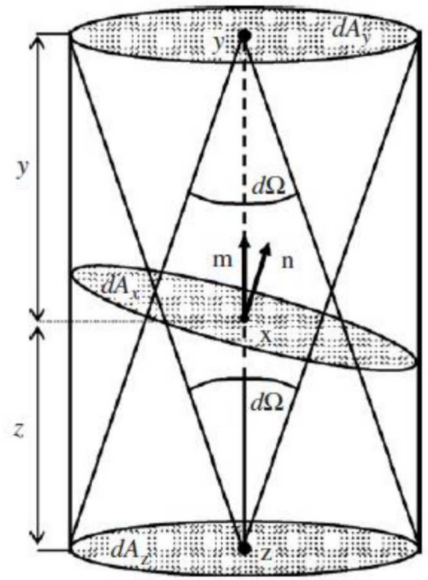
Motivation for Neumann Boundary Conditions

- **Result of Weckner and Abeyaratne was generalized to 3D in 2008 by Silling & Lehoucq*.**

- **Given PD EOM**

$$\int_R \mathbf{f}(\mathbf{y},\mathbf{x})\,d\mathbf{V_y} + \mathbf{b}(\mathbf{x},t) = 0$$

- **Peridynamic force flux vector at x in the direction of unit vector n is given by***



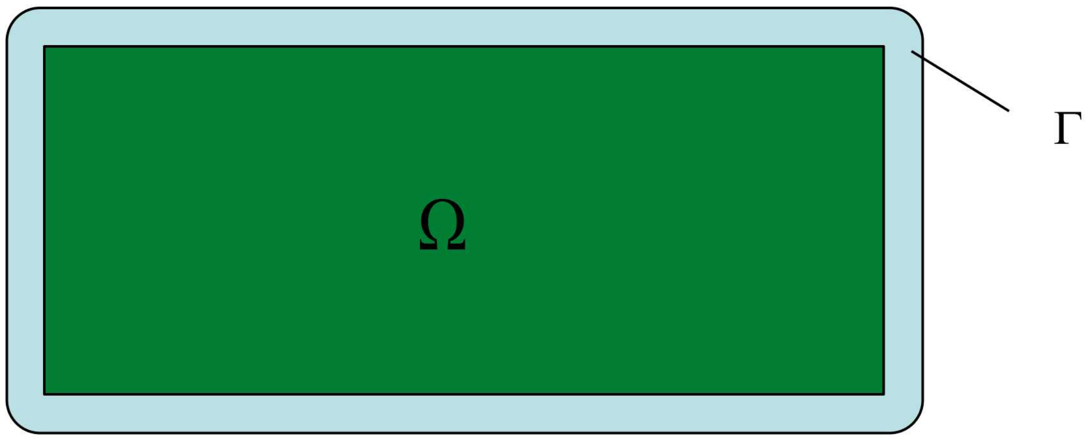
$$\tau(\mathbf{x},\mathbf{n}) = \frac{1}{2}\int_{\mathcal{L}}\int_0^{\delta}\int_0^{\delta}(\mathbf{y}+\mathbf{z})^2\mathbf{f}(\mathbf{x}+y\mathbf{m},\mathbf{x}-z\mathbf{m})\mathbf{m}\cdot\mathbf{n}\;\mathbf{d}z\mathbf{d}y\mathbf{d}\Omega_{\mathbf{m}}$$

- **Physical interpretation*: "According to Timoshenko (1983), the total stress on an infinitesimal element of a plane taken within a deformed elastic body is defined as the resultant of all the actions of the molecules situated on one side of the plane upon the molecules on the other, the directions of which (actions) intersect the element under consideration. *Replacing molecule with peridynamic particle results in a definition that is consistent with our interpretation.*"**
- **Motivation was to postprocess numerical solution to compute stresses, not to apply a traction b.c.**

*R.B. Lehoucq and S.A. Silling, Force flux and the peridynamic stress tensor, Journal of the Mechanics and Physics of Solids, 56, pp. 1566–1577, 2008.

Motivation for Neumann Boundary Conditions

- **If I know solution in nonlocal boundary, I can compute the flux at (local) domain boundary!**



- **This is good to know, but problematic in at least several ways:**
  - **Requires we know u outside domain -- Like need a nonlocal Dirichlet boundary condition in order to compute Neumann boundary condition!**
  - **If we know what we want flux to be, it's not clear how to determine what solution outside the domain should be**
  - **This isn't how things work locally -- I just want to apply a Neumann boundary condition and solve the problem without jumping through hoops going from Dirichlet b.c. to Neumann b.c.**

Literature Review (Incomplete)

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- H. You, X.Y. Lu, N. Trask, and Y. Yu. A Neumann-type boundary condition for nonlocal problems. Preprint.

- **Observation: This is an active area of research!**
- **Bad News: This means we don't fully understand it yet….**
- **Good News: You shouldn't feel bad if you don't fully understand it yet!**

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Review of Local Neumann

- ❑ Let's review how Neumann boundary conditions are applied for differential equations
- ❑ Example: Finite Difference solution to Poisson's equation in 1D

$$-k\frac{d^2u}{dx^2}(x) = f(x) \qquad x \in (0,1)$$

$$\frac{du}{dx} = 0 \qquad x = 0,1$$

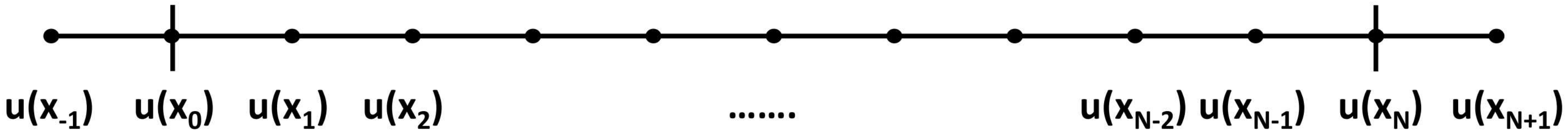
Stencil for Laplace operator:

$$-k\frac{d^2u}{dx^2}(x_i) = k\frac{-u(x_{i+1}) + 2u(x_i) - u(x_{i-1})}{h^2} + O(h^2), \quad i = 0,\dots,N$$

Stencil for Neumann b.c.:

$$\frac{du}{dx}(x_i) = \frac{u(x_{i+1}) - u(x_{i-1})}{2h} + O(h^2), \quad i=0,N$$

- ❑ Requires extending mesh by two "fictitious" nodes outside of Ω



- ❑ **In nonlocal setting, do something very similar and discretize nonlocal Neumann boundary condition and incorporate it into linear system of equations!**

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Nonlocal Neumann Boundary Condition: Theory

- We will utilize the following operators from nonlocal calculus*,**

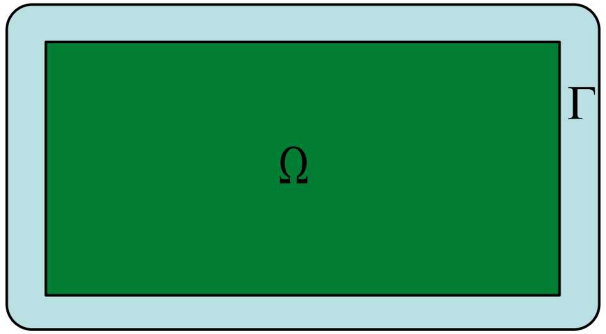
$$\alpha(x,y):\mathbb{R}^n\times\mathbb{R}^n\to\mathbb{R}^k$$
$$\mu(x,y)=\alpha(x,y)\cdot\alpha(x,y)$$

- Nonlocal point divergence

$$\mathcal{D}[\nu](x)=\int_{\Omega\cup\Gamma}\left(v(x,y)\cdot\alpha(x,y)-v(y,x)\cdot\alpha(y,x)\right)dy \quad \text{for } x\in\Omega$$

- Nonlocal two-point gradient

$$\mathcal{G}[u](x,y)=\left(u(y)-u(x)\right)\alpha(y,x) \quad \text{for } (x,y)\in\mathbb{R}^n\times\mathbb{R}^n$$



- Nonlocal normal operator

$$\mathcal{N}[\nu](x)=-\int_{\Omega\cup\Gamma}\left(v(x,y)\cdot\alpha(x,y)-v(y,x)\cdot\alpha(y,x)\right)dy \quad \text{for } x\in\Gamma$$

- Nonlocal Laplacian

$$\mathcal{L}[u](x)=\mathcal{D}\left[\mathcal{G}[u]\right](x)=2\int_{\Omega\cup\Gamma}\left(u(y)-u(x)\right)\mu(y,x)dy \quad \text{for } x\in\Omega$$

*Q. Du, M. Gunzburger, R. Lehoucq, and K. Zhou, A nonlocal vector calculus, nonlocal volume-constrained problems, and nonlocal balance laws, Mathematical Models and and Methods in Applied Sciences, 23 (2013), pp. 493-540.

** B. Hinds and P. Radu., Dirichlet's principle and wellposedness of steady state solutions for a nonlocal peridynamics model, Appl. Math. and Comput., 219 (2012), pp. 1411-1419.

Nonlocal Neumann Boundary Condition: Theory

Define energy of function u(x) as

$$\mathcal{E}[\mathrm{u}] = \frac{1}{2}\int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} \left|\mathcal{G}\mathrm{u}\right|^2 \, dV_x \, dV_y - \int_{\Omega} u(x)\, f(x)\, dV_x + \int_{\Gamma} u(x)\, g(x)\, dV_x$$

- **Theorem: H_μ gradient flow of energy over Hilbert space H_μ defined by**

$$H_\mu := \left\{ u \in L_2(\Omega\cup\Gamma) \,\middle|\, \int_{(\Omega\cup\Gamma)\times(\Omega\cup\Gamma)} \left|u(y) - u(x)\right|^2 \mu(y - x)\, dV_x \, dV_y < \infty \right\}$$

with $$\langle u, v \rangle_H = \int_{(\Omega\cup\Gamma)\times(\Omega\cup\Gamma)} \big(u(y) - u(x)\big)\big(v(y) - v(x)\big)\mu(y - x)\, dV_x \, dV_y$$

yields nonlocal boundary value problem

$$-\mathcal{L}[u](x) = -\int_{\Omega\cup\Gamma} \left[u(y) - u(x)\right] \mu(y - x)\, dV_y = f(x), \qquad x \in \Omega$$

$$\mathcal{N}[\mathcal{G}u](x) = 2\int_{\Omega\cup\Gamma} \left[u(y) - u(x)\right] \mu(y - x)\, dV_y = g(x), \qquad x \in \Gamma$$

Nonlocal Neumann Boundary Condition: Theory

Proof:

- **Let u(x) be a minimizer of the energy functional E[u] over the Hilbert space H_μ and let $v \in H_\mu$ be a test function. Using the classical direct method in calculus of variations, we will show that u is a solution to the nonlocal BVP. Using differentiation in Hilbert spaces and (nonlocal) integration by parts, compute:**

$$0 = \frac{d}{dt} E[u + tv]\Big|_{t=0}$$

$$= \int_{\Omega\cup\Gamma} \int_{\Omega\cup\Gamma} \mathcal{G}u\,\mathcal{G}v \; dV_x \, dV_y - \int_{\Omega} v(x)\, f(x)\, dV_x + \int_{\Gamma} v(x)\, g(x)\, dV_x$$

$$= -\int_{\Omega\cup\Gamma} \mathcal{L}[u](x)\; v(x)\; dV_x - \int_{\Omega} v(x)\, f(x)\, dV_x + \int_{\Gamma} v(x)\, g(x)\, dV_x$$

$$= -\int_{\Omega} \left[\mathcal{L}[u](x) \; - f(x)\right] v(x)\; dV_x - \int_{\Gamma} \left[\int_{\Omega\cup\Gamma} 2\big(u(y) - u(x)\big)\, \mu(y - x)\, dV_y - g(x) \right] v(x)\, dV_x$$

- **Since H_μ is complete, u(x) must satisfy nonlocal BVP.**

Nonlocal Neumann Boundary Condition: Theory

- How should we interpret Neumann boundary condition operator?

$$\mathcal{N}[\mathcal{G}u](x) = 2\int_{\Omega\cup\Gamma}\left[u(y)-u(x)\right]\mu(y-x)\,dV_y, \quad x\in\Gamma$$

- Under assumptions, can show convergence to local limit

$$\lim_{\delta\to 0}\int_{\Gamma}\int_{\Omega\cup\Gamma}\left[u(y)-u(x)\right]\mu(y-x)\,dV_y = \nabla u\cdot n$$

- How does this operator compare with flux operator we saw earlier? Compare in 1D:

$$\int_{\Gamma}\int_{\Omega\cup\Gamma}\left[u(y)-u(x)\right]\mu(y-x)\,dV_y = \int_{\Gamma}\int_{\Gamma}\left[u(y)-u(x)\right]\mu(y-x)\,dV_y$$

$$+\int_{\Gamma}\int_{\Omega}\left[u(y)-u(x)\right]\mu(y-x)\,dV_y$$

Nonlocal Neumann Boundary Condition: Theory

- How should we interpret the Neumann boundary condition operator?

$$\mathcal{N}[\mathcal{G}u](x) = 2\int_{\Omega\cup\Gamma} [u(y)-u(x)]\,\mu(y-x)\,dV_y, \quad x\in\Gamma$$

- Under assumptions, can show convergence to local limit at rate of $O(\delta^2)$

$$\lim_{\delta\to 0}\int_{\Gamma}\int_{\Omega\cup\Gamma}[u(y)-u(x)]\,\mu(y-x)\,dV_y = \nabla u\cdot n$$

- How does this operator compare with flux operator we saw earlier? Compare in 1D:

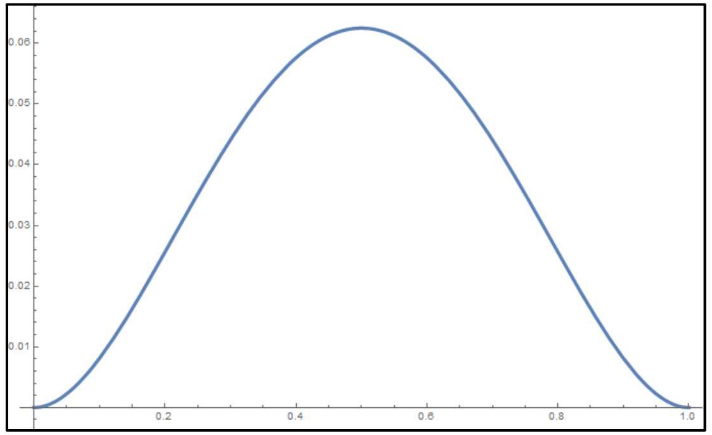
$$\int_{\Gamma}\int_{\Omega\cup\Gamma}[u(y)-u(x)]\,\mu(y-x)\,dV_y = \underbrace{\cancel{\int_{\Gamma}\int_{\Gamma}[u(y)-u(x)]\,\mu(y-x)\,dV_y}}_{\to 0}$$

$$+\underbrace{\int_{\Gamma}\int_{\Omega}[u(y)-u(x)]\,\mu(y-x)\,dV_y}_{\text{Flux operator from Weckner \& Abeyaratne}}$$

- **We can now apply a nonlocal boundary condition to prescribe a flux without ever needing to know u(x) in Γ, just as we do locally!**

Nonlocal Neumann Boundary Condition: Theory

- In local models, we know characteristic shape of solution associated with Neumann boundary condition.
  - Example: zero Neumann has zero slope at boundary
- What do solutions associated with nonlocal Neumann boundary conditions look like?
  - Given u(x) for $x \in \Omega$, we can solve analytically for u(x) for $x \in \Gamma$
  - This is not required for numerical solution; We do so here for curiosity
- Let
  - $u(x) = x^2 (1-x)^2$, $x \in \Omega = (0,1)$
  - $\delta = 0.1$
  - $\mathcal{N}[\mathcal{G}u](x) = 0$, $x \in \Gamma$
- Observations:
  - u(x), $x \in \Gamma$, is smooth except for discontinuity at boundary

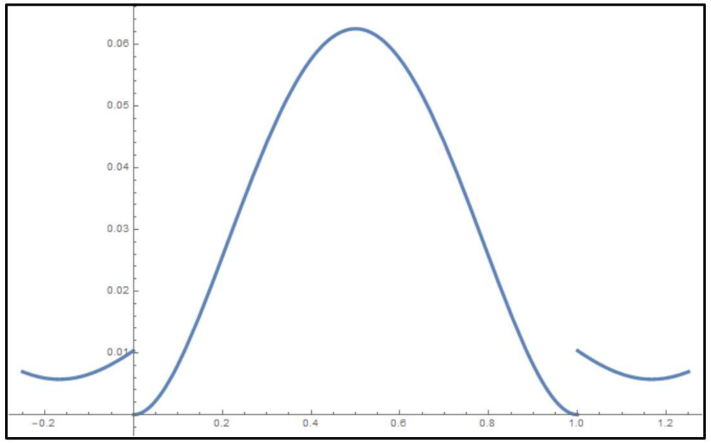


$$-\nabla^2 u(x) = f(x), \quad x \in \Omega$$
$$\nabla u(x) \cdot n = 0, \quad x = \Gamma$$

Local Poisson's Equation

$$-\mathcal{L}[u](x) = f(x), \quad x \in \Omega$$
$$\mathcal{N}[\mathcal{G}u](x) = 0, \quad x \in \Gamma$$

Nonlocal Poisson's Equation



Nonlocal Neumann Boundary Condition: Computation

- Goal: Numerical solution of Nonlocal Poisson's equation:

$$-\mathcal{L}[u](x) = f(x), \quad x \in \Omega$$
$$\mathcal{N}[\mathcal{G}u](x) = g(x), \quad x \in \Gamma$$

- Consider manufactured solution
  - $u(x) = x^2 (1-x)^2$, $x \in \Omega = (0,1)$
  - Verify h-convergence
  - Verify δ-convergence

- Issue #1: Asymptotic incompatibility for certain discretizations*
  - Use piecewise linear discretization
- Issue #2: Solution may be discontinuous in $\Omega = (0,1)$, and definitely has discontinuity at x = 0,1.
  - Use discontinuous Galerkin discretization

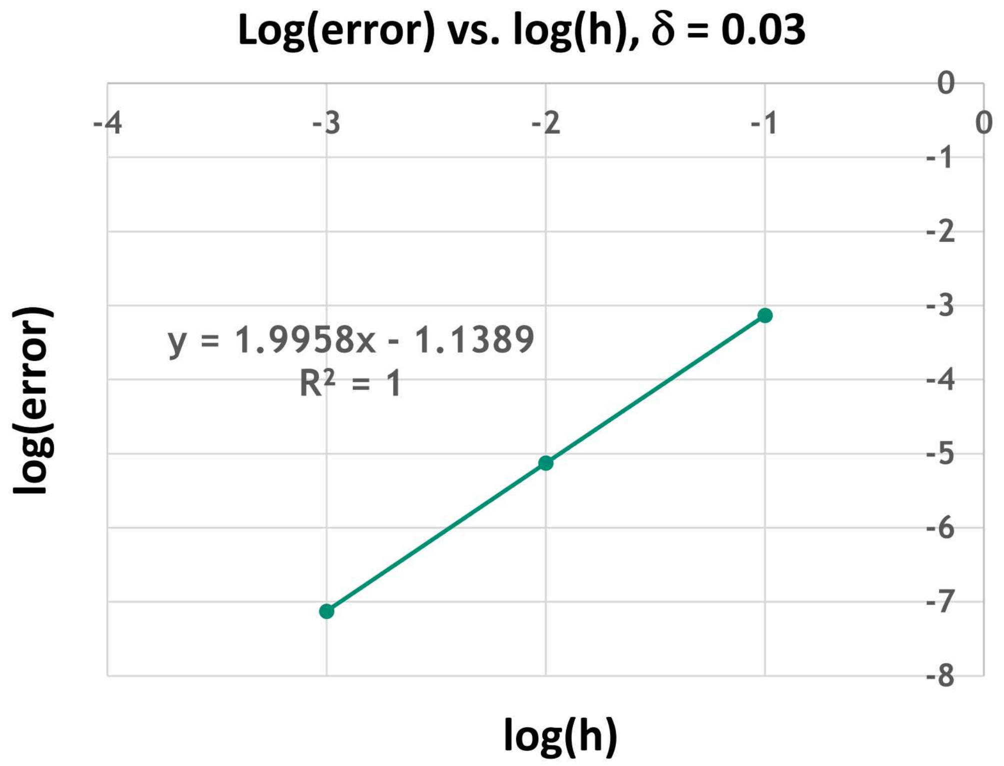
* X. Tian and Q. Du, Asymptotically compatible schemes and applications to robust discretization of nonlocal models. *SIAM J. Numer. Anal.* 52, 1641–1665, 2014.

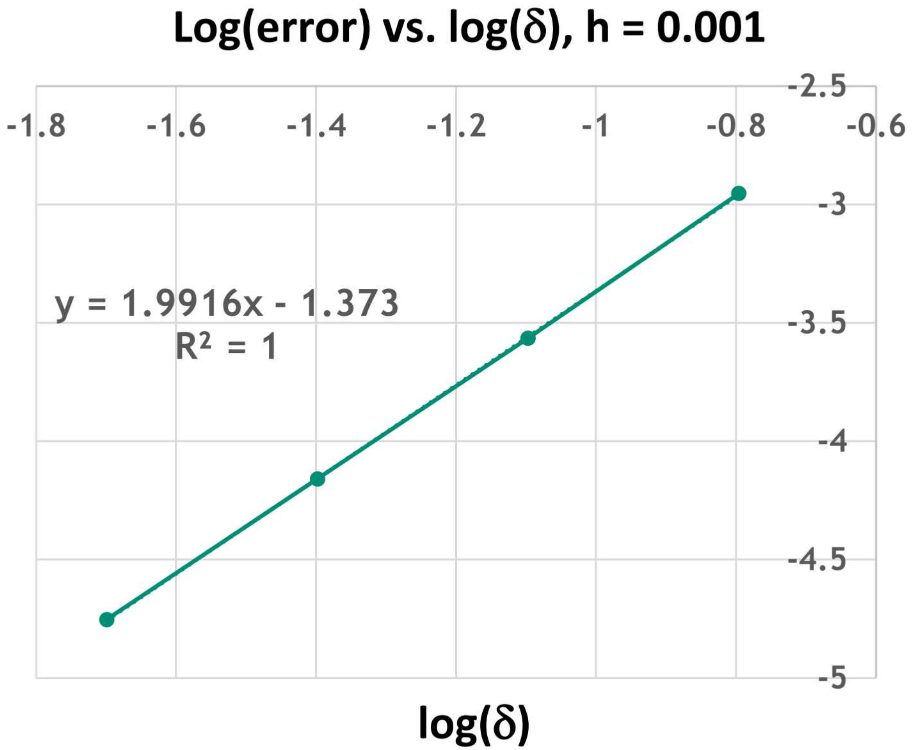
Nonlocal Neumann Boundary Condition: Computation

- **Nonlocal Poisson's equation with nonlocal Neumann boundary conditions (homogeneous)**
- **Piecewise linear DG**

$$-\mathcal{L}[u](x) = f(x), \quad x \in \Omega$$

$$\mathcal{N}[\mathcal{G}u](x) = 0, \quad x \in \Gamma$$





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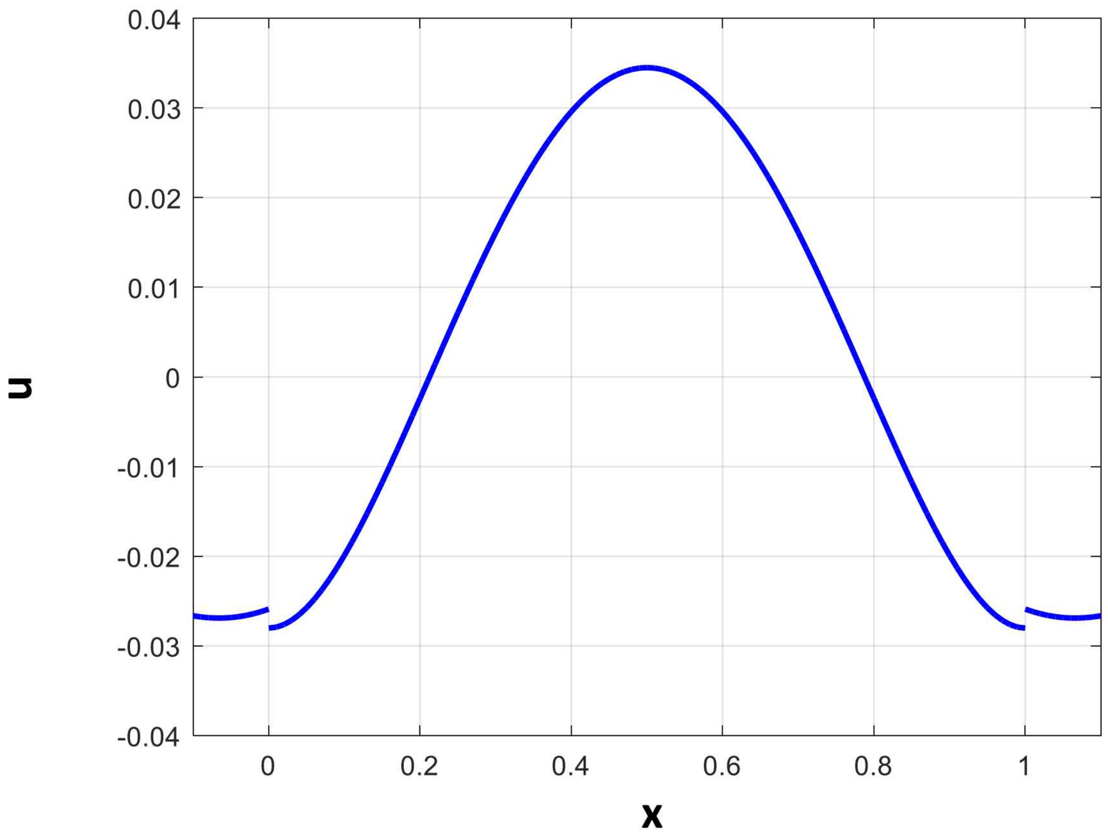

Conclusions

- ❑ **Demonstrated nonlocal Neumann boundary condition derived from energy principle**

- ❑ **Advantages**
  - ❑ **No need to determine u(x) in nonlocal boundary**
  - ❑ **Consistent with local Neumann boundary condition**
  - ❑ **Implement and apply just like a local boundary condition**

- ❑ **Questions?**