

Connecting peridynamic models and coupling local and nonlocal systems

Pablo Seleson

Collaborators: Max Gunzburger (FSU) and Michael L. Parks (Sandia)

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Outline

- 1 Overview of peridynamics
- 2 Connecting peridynamic models
- 3 The role of influence functions
- 4 Coupling local/nonlocal systems

Part I: Overview of peridynamics

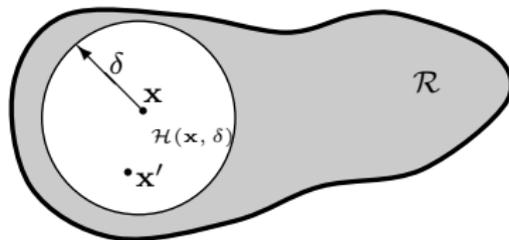
What is peridynamics (PD)?*

Generalized **continuum** theory with an integral formulation,
that employs **nonlocal** model of force interaction

$$\rho(\mathbf{x}) \frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x}, t) = \int_{\mathcal{R}} \{ \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle \} dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t)$$

Model features

- 1 Continuum model
- 2 Integral formulation
- 3 Nonlocal model



The neighborhood: $\mathcal{H}(\mathbf{x}, \delta) := \{ \mathbf{x}' \in \mathcal{R} : \|\mathbf{x}' - \mathbf{x}\| \leq \delta \}$

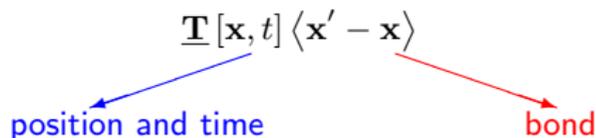
$$\underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = \mathbf{0}, \text{ for } \|\mathbf{x}' - \mathbf{x}\| > \delta$$

* S. A. Silling, J. Mech. Phys. Solids, 48 (2000), pp. 175–209.

State-based PD model (multibody interactions)*

$$\rho(\mathbf{x}) \frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x}, t) = \int_{\mathcal{H}(\mathbf{x}, \delta)} \{ \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle \} dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t)$$

$\underline{\mathbf{T}}[\mathbf{x}', t]$ is a general transformation, occurring at point \mathbf{x} at time t , applied to the bond $\langle \mathbf{x}' - \mathbf{x} \rangle$.



$\underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle$:

- mapping the bond $\langle \mathbf{x}' - \mathbf{x} \rangle$ to force density per volume
- contains constitutive relationship
- vanishes outside some horizon (like MD cutoff radius)

* S. A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, J. Elasticity, 88 (2007), pp. 151–184.

Deformation

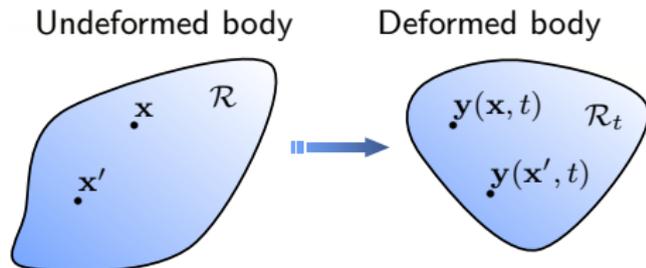
Definitions:

- \mathbf{x} : *reference* position
- \mathbf{y} : *current* position
- \mathbf{u} : displacement

$$\mathbf{y}(\mathbf{x}', t) = \mathbf{x} + \mathbf{u}(\mathbf{x}', t)$$

$$\mathbf{y}(\mathbf{x}, t) = \mathbf{x} + \mathbf{u}(\mathbf{x}, t)$$

$$\begin{aligned} \mathbf{y}(\mathbf{x}', t) - \mathbf{y}(\mathbf{x}, t) &= (\mathbf{x}' - \mathbf{x}) + \mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t) \\ &= \underbrace{(\mathbf{I} + \nabla \mathbf{u}(\mathbf{x}, t))}_{\text{deformation gradient}} (\mathbf{x}' - \mathbf{x}) + O(\|\mathbf{x}' - \mathbf{x}\|^2) \end{aligned}$$



Deformation gradient is a local linear approximation of the true deformation

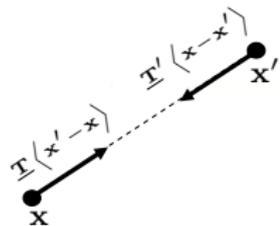
Notation: $\mathbf{y}' := \mathbf{y}(\mathbf{x}', t)$; $\mathbf{y} := \mathbf{y}(\mathbf{x}, t)$; $\mathbf{u}' := \mathbf{u}(\mathbf{x}', t)$; $\mathbf{u} := \mathbf{u}(\mathbf{x}, t)$

Bond-based PD model (pairwise interactions)

Ordinary material

$$\underline{\mathbf{T}} = \underline{t} \underline{\mathbf{M}},$$

$$\underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = \underbrace{\underline{t}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle}_{\text{scalar-valued}} \underbrace{\frac{\mathbf{y}' - \mathbf{y}}{|\mathbf{y}' - \mathbf{y}|}}_{\text{bond direction}}$$



Let choose*

$$\underline{t}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = \frac{1}{2} \kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x})$$

$$\rho(\mathbf{x}) \frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x}, t) = \int_{\mathcal{H}(\mathbf{x}, \delta)} \kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t)$$

Bond-based PD is a special case of state-based PD

* S. A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, J. Elasticity, 88 (2007), pp. 151–184.

Chronology of some PD models

- 1 2000: Bond-based PD model*
→ pairwise interactions in PD
- 2 2000: EAM-like PD model¹
→ generalization of bond-based PD models
(based on the embedded-atom model (EAM))
- 3 2005: Prototype microelastic brittle (PMB) model[†]
→ bond-based PD constitutive model
- 4 2007: State-based PD model[‡]
→ the most general PD model
- 5 2007: Linear peridynamic solid (LPS) model³
→ state-based PD constitutive model

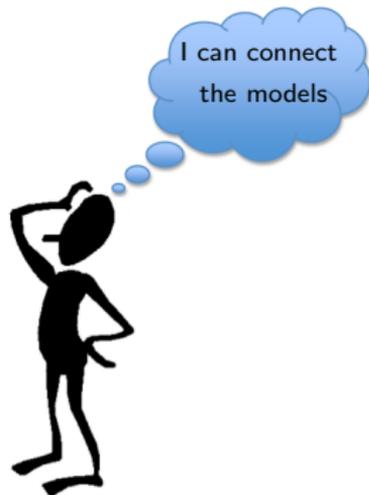
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Part II: Connecting peridynamic models

EAM-like PD model

Macroelastic energy density:

$$\widehat{W}(\mathbf{x}, t) = \underbrace{E(\vartheta(\mathbf{x}, t))}_{\text{multibody}} + \underbrace{W(\mathbf{x}, t)}_{\text{pairwise}}$$

Weighted deformed
volume

$$\vartheta(\mathbf{x}, t) = \int_{\mathcal{R}} j(\|\mathbf{x}' - \mathbf{x}\|) \|\mathbf{y}' - \mathbf{y}\| dV_{\mathbf{x}'}$$

Macroscopic pairwise
energy density

$$W(\mathbf{x}, t) = \frac{1}{2} \int_{\mathcal{R}} w(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) dV_{\mathbf{x}'}$$

EAM-like PD model

Macroelastic energy density:

$$\widehat{W}(\mathbf{x}, t) = E(\vartheta(\mathbf{x}, t)) + W(\mathbf{x}, t)$$

multibody
pairwise

Weighted deformed
volume

$$\vartheta(\mathbf{x}, t) = \int_{\mathcal{R}} j(\|\mathbf{x}' - \mathbf{x}\|) \|\mathbf{y}' - \mathbf{y}\| dV_{\mathbf{x}'}$$

Macroscopic pairwise
energy density

$$W(\mathbf{x}, t) = \frac{1}{2} \int_{\mathcal{R}} w(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) dV_{\mathbf{x}'}$$

EAM-like PD equation of motion:

$$\rho(\mathbf{x}) \frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x}, t) = \int_{\mathcal{H}(\mathbf{x}, \delta)} \left[-(P(\mathbf{x}', t) + P(\mathbf{x}, t)) j(\|\mathbf{x}' - \mathbf{x}\|) + \kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) \right] \frac{\mathbf{y}' - \mathbf{y}}{\|\mathbf{y}' - \mathbf{y}\|} dV_{\mathbf{x}'}$$

$$+ \mathbf{b}(\mathbf{x}, t)$$

$$P(\mathbf{x}, t) = -\frac{dE}{d\vartheta}(\vartheta(\mathbf{x}, t))$$

EAM-like: a state-based PD model

Choose

$$\underline{t}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = -P(\mathbf{x}, t) j(\|\mathbf{x}' - \mathbf{x}\|) + \frac{1}{2} \kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x})$$

and assume an ordinary material, i.e., $\underline{\mathbf{T}} = \underline{t} \underline{\mathbf{M}}$, then

$$\rho(\mathbf{x}) \frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x}, t) = \int_{\mathcal{H}(\mathbf{x}, \delta)} \{ \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle \} dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t)$$

EAM-like PD is a particular state-based PD model

$$P(\mathbf{x}', t) \equiv 0 \Rightarrow \underline{t}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = \frac{1}{2} \kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) \text{ (bond-based PD)}$$

If volume-dependent part vanishes we recover a pairwise interaction

LPS : An EAM-like PD model

$$\underline{t}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = -P(\mathbf{x}, t) j(\|\mathbf{x}' - \mathbf{x}\|) + \frac{1}{2} \kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x})$$

$$P(\mathbf{x}, t) = -\frac{dE}{d\vartheta}(\vartheta(\mathbf{x}, t)); \quad \vartheta(\mathbf{x}, t) = \int_{\mathcal{R}} j(\|\mathbf{x}' - \mathbf{x}\|) \|\mathbf{y}' - \mathbf{y}\| dV_{\mathbf{x}'}$$

Let

Weighted volume (1) $m := \int_{\mathcal{R}} \underline{\omega} \langle \mathbf{x}' - \mathbf{x} \rangle \|\mathbf{x}' - \mathbf{x}\|^2 dV_{\mathbf{x}'}$

LPS : An EAM-like PD model

$$\underline{t}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = -P(\mathbf{x}, t) j(\|\mathbf{x}' - \mathbf{x}\|) + \frac{1}{2} \kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x})$$

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Let

Weighted volume (1) $m := \int_{\mathcal{R}} \underline{\omega} \langle \mathbf{x}' - \mathbf{x} \rangle \|\mathbf{x}' - \mathbf{x}\|^2 dV_{\mathbf{x}'}$

Influence function (2) $\underline{\omega} \langle \mathbf{x}' - \mathbf{x} \rangle = \frac{j(\|\mathbf{x}' - \mathbf{x}\|)}{\|\mathbf{x}' - \mathbf{x}\|} \Rightarrow \boxed{m = \vartheta(\mathbf{x}, 0)}$

LPS : An EAM-like PD model

$$\underline{t}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = -P(\mathbf{x}, t) j(\|\mathbf{x}' - \mathbf{x}\|) + \frac{1}{2} \kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x})$$

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(3) $E(\vartheta) = \frac{3K-5G}{m} \left(\frac{3}{m} \frac{\vartheta^2}{2} - 3\vartheta + C \right); \quad K, G : \text{bulk, shear modulus}$

$$\Rightarrow P(\mathbf{x}, t) = -\frac{3K-5G}{m} \left(\frac{3}{m} \vartheta(\mathbf{x}, t) - 3 \right)$$

LPS : An EAM-like PD model

$$\underline{t}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = -P(\mathbf{x}, t) j(\|\mathbf{x}' - \mathbf{x}\|) + \frac{1}{2} \kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x})$$

$$P(\mathbf{x}, t) = -\frac{dE}{d\vartheta}(\vartheta(\mathbf{x}, t)); \quad \vartheta(\mathbf{x}, t) = \int_{\mathcal{R}} j(\|\mathbf{x}' - \mathbf{x}\|) \|\mathbf{y}' - \mathbf{y}\| dV_{\mathbf{x}'}$$

Let

Weighted volume (1) $m := \int_{\mathcal{R}} \underline{\omega} \langle \mathbf{x}' - \mathbf{x} \rangle \|\mathbf{x}' - \mathbf{x}\|^2 dV_{\mathbf{x}'}$

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$$\Rightarrow P(\mathbf{x}, t) = -\frac{3K-5G}{m} \left(\frac{3}{m} \vartheta(\mathbf{x}, t) - 3 \right)$$

(4) $\kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) = \frac{30G}{m} j(\|\mathbf{x}' - \mathbf{x}\|) s(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x})$

Stretch

$$s(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) := \frac{\|\mathbf{y}' - \mathbf{y}\| - \|\mathbf{x}' - \mathbf{x}\|}{\|\mathbf{x}' - \mathbf{x}\|}$$

LPS : An EAM-like PD model

We define the *dilatation*

$$\theta[\mathbf{x}, t] = \frac{3}{m} \int_{\mathcal{R}} \omega \langle \mathbf{x}' - \mathbf{x} \rangle \|\mathbf{x}' - \mathbf{x}\| \underline{e}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle dV_{\mathbf{x}'}$$

with extension $\underline{e}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = \|\mathbf{y}' - \mathbf{y}\| - \|\mathbf{x}' - \mathbf{x}\|$
 and deviatoric part

$$\underline{e}^d[\mathbf{x}, t] = \underline{e}[\mathbf{x}, t] - \frac{\theta[\mathbf{x}, t] \|\mathbf{x}' - \mathbf{x}\|}{3} = \underline{e}[\mathbf{x}, t] - \underline{e}^i[\mathbf{x}, t]$$

We obtain:

$$\boxed{\theta[\mathbf{x}, t] = \frac{3}{m} \vartheta(\mathbf{x}, t) - 3} \Rightarrow P(\mathbf{x}, t) = -\frac{3K - 5G}{m} \theta[\mathbf{x}, t].$$

LPS : An EAM-like PD model

We define the *dilatation*

$$\theta[\mathbf{x}, t] = \frac{3}{m} \int_{\mathcal{R}} \underline{\omega} \langle \mathbf{x}' - \mathbf{x} \rangle \|\mathbf{x}' - \mathbf{x}\| \underline{e}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle dV_{\mathbf{x}'}$$

with extension $\underline{e}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = \|\mathbf{y}' - \mathbf{y}\| - \|\mathbf{x}' - \mathbf{x}\|$
 and deviatoric part

$$\underline{e}^d[\mathbf{x}, t] = \underline{e}[\mathbf{x}, t] - \frac{\theta[\mathbf{x}, t] \|\mathbf{x}' - \mathbf{x}\|}{3} = \underline{e}[\mathbf{x}, t] - \underline{e}^i[\mathbf{x}, t]$$

We obtain:

$$\boxed{\theta[\mathbf{x}, t] = \frac{3}{m} \vartheta(\mathbf{x}, t) - 3} \Rightarrow P(\mathbf{x}, t) = -\frac{3K - 5G}{m} \theta[\mathbf{x}, t].$$

Let $\alpha := \frac{15G}{m}$ and $\underline{x} \langle \mathbf{x}' - \mathbf{x} \rangle := \mathbf{x}' - \mathbf{x}$

$$\underline{t} = \frac{3K\theta}{m} \underline{\omega} \underline{x} + \alpha \underline{\omega} \underline{e}^d$$

$$\theta[\mathbf{x}, t] = 3 \left(\frac{\vartheta(\mathbf{x}, t)}{\vartheta(\mathbf{x}, 0)} - 1 \right)$$

LPS is an EAM-like model; we related their volume-dependent variables

PMB : an LPS model

LPS force scalar state

$$\underline{t} = \frac{3K\theta}{m} \underline{\omega} \underline{x} + \alpha \underline{\omega} \underline{e}^d$$

Assume a Poisson's ratio $\nu = 1/4$, then $G = \frac{3}{5}K$ and we can write

$$\underline{t} = \frac{9K}{m} \underline{\omega} \underline{e}$$

Let an influence function be

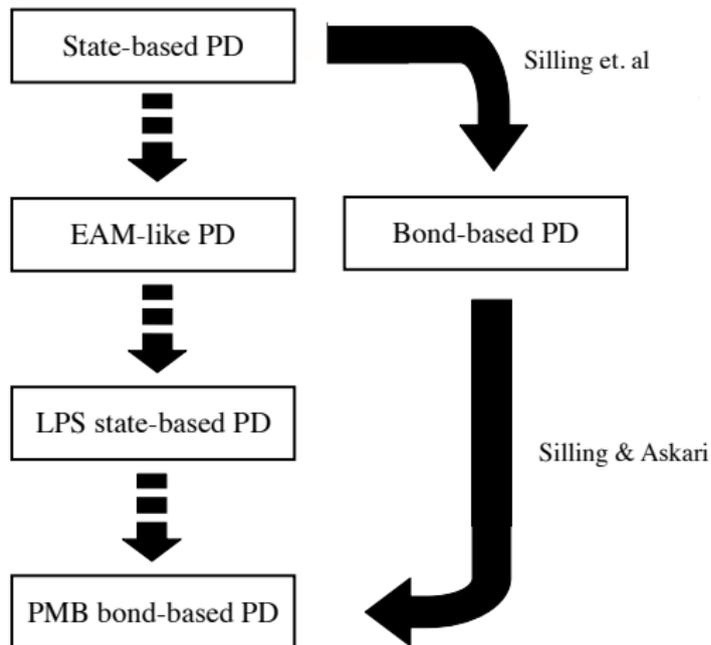
$$\underline{\omega} \langle \mathbf{x}' - \mathbf{x} \rangle = \begin{cases} \frac{1}{\|\mathbf{x}' - \mathbf{x}\|} & \|\mathbf{x}' - \mathbf{x}\| \leq \delta \\ 0 & \text{otherwise} \end{cases}$$

$$\kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) = c s(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x})$$

with $c = \left(\frac{18K}{\pi\delta^4}\right)$, s the stretch, and $\kappa(\cdot, \cdot) = 0$ for $\|\mathbf{x}' - \mathbf{x}\| > \delta$

PMB is an LPS model for $\nu = 1/4$ and particular influence function

Summary of part II: hierarchy of PD models*



* Silling et al. : S. A. Silling, M. Epton, O. Weckner, J.Xu, and E. Askari, *J. Elasticity*, 88 (2007), pp. 151–184.
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Part III

The role of influence functions

What is an influence function?

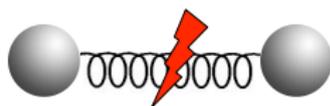
An influence function is a nonnegative scalar state $\underline{\omega}$ defined on $\mathcal{H}(\mathbf{x}, \delta)$. If $\underline{\omega}$ depends only upon $\|\mathbf{x}' - \mathbf{x}\|$, then is a *spherical* influence function.

What are influence functions used for?



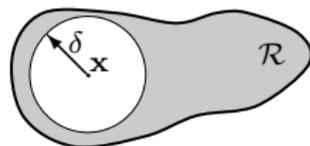
Breaking bonds

$$\underline{\omega}(\mathbf{x}' - \mathbf{x}) = \begin{cases} 1 & \text{stretch}(\mathbf{x}', \mathbf{x}) \leq s_0, \\ 0 & \text{otherwise.} \end{cases}$$



Imposing cutoff radius

$$\underline{\omega}(\mathbf{x}' - \mathbf{x}) = \begin{cases} 1 & \|\mathbf{x}' - \mathbf{x}\| \leq \delta, \\ 0 & \text{otherwise.} \end{cases}$$



Both implement only boolean variables

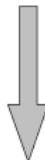
Beyond boolean variables

EAM-like PD Model



$$\underline{\omega} \langle \mathbf{x}' - \mathbf{x} \rangle = \frac{j \left(\|\mathbf{x}' - \mathbf{x}\| \right)}{\|\mathbf{x}' - \mathbf{x}\|}$$

LPS State-Base PD Model



$$\underline{\omega} \langle \mathbf{x}' - \mathbf{x} \rangle = \begin{cases} \frac{1}{\|\mathbf{x}' - \mathbf{x}\|} & \|\mathbf{x}' - \mathbf{x}\| \leq \delta \\ 0 & \text{otherwise} \end{cases}$$

PMB Bond-Base PD Model



What would be the effect of using more general influence functions?

Generalized PMB (GPMB) models

Linear peridynamic solid (LPS) force scalar state

$$\underline{t} = \frac{3K\theta}{m} \underline{\omega} \underline{x} + \alpha \underline{\omega} \underline{e}^d$$

Assume a Poisson's ratio $\nu = 1/4$, then $G = \frac{3}{5}K$ and we can write

$$\underline{t} = \frac{9K}{m} \underline{\omega} \underline{e}$$

Let an influence function be

$$\underline{\omega} \langle \mathbf{x}' - \mathbf{x} \rangle = \begin{cases} \frac{\omega_g(\|\mathbf{x}' - \mathbf{x}\|)}{\|\mathbf{x}' - \mathbf{x}\|} & \|\mathbf{x}' - \mathbf{x}\| \leq \delta \\ 0 & \text{otherwise} \end{cases}$$

$$\kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) = c_g s(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) \omega_g(\|\mathbf{x}' - \mathbf{x}\|)$$

with c_g a constant, s the stretch, and $\kappa(\cdot, \cdot) = 0$ for $\|\mathbf{x}' - \mathbf{x}\| > \delta$

We develop a family of GPMB models; all are special cases of LPS

Generalized PMB (GPMB) models

The following relations hold

$$\left\{ \begin{array}{l} \kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) = c_g s(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) \omega_g(\|\mathbf{x}' - \mathbf{x}\|), \\ w(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) = \frac{1}{2} c_g s(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x})^2 \|\mathbf{x}' - \mathbf{x}\| \omega_g(\|\mathbf{x}' - \mathbf{x}\|), \\ c_g = \frac{18K}{\int_{\mathcal{H}(\mathbf{0}, \delta)} \|\boldsymbol{\xi}\| \omega_g(\|\boldsymbol{\xi}\|) dV_{\boldsymbol{\xi}}}, \\ \underline{\omega} \langle \mathbf{x}' - \mathbf{x} \rangle = \frac{\omega_g(\|\mathbf{x}' - \mathbf{x}\|)}{\|\mathbf{x}' - \mathbf{x}\|}. \end{array} \right.$$

Note that:

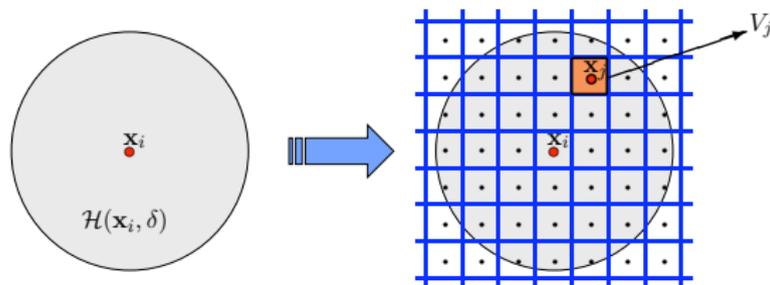
- c_g is found matching energy densities to classical elasticity.
- this influence function allows to connect GPMB to LPS.
- $\kappa(\boldsymbol{\eta}, \boldsymbol{\xi}) = \frac{\partial w}{\partial \boldsymbol{\eta}}(\boldsymbol{\eta}, \boldsymbol{\xi})$.

Particle-type discretization of PD

Given the PD equation of motion

$$\rho(\mathbf{x}) \frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x}, t) = \int_{\mathcal{H}(\mathbf{x}, \delta)} \kappa(\mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t), \mathbf{x}' - \mathbf{x}) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t)$$

we discretize the body \mathcal{R} into particles forming a cubic lattice



to get

$$\rho_i \frac{d^2 \mathbf{u}_i}{dt^2} = \sum_{j \in \mathcal{F}_i} \kappa(\mathbf{u}_j - \mathbf{u}_i, \mathbf{x}_j - \mathbf{x}_i) V_j + \mathbf{b}_i$$

$$\mathcal{F}_i = \{j : \|\mathbf{x}_j - \mathbf{x}_i\| \leq \delta, j \neq i\}$$

Example 1: 1D wave propagation for GPMB

We choose

$$\omega_g(|x' - x|) := \begin{cases} \left(\frac{1}{|x' - x| + \varepsilon} \right)^p & |x' - x| \leq \delta \\ 0 & \text{otherwise} \end{cases}$$

with ε a smoothing length. The PD equation of motion is

$$\rho(x) \frac{\partial^2 u}{\partial t^2}(x, t) = \int_{x-\delta}^{x+\delta} \kappa(u' - u, x' - x) dx' + b(x, t)$$

with

$$\kappa(u' - u, x' - x) = \frac{\gamma_p}{|x' - x|} (u' - u) \left(\frac{1}{|x' - x| + \varepsilon} \right)^p$$

We want to investigate how p affects the model behavior

Example 1: 1D wave propagation for GPMB

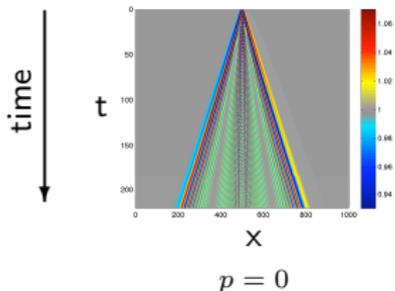
$$\begin{aligned}\Omega &= (0, 1000) \\ \Delta x &= 0.25 \\ \rho &= 1 \\ \delta &= 5 \\ \varepsilon &= 1 \\ \Delta t &= 0.1 \\ T &= [0, 220] \\ K &= 1\end{aligned}$$

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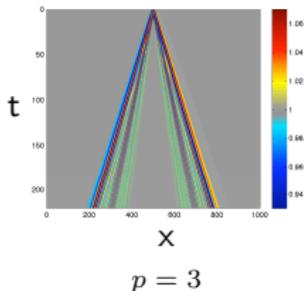
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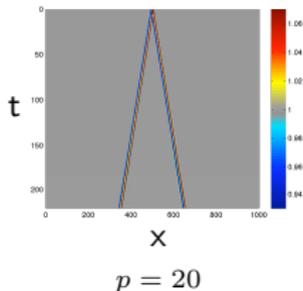
x
 $p = 0$



x
 $p = 3$



x
 $p = 20$



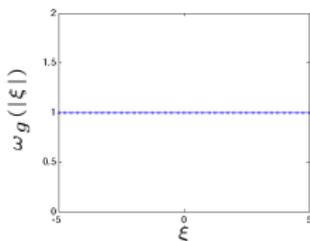
Plot style
from A/G*

The larger the value of p the less dispersive the wave

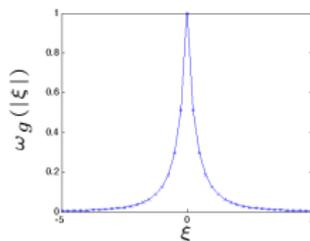
* M. Arndt and M. Griebel, Multiscale Model. Simul., 4 (2005), pp. 531–562.

Example 1: 1D wave propagation for GPMB

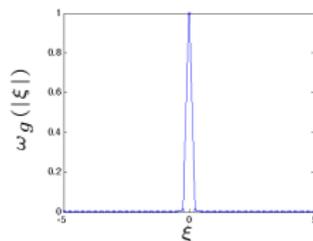
$$\omega_g(|x' - x|) := \begin{cases} \left(\frac{1}{|x' - x| + \varepsilon} \right)^p & |x' - x| \leq \delta \\ 0 & \text{otherwise} \end{cases}$$



(a) $p = 0$



(b) $p = 3$



(c) $p = 20$

The larger the value of p the more singular the influence function

Example 1: 1D wave propagation for GPMB

The dispersion relation for the GPMB model is

$$\Omega_p^2(k) = \frac{9K}{5\rho} k^2 \left[1 - \frac{2}{4!} \frac{I_{\delta,\varepsilon}(p, 3)}{I_{\delta,\varepsilon}(p, 1)} k^2 + \frac{2}{6!} \frac{I_{\delta,\varepsilon}(p, 5)}{I_{\delta,\varepsilon}(p, 1)} k^4 + \dots \right]$$

with

$$I_{\delta,\varepsilon}(p, n) := \int_0^\delta \xi^n \left(\frac{1}{\xi + \varepsilon} \right)^p d\xi$$

We compute the coefficients $\frac{2}{(n+1)!} \frac{I_{\delta,\varepsilon}(p, n)}{I_{\delta,\varepsilon}(p, 1)}$ for $\varepsilon = 1$ and $\delta = 5$

p	$n = 1$	$n = 3$	$n = 5$
0	1.00e+00	1.042e+00	5.787e-01
3	1.00e+00	3.933e-01	1.594e-01
5	1.00e+00	1.225e-01	3.126e-02
20	1.00e+00	1.838e-03	5.836e-06
100	1.00e+00	5.369e-05	4.009e-09
1000	1.00e+00	5.035e-07	3.394e-13

The larger the value of p the smaller the higher-order coefficients

Example 2: 3D fracture dynamics for GPMB

Choose the scalar force function

$$\kappa(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) = \gamma_p^{(3d)} s(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) \omega_g(\|\mathbf{x}' - \mathbf{x}\|),$$

with

$$\omega_g(t, \mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) = \begin{cases} \left(\frac{1}{\|\mathbf{x}' - \mathbf{x}\| + \varepsilon} \right)^p \mu(t, \mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) & \|\mathbf{x}' - \mathbf{x}\| \leq \delta \\ 0 & \text{otherwise} \end{cases}$$

the function μ is boolean with nonzero value for unbroken bonds.

The function ω_g has three roles:

- Define the neighborhood $\mathcal{H}(\mathbf{x}, \delta)$.
- Implement bond-breaking mechanism.
- Modulate the strength of nonlocal interactions.

Example 2: 3D fracture dynamics for GPMB

Damage at a point \mathbf{x} :*

$$\varphi(\mathbf{x}, t) = 1 - \frac{\int_{\mathcal{H}(\mathbf{x}, \delta)} \mu(t, \mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) dV_{\mathbf{x}'}}{\int_{\mathcal{H}(\mathbf{x}, \delta)} dV_{\mathbf{x}'}}$$

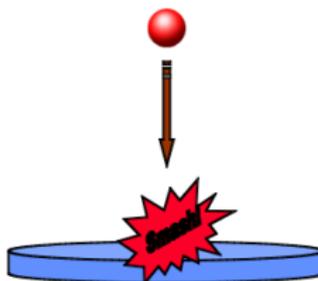
where $0 \leq \varphi(\mathbf{x}, t) \leq 1$

- Damage of zero corresponds to pristine material
- Maximum sustainable damage is one

* S. A. Silling and E. Askari, *Comp. Struct.*, 83 (2005), pp. 1526–1535.

Example 2: 3D fracture dynamics for GPMB

PD in LAMMPS * (<http://lammps.sandia.gov>)



<ul style="list-style-type: none"> ● Projectile <ul style="list-style-type: none"> - Sphere: diameter 10 mm 	<ul style="list-style-type: none"> ● Disc <ul style="list-style-type: none"> - diameter 74 mm - thickness 2.5 mm
<ul style="list-style-type: none"> ● Target Material <ul style="list-style-type: none"> - Bulk modulus 14.9 GPa - Density 2200 kg/m³ - Horizon 1.5 mm 	<ul style="list-style-type: none"> Discretization <ul style="list-style-type: none"> - Mesh spacing 0.5 mm - 100,000 particles - 0.15 msec

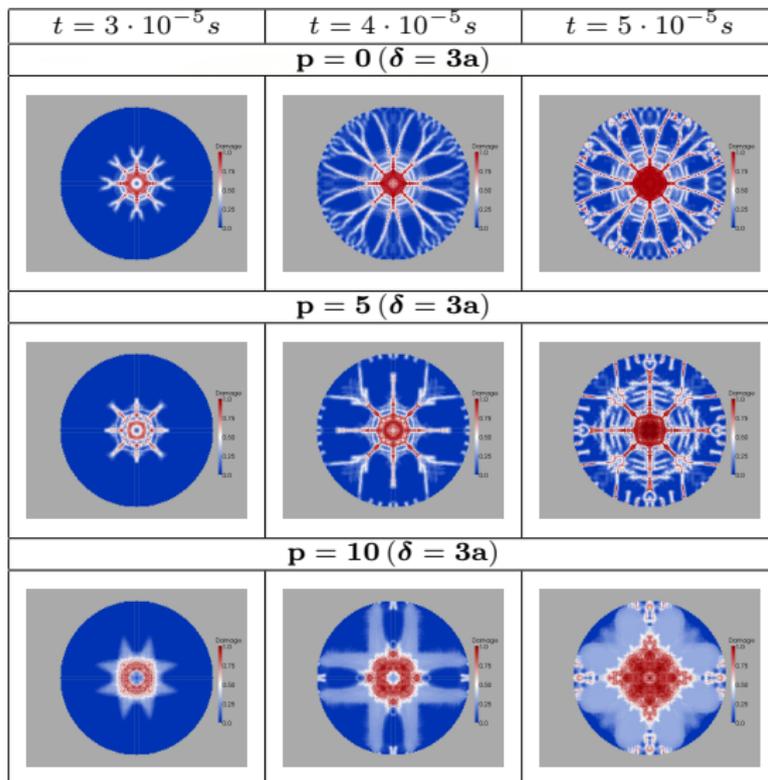
* M. L. Parks, R. B. Lehoucq, S. J. Plimpton, and S. A. Silling, *Comp. Phys. Comm.*, 179 (2008), pp. 777–783
S. A. Silling and E. Askari, *Comp. Struct.*, 83 (2005), pp. 1526–1535.

Example 2: 3D fracture dynamics for GPMB

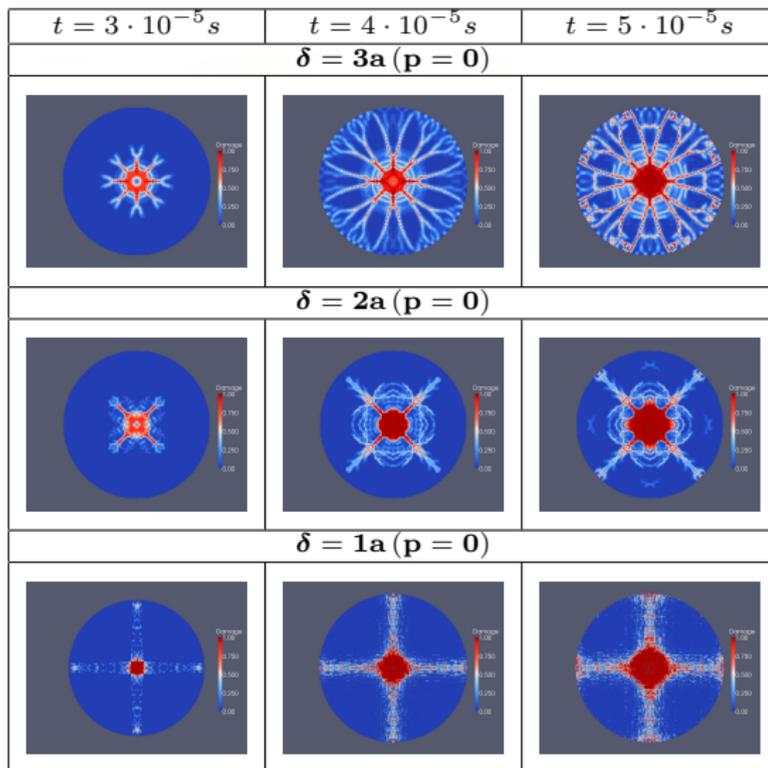
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Impact on a disc of brittle material

Example 2: 3D fracture dynamics (p-dependence)



Example 2: 3D fracture dynamics (δ -dependence)



Calibration and validation

- Use PD influence functions is unexplored in nonlocal modeling.
- Influence functions enable a rich spectrum of behavior in nonlocal dynamical systems, even when the peridynamic horizon is fixed.
- **Question 1: Which influence function should be used?**



Calibration and validation

Summary of part III

Explored role of influence functions within PD theory:

- 1 Influence functions can be used to:
 - connect peridynamic models,
 - break bonds,
 - impose a finite interaction range.
- 2 Influence functions can modulate nonlocal interactions
- 3 Demonstrate by numerical experiments:
 - wave propagation in 1D,
 - fracture dynamics in 3D.

Part IV

Coupling local/nonlocal systems

Some motivation ...

This part is motivated by the **multiscale implementation** of PD. PD has a **length scale** δ in contrast to classical mechanics. We can use this property to couple systems with different interactions ranges of which **local/nonlocal coupling** is a special case.

Classical local interface problems

Classical local problem

$$\begin{cases} \mathcal{L}_u^l(\mathbf{x}) = b(\mathbf{x}), & \mathbf{x} \in \Omega \\ u(\mathbf{x}) = 0, & \mathbf{x} \in \partial\Omega \end{cases}$$

$$\mathcal{L}_u^l(\mathbf{x}) := -\nabla \cdot [\mathbf{D}(\mathbf{x})\nabla u(\mathbf{x})]$$

Weak formulation: Given $b(\mathbf{x}) \in L_2(\Omega)$, find $u(\mathbf{x}) \in V^l$ s.t.

$$a_\Omega^l(u, v) = (b, v)_\Omega, \quad \forall v \in V^l$$

$$a_\Omega^l(u, v) := \int_\Omega \nabla v(\mathbf{x}) \cdot (\mathbf{D}(\mathbf{x})\nabla u(\mathbf{x})) d\mathbf{x}$$

$$(u, v)_\Omega := \int_\Omega v(\mathbf{x})u(\mathbf{x})d\mathbf{x}$$

$$V^l := H_0^1 = \{v \in H^1(\Omega) : v|_{\partial\Omega} = 0\}$$

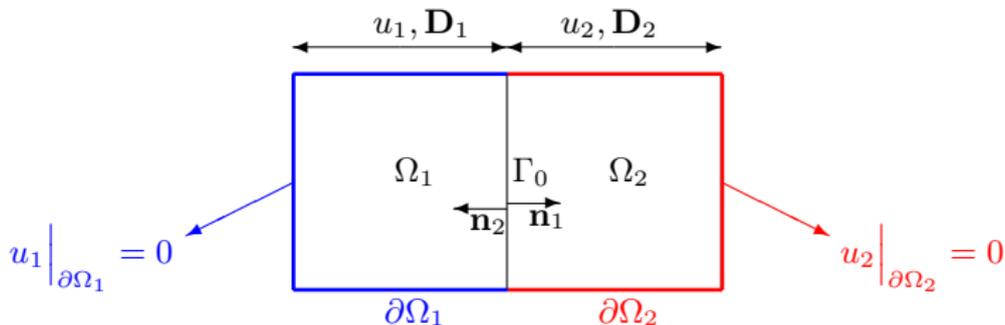
We assume u to be a scalar-valued function

Classical local interface problems

Two-domain formulation

$$\begin{cases} \mathcal{L}_u^{l,(i)}(\mathbf{x}) = b_i(\mathbf{x}), & \mathbf{x} \in \Omega_i \\ u_i(\mathbf{x}) = 0, & \mathbf{x} \in \partial\Omega_i \end{cases}; \quad i = 1, 2$$

$$\mathcal{L}_u^{l,(i)}(\mathbf{x}) := -\nabla \cdot [\mathbf{D}_i(\mathbf{x}) \nabla u_i(\mathbf{x})]$$

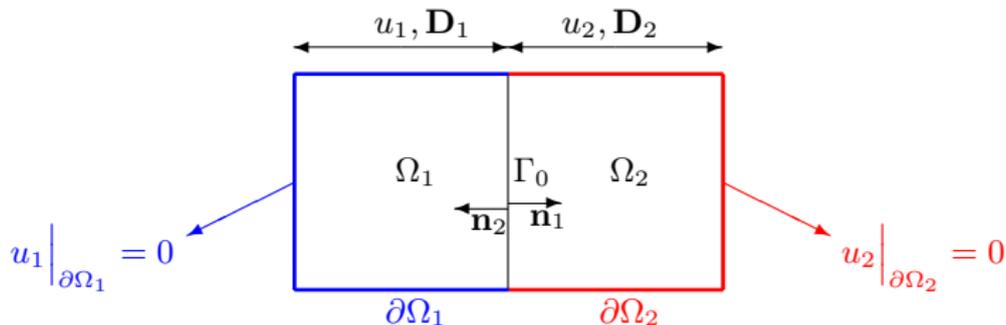


Classical local interface problems

Two-domain formulation

$$\begin{cases} \mathcal{L}_u^{l,(i)}(\mathbf{x}) = b_i(\mathbf{x}), & \mathbf{x} \in \Omega_i \\ u_i(\mathbf{x}) = 0, & \mathbf{x} \in \partial\Omega_i \end{cases}; \quad i = 1, 2$$

$$\mathcal{L}_u^{l,(i)}(\mathbf{x}) := -\nabla \cdot [\mathbf{D}_i(\mathbf{x}) \nabla u_i(\mathbf{x})]$$



What are the conditions on the interface Γ_0 that make subdomain solutions identical to one-domain solution? \rightarrow transmission conditions



Classical local interface problems

Two-domain formulation

Weak formulation: Given $b_i(\mathbf{x}) \in L_2(\Omega_i)$, find $u_i(\mathbf{x}) \in V_i^l$ s.t.

$$a_{\Omega_i}^{l,(i)}(u_i, v_i) = (b_i, v_i)_{\Omega_i} + \lambda_{\Gamma_0}^{l,(i)}(u_i, v_i), \quad \forall v_i \in V_i^l, i = 1, 2$$

Local flux

$$a_{\Omega}^{l,(i)}(u, v) := \int_{\Omega} \nabla v(\mathbf{x}) \cdot (\mathbf{D}_i(\mathbf{x}) \nabla u(\mathbf{x})) d\Omega$$

$$\lambda_{\Gamma}^{l,(i)}(u, v) := \int_{\Gamma} v(\mathbf{x}) (\mathbf{D}_i(\mathbf{x}) \nabla u(\mathbf{x})) \cdot \mathbf{n}_i dS$$

$$V_i^l := \left\{ v \in H^1(\Omega_i) : v|_{\partial\Omega_i} = 0 \right\}$$

Classical local interface problems

Transmission conditions

- Transmission condition I : “Continuity of the fields”

$$u_1(\mathbf{x}) = u_2(\mathbf{x}), \quad \text{for } \mathbf{x} \in \Gamma_0$$

- Transmission condition II: “Flux balance condition”

$$(\mathbf{D}_1(\mathbf{x})\nabla u_1(\mathbf{x})) \cdot \mathbf{n}_1 = -(\mathbf{D}_2(\mathbf{x})\nabla u_2(\mathbf{x})) \cdot \mathbf{n}_2, \quad \text{for } \mathbf{x} \in \Gamma_0$$

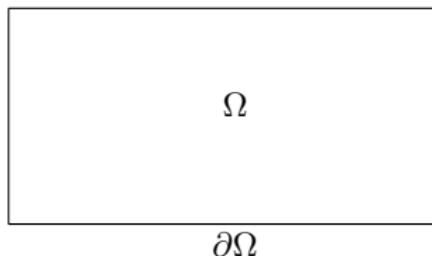
$\left\{ \begin{array}{l} \text{i- add subdomain weak formulations} \\ \text{ii- recover one-domain weak formulation} \end{array} \right. \Rightarrow \text{transmission conditions}$

Nonlocal interface problems

Nonlocal problem *

$$\begin{cases} \mathcal{L}_u^{nl}(\mathbf{x}) = b(\mathbf{x}), & \mathbf{x} \in \Omega \\ u(\mathbf{x}) = 0, & \mathbf{x} \in \mathcal{B}\Omega \end{cases}$$

$$\mathcal{L}_u^{nl}(\mathbf{x}) := -\frac{1}{2} \int_{\overline{\Omega}} \{T(\mathbf{x}', \mathbf{x}) - T(\mathbf{x}, \mathbf{x}')\} d\mathbf{x}'$$



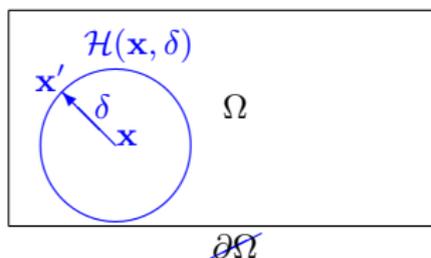
*Based on S. A. Silling, M. Epton, O. Weckner, J.Xu, and E. Askari, J. Elasticity, 88 (2007), pp. 151–184.

Nonlocal interface problems

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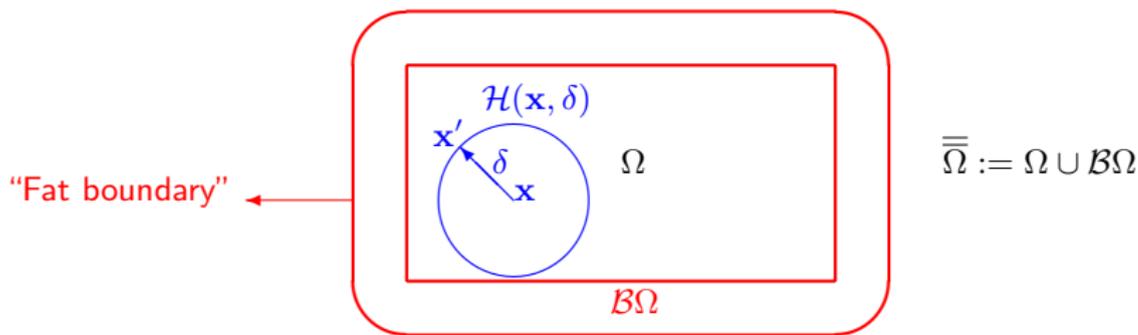
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Nonlocal interface problems

Nonlocal problem *

$$\begin{cases} -\frac{1}{2} \int_{\overline{\Omega}} \{T(\mathbf{x}', \mathbf{x}) - T(\mathbf{x}, \mathbf{x}')\} d\mathbf{x}' = b(\mathbf{x}), & \mathbf{x} \in \Omega \\ u(\mathbf{x}) = 0, & \mathbf{x} \in \mathcal{B}\Omega \end{cases}$$

Some choices for $T(\mathbf{x}', \mathbf{x})$:

- 1 $\underline{T}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = J(\mathbf{x}' - \mathbf{x}) |u(\mathbf{x}', t) - u(\mathbf{x}, t)|^{p-2} (u(\mathbf{x}', t) - u(\mathbf{x}, t))$
 \rightarrow recover spatial operator of nonlocal p -Laplacian equation. †

* Based on S. A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, *J. Elasticity*, 88 (2007), pp. 151–184.

† F. Andreu, J. M. Mazón, J. D. Rossi, and J. Toledo, *SIAM J. Math. Anal.*, 40 (2009), pp. 1815–1851.

Nonlocal interface problems

Nonlocal problem *

$$\begin{cases} -\frac{1}{2} \int_{\overline{\Omega}} \{T(\mathbf{x}', \mathbf{x}) - T(\mathbf{x}, \mathbf{x}')\} d\mathbf{x}' = b(\mathbf{x}), & \mathbf{x} \in \Omega \\ u(\mathbf{x}) = 0, & \mathbf{x} \in \mathcal{B}\Omega \end{cases}$$

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 \rightarrow recover spatial operator of nonlocal p -Laplacian equation. †
- 2 $\underline{T}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = \frac{k(\mathbf{x}', \mathbf{x})}{\rho c \|\mathbf{x}' - \mathbf{x}\|^2} (\theta(\mathbf{x}', t) - \theta(\mathbf{x}, t))$
 \rightarrow recover spatial operator of nonlocal heat transfer equation. ‡

* Based on S. A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, *J. Elasticity*, 88 (2007), pp. 151–184.

† F. Andreu, J. M. Mazón, J. D. Rossi, and J. Toledo, *SIAM J. Math. Anal.*, 40 (2009), pp. 1815–1851.

‡ F. Bobaru & M. Duangpanya, *Int. J. Heat Mass Transfer*, (2010), In press.

Nonlocal interface problems

Nonlocal problem *

$$\begin{cases} -\frac{1}{2} \int_{\overline{\Omega}} \{T(\mathbf{x}', \mathbf{x}) - T(\mathbf{x}, \mathbf{x}')\} d\mathbf{x}' = b(\mathbf{x}), & \mathbf{x} \in \Omega \\ u(\mathbf{x}) = 0, & \mathbf{x} \in \mathcal{B}\Omega \end{cases}$$

Some choices for $T(\mathbf{x}', \mathbf{x})$:

- 1 $\underline{T}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = J(\mathbf{x}' - \mathbf{x}) |u(\mathbf{x}', t) - u(\mathbf{x}, t)|^{p-2} (u(\mathbf{x}', t) - u(\mathbf{x}, t))$
 \rightarrow recover spatial operator of nonlocal p -Laplacian equation. †
- 2 $\underline{T}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = \frac{k(\mathbf{x}', \mathbf{x})}{\rho c \|\mathbf{x}' - \mathbf{x}\|^2} (\theta(\mathbf{x}', t) - \theta(\mathbf{x}, t))$
 \rightarrow recover spatial operator of nonlocal heat transfer equation. ‡
- 3 We choose

$$T(\mathbf{x}', \mathbf{x}) = c(\mathbf{x}', \mathbf{x}) (u(\mathbf{x}') - u(\mathbf{x}))$$

Note: $c(\mathbf{x}', \mathbf{x})$ is not necessarily symmetric.

* Based on S. A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, *J. Elasticity*, 88 (2007), pp. 151–184.

† F. Andreu, J. M. Mazón, J. D. Rossi, and J. Toledo, *SIAM J. Math. Anal.*, 40 (2009), pp. 1815–1851.

‡ F. Bobaru & M. Duangpanya, *Int. J. Heat Mass Transfer*, (2010), In press.

Nonlocal interface problems

Nonlocal problem

Weak formulation: Given $b(\mathbf{x}) \in L_2(\Omega)$, find $u(\mathbf{x}) \in V^{nl}$ s.t.

$$a_{\overline{\Omega}}^{nl}(u, v) = (b, v)_{\overline{\Omega}}, \quad \forall v \in V^{nl}$$

where *

$$a_{\Omega}^{nl}(u, v) := \frac{1}{2} \int_{\Omega} \int_{\Omega} (v(\mathbf{x}') - v(\mathbf{x})) c(\mathbf{x}', \mathbf{x}) (u(\mathbf{x}') - u(\mathbf{x})) d\mathbf{x}' d\mathbf{x}$$

$$(u, v)_{\Omega} := \int_{\Omega} v(\mathbf{x}) u(\mathbf{x}) d\mathbf{x}$$

- V^{nl} depends on the form of $c(\mathbf{x}', \mathbf{x})$, and $v \in V^{nl}$ satisfies $v|_{B\Omega} = 0$
- No assumption of smoothness

*M. Gunzburger and R. B. Lehoucq, Multiscale Model. Simul., 8(5) (2010), pp. 1581–1598.
 B. Aksoylu and M. L. Parks, Applied Mathematics and Computation, (2010). Accepted for publication.
 E. Emmrich and O. Weckner, Commun. Math. Sci., 5(4) (2007), pp. 851–864.

Nonlocal interface problems

Connection to the classical local problem

We need to relate a scalar-valued $c(\mathbf{x}', \mathbf{x})$ to a tensor-valued $\mathbf{D}(\mathbf{x})$

$$c(\mathbf{x} + \boldsymbol{\xi}, \mathbf{x}) = \begin{cases} \gamma_\delta^d \frac{\boldsymbol{\xi} \cdot \mathbf{K}(\mathbf{x}, \boldsymbol{\xi}) \boldsymbol{\xi}}{|\boldsymbol{\xi}|^{2+\alpha}} & |\boldsymbol{\xi}| < \delta, \\ 0 & \text{otherwise} \end{cases},$$

with $\alpha < d + 2$, d the problem dimension, and γ_δ^d a constant

We can relate $\mathbf{K}(\mathbf{x}, \boldsymbol{\xi})$ and $\mathbf{D}(\mathbf{x})$ in the limit $\delta \rightarrow 0$

For simplicity let's assume $\mathbf{K}(\mathbf{x}, \boldsymbol{\xi}) = \mathbf{K}(\mathbf{x})$

Nonlocal interface problems

Convergence to the local problem in strong form

$$-\int_{\overline{\Omega}} c_{\text{sym}}(\mathbf{x}', \mathbf{x}) (u(\mathbf{x}') - u(\mathbf{x})) d\mathbf{x}' = b(\mathbf{x}); \quad c_{\text{sym}}(\mathbf{x}', \mathbf{x}) = \frac{c(\mathbf{x}', \mathbf{x}) + c(\mathbf{x}, \mathbf{x}')}{2}$$

Assume u and \mathbf{K} smooth enough; by Taylor expansion

$$c_{\text{sym}}(\mathbf{x}', \mathbf{x}) = \gamma_{\delta}^d \frac{1}{|\boldsymbol{\xi}|^2} \boldsymbol{\xi} \cdot \left(\mathbf{K}(\mathbf{x}) + \frac{1}{2} \boldsymbol{\xi} \cdot \nabla \mathbf{K}(\mathbf{x}) \right) \boldsymbol{\xi} + O(|\boldsymbol{\xi}|^2)$$

$$\Rightarrow \underbrace{-\nabla \cdot [\mathbf{D}(\mathbf{x}) \nabla u(\mathbf{x})]}_{\text{Classical local problem}} = b(\mathbf{x}) + \text{h.o.t.}$$

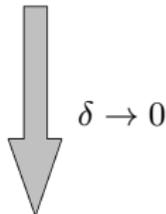
$$\mathbf{D}(\mathbf{x}) = \int_{\mathcal{H}(\mathbf{0}, \delta)} \left[\gamma_{\delta}^d \frac{1}{2|\boldsymbol{\xi}|^{2+\alpha}} (\boldsymbol{\xi} \otimes \boldsymbol{\xi}) \mathbf{K}(\mathbf{x}) (\boldsymbol{\xi} \otimes \boldsymbol{\xi}) \right] dV_{\boldsymbol{\xi}} = \frac{\mathbf{K}(\mathbf{x}, \mathbf{0}) + \mathbf{K}^{\text{T}}(\mathbf{x}, \mathbf{0})}{2} + \frac{1}{2} \text{tr}(\mathbf{K})(\mathbf{x}, \mathbf{0}) \mathbf{I}$$

$$\gamma_{\varepsilon}^1 = \frac{3}{2} \frac{3-\alpha}{\delta^{3-\alpha}}; \quad \gamma_{\varepsilon}^2 = \frac{4}{\pi} \frac{4-\alpha}{\delta^{4-\alpha}}; \quad \gamma_{\varepsilon}^3 = \frac{15}{4\pi} \frac{5-\alpha}{\delta^{5-\alpha}}$$

Nonlocal interface problems

Convergence to the local problem in weak form

$$a_{\overline{\Omega}}^{nl}(u, v) = (b, v)_{\overline{\Omega}}$$



$$a_{\Omega}^l(u, v) = (b, v)_{\Omega}$$

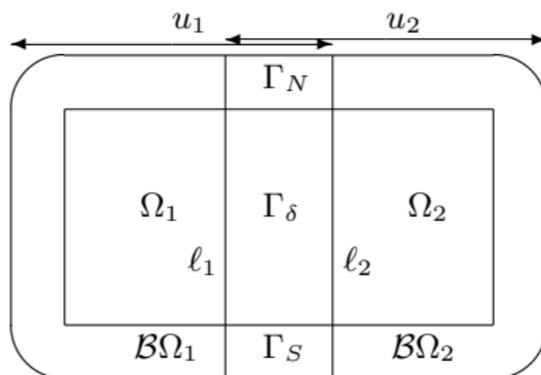
Nonlocal problem \rightarrow Classical local problem, in the limit $\delta \rightarrow 0$

Nonlocal interface problems

Two domain formulation

$$\begin{cases} \mathcal{L}_u^{nl,(i)} = b_i(\mathbf{x}), & \mathbf{x} \in \Omega^{(i)} \\ u_i(\mathbf{x}) = 0, & \mathbf{x} \in \mathcal{B}\Omega^{(i)} \end{cases}$$

$$\begin{aligned} \mathcal{L}_u^{nl,(i)}(\mathbf{x}) = & \int_{\Omega^{(i)} \cup \mathcal{B}\Omega^{(i)}} c_{\text{sym}}(\mathbf{x}', \mathbf{x}) (u_i(\mathbf{x}') - u_i(\mathbf{x})) dV_{\mathbf{x}'} \\ & + \int_{\Omega_j \cup \mathcal{B}\Omega_j} c_{\text{sym}}(\mathbf{x}', \mathbf{x}) (u_j(\mathbf{x}') - u_i(\mathbf{x})) dV_{\mathbf{x}'}, \quad i, j = 1, 2, i \neq j. \end{aligned}$$



$$\Omega^{(i)} := \Omega_i \cup \ell_i \cup \Gamma_\delta,$$

$$\mathcal{B}\Omega^{(i)} := \mathcal{B}\Omega_i \cup \Gamma_S \cup \Gamma_N,$$

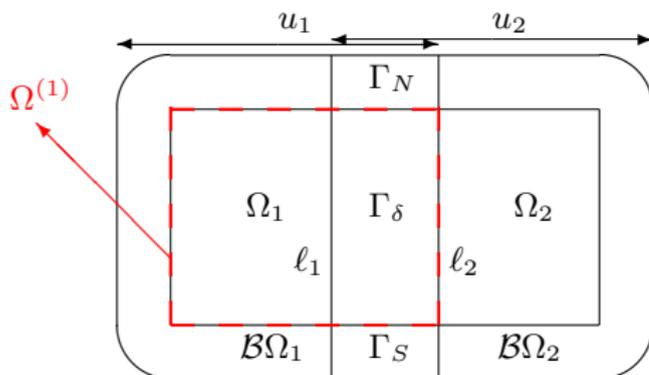
$$|\Gamma_\delta| = 2\delta.$$

Nonlocal interface problems

Two domain formulation

$$\begin{cases} \mathcal{L}_u^{nl,(i)} = b_i(\mathbf{x}), & \mathbf{x} \in \Omega^{(i)} \\ u_i(\mathbf{x}) = 0, & \mathbf{x} \in \mathcal{B}\Omega^{(i)} \end{cases}$$

$$\begin{aligned} \mathcal{L}_u^{nl,(i)}(\mathbf{x}) = & \int_{\Omega^{(i)} \cup \mathcal{B}\Omega^{(i)}} c_{\text{sym}}(\mathbf{x}', \mathbf{x}) (u_i(\mathbf{x}') - u_i(\mathbf{x})) dV_{\mathbf{x}'} \\ & + \int_{\Omega_j \cup \mathcal{B}\Omega_j} c_{\text{sym}}(\mathbf{x}', \mathbf{x}) (u_j(\mathbf{x}') - u_i(\mathbf{x})) dV_{\mathbf{x}'}, \quad i, j = 1, 2, i \neq j. \end{aligned}$$



$$\begin{aligned} \Omega^{(i)} &:= \Omega_i \cup \ell_i \cup \Gamma_\delta, \\ \mathcal{B}\Omega^{(i)} &:= \mathcal{B}\Omega_i \cup \Gamma_S \cup \Gamma_N, \\ |\Gamma_\delta| &= 2\delta. \end{aligned}$$

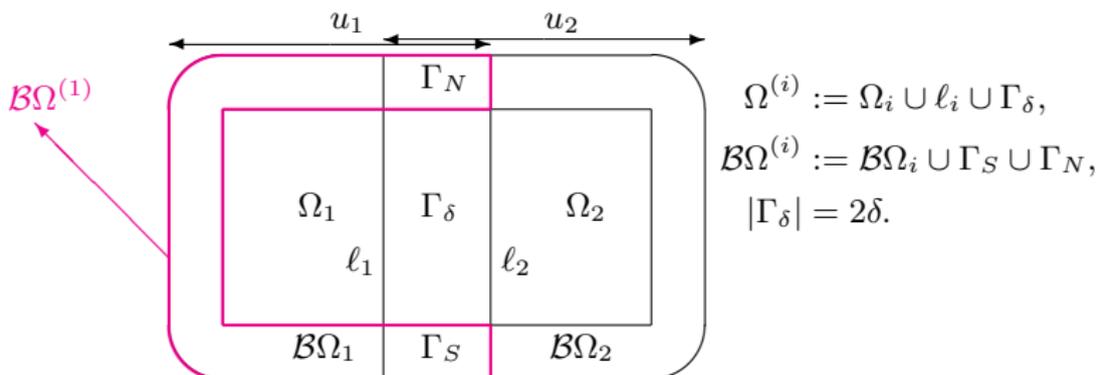
The interaction between $\Omega^{(1)}$ and $\Omega^{(2)}$ occurs only along Γ_δ

Nonlocal interface problems

Two domain formulation

$$\begin{cases} \mathcal{L}_u^{nl,(i)} = b_i(\mathbf{x}), & \mathbf{x} \in \Omega^{(i)} \\ u_i(\mathbf{x}) = 0, & \mathbf{x} \in \mathcal{B}\Omega^{(i)} \end{cases}$$

$$\begin{aligned} \mathcal{L}_u^{nl,(i)}(\mathbf{x}) = & \int_{\Omega^{(i)} \cup \mathcal{B}\Omega^{(i)}} c_{\text{sym}}(\mathbf{x}', \mathbf{x}) (u_i(\mathbf{x}') - u_i(\mathbf{x})) dV_{\mathbf{x}'} \\ & + \int_{\Omega_j \cup \mathcal{B}\Omega_j} c_{\text{sym}}(\mathbf{x}', \mathbf{x}) (u_j(\mathbf{x}') - u_i(\mathbf{x})) dV_{\mathbf{x}'}, \quad i, j = 1, 2, i \neq j. \end{aligned}$$



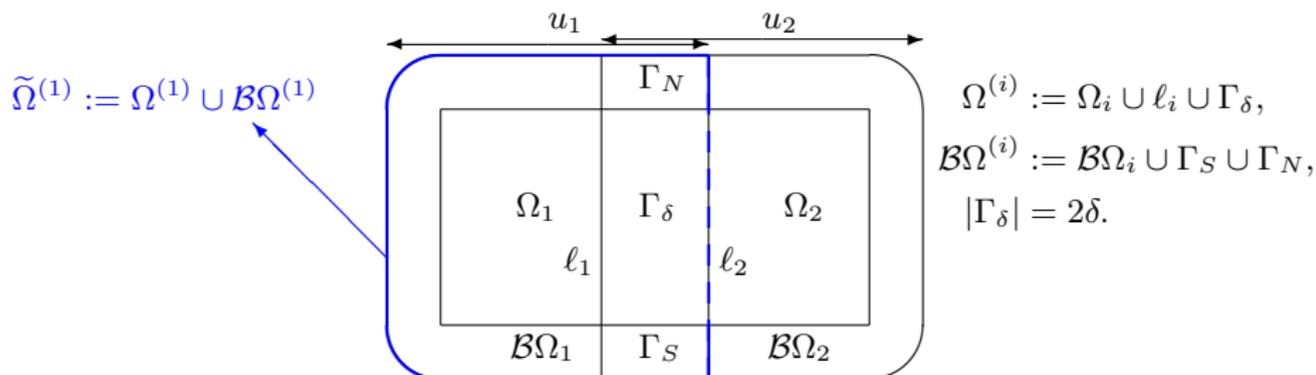
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The interaction between $\Omega^{(1)}$ and $\Omega^{(2)}$ occurs only along Γ_δ

Nonlocal interface problems

Two domain formulation

Weak formulation: Given $b_i(\mathbf{x}) \in L_2(\Omega^{(i)})$, find $u_i(\mathbf{x}) \in V_i^{nl}$ s.t.

$$a_{\tilde{\Omega}^{(i)}}(u_i, v_i) = (b_i, v_i)_{\tilde{\Omega}^{(i)}} + \lambda_{\tilde{\Omega}^{(i)}}(u_j, v_i), \quad \forall v_i \in V_i^{nl}$$

where $i, j = 1, 2$, $i \neq j$, and

Nonlocal flux

$$\lambda_{\tilde{\Omega}^{(i)}}(u_j, v_i) := \int_{\tilde{\Omega}^{(i)}} v_i(\mathbf{x}) \int_{\overline{\tilde{\Omega} \setminus \tilde{\Omega}^{(i)}}} c_{\text{sym}}(\mathbf{x}', \mathbf{x}) (u_j(\mathbf{x}') - u_j(\mathbf{x})) d\mathbf{x}' d\mathbf{x}$$

V_i^{nl} depends on the form of $c(\mathbf{x}', \mathbf{x})$, and $v_i \in V_i^{nl}$ satisfies $v_i|_{\mathcal{B}\Omega^{(i)}} = 0$

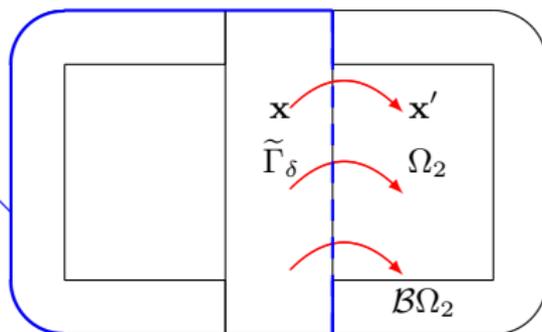
$$\tilde{\Omega}^{(i)} := \Omega^{(i)} \cup \mathcal{B}\Omega^{(i)}; \quad \overline{\tilde{\Omega}} := \Omega \cup \mathcal{B}\Omega$$

Nonlocal interface problems

The nonlocal flux

$$\lambda_{\tilde{\Omega}^{(1)}}(u_2, v_1) = \int_{\tilde{\Gamma}_\delta} v_1(\mathbf{x}) \int_{\Omega_2 \cup \mathcal{B}\Omega_2} c_{\text{sym}}(\mathbf{x}', \mathbf{x}) (u_2(\mathbf{x}') - u_2(\mathbf{x})) d\mathbf{x}' d\mathbf{x}$$

$$\tilde{\Omega}^{(1)} := \Omega^{(1)} \cup \mathcal{B}\Omega^{(1)}$$



$$\tilde{\Gamma}_\delta := \Gamma_\delta \cup \Gamma_N \cup \Gamma_S$$

Nonlocal interface problems

Transmission conditions

- Transmission condition I : “Continuity of the fields”

$$u_1(\mathbf{x}) = u_2(\mathbf{x}), \quad \text{for } \mathbf{x} \in \Gamma_\delta$$

- Transmission condition II : “Nonlocal flux balance condition”

$$\underbrace{\lambda_{\tilde{\Omega}^{(1)}}(u_2, v_1) = -\lambda_{\tilde{\Omega}^{(2)}}(u_1, v_2)}_{\text{“local flux balance”}} + \frac{1}{2} \sum_{i=1}^2 \left[a_{\tilde{\Gamma}_\delta}(u_i, v_i) - (b_i, v_i)_{\tilde{\Gamma}_\delta} \right]$$



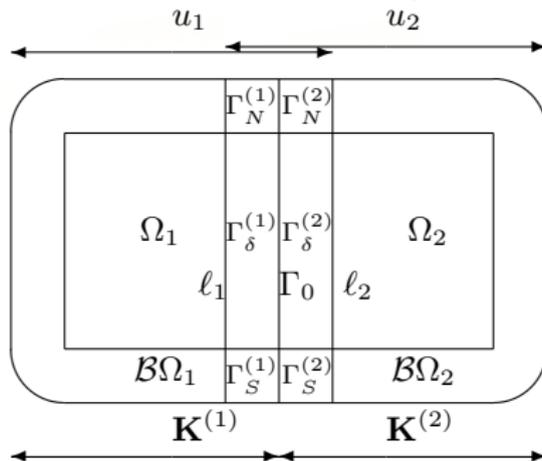
$$u(\mathbf{x}, t) := \begin{cases} u_1(\mathbf{x}, t) & \mathbf{x} \in \Omega^{(1)} \\ u_2(\mathbf{x}, t) & \mathbf{x} \in \Omega^{(2)} \end{cases} ; \text{etc.}$$

$$\int_{\Gamma_\delta} v(\mathbf{x}) \left\{ - \int_{\tilde{\Omega}} c_{\text{sym}}(\mathbf{x}', \mathbf{x}) (u(\mathbf{x}') - u(\mathbf{x})) d\mathbf{x}' - b(\mathbf{x}) \right\} d\mathbf{x} = 0$$

Transmission condition II \rightarrow Interface nonlocal equation

Nonlocal interface problems

Convergence to the classical two-domain problem

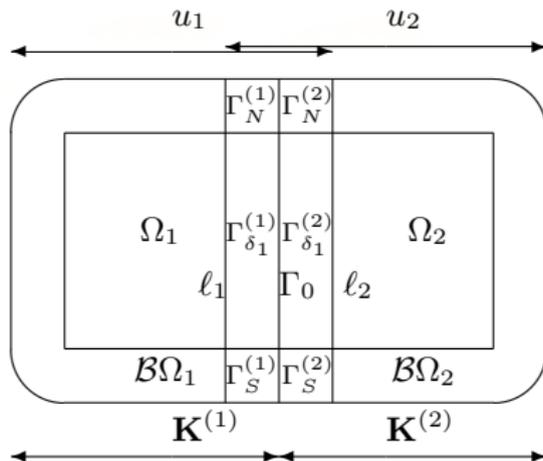


In the limit of $\delta \rightarrow 0$ we can show

- Transmission condition II:
Nonlocal flux balance \rightarrow local flux balance
- Subdomains weak formulations :
Nonlocal formulation \rightarrow local formulation

Nonlocal interface problems

Local/nonlocal transmission condition



Some considerations:

- We have a two-materials system (with $\delta_1 > \delta_2$)
- $|\Gamma_{\delta}| = 2 \max(\delta_1, \delta_2) = 2\delta_1$
- The nonlocal flux balance is the interface equation!
- We let $\delta_2 \rightarrow 0$, while holding δ_1 finite

Nonlocal interface problems

Local/nonlocal transmission condition

The diffusion equation for the interface is

$$- \int_{\overline{\Omega}} c_{\text{sym}}(\mathbf{x}', \mathbf{x}) (u(\mathbf{x}') - u(\mathbf{x})) dV_{\mathbf{x}'} = b(\mathbf{x}), \quad \mathbf{x} \in \Gamma_{\delta}.$$

In weak form we have

$$- \int_{\Gamma_{\delta}} v(\mathbf{x}) \int_{\overline{\Omega}} c_{\text{sym}}(\mathbf{x}', \mathbf{x}) (u(\mathbf{x}') - u(\mathbf{x})) dV_{\mathbf{x}'} dV_{\mathbf{x}} = \int_{\Gamma_{\delta}} v(\mathbf{x}) b(\mathbf{x}) dV_{\mathbf{x}}.$$

Let

$$c(\mathbf{x} + \boldsymbol{\xi}, \mathbf{x}) = \chi_{\delta(\mathbf{x})}(\boldsymbol{\xi}) \gamma_{\delta(\mathbf{x})}^d \frac{\boldsymbol{\xi} \cdot \mathbf{K}(\mathbf{x}, \boldsymbol{\xi}) \boldsymbol{\xi}}{\|\boldsymbol{\xi}\|^{2+\alpha}}; \quad \chi_{\delta}(\boldsymbol{\xi}) = \begin{cases} 1 & \|\boldsymbol{\xi}\| \leq \delta, \\ 0 & \text{otherwise.} \end{cases}$$

Therefore,

$$c_{\text{sym}}(\mathbf{x} + \boldsymbol{\xi}, \mathbf{x}) = \boldsymbol{\xi} \cdot \left(\frac{\chi_{\delta(\mathbf{x})}(\boldsymbol{\xi}) \gamma_{\delta(\mathbf{x})}^d \mathbf{K}(\mathbf{x}, \boldsymbol{\xi}) + \chi_{\delta(\mathbf{x} + \boldsymbol{\xi})}(\boldsymbol{\xi}) \gamma_{\delta(\mathbf{x} + \boldsymbol{\xi})}^d \mathbf{K}(\mathbf{x} + \boldsymbol{\xi}, -\boldsymbol{\xi})}{2 \|\boldsymbol{\xi}\|^{2+\alpha}} \right) \boldsymbol{\xi}$$

Nonlocal interface problems

Local/nonlocal transmission condition

Let $\tilde{\Omega}_i := \Omega_i \cup \mathcal{B}\Omega_i$ and $\tilde{\Gamma}_\delta^{(i)} := \Gamma_\delta^{(i)} \cup \Gamma_N^{(i)} \cup \Gamma_S^{(i)}$, $i = 1, 2$

$$\mathbf{K}(\mathbf{x}, \boldsymbol{\xi}) = \begin{cases} \mathbf{K}^{(1)}(\|\boldsymbol{\xi}\|) & \mathbf{x} \in \tilde{\Omega}_1 \cup \tilde{\Gamma}_{\delta_1}^{(1)}, \\ \mathbf{K}^{(2)}(\|\boldsymbol{\xi}\|) & \mathbf{x} \in \tilde{\Omega}_2 \cup \tilde{\Gamma}_{\delta_1}^{(2)}. \end{cases}; \quad \delta(\mathbf{x}) = \begin{cases} \delta_1 & \mathbf{x} \in \tilde{\Omega}_1 \cup \tilde{\Gamma}_\delta^{(1)}, \\ \delta_2 & \mathbf{x} \in \tilde{\Omega}_2 \cup \tilde{\Gamma}_\delta^{(2)}. \end{cases}$$

We obtain for $\delta_2 \rightarrow 0$

$$\begin{aligned} & \left. \begin{array}{l} \text{Nonlocal} \\ \text{Local} \end{array} \right\} \begin{aligned} & - \int_{\Gamma_{\delta_1}^{(1)}} v(\mathbf{x}) \int_{\tilde{\Omega}_1} \frac{\chi_{\delta_1}(\boldsymbol{\xi}) \gamma_{\delta_1}^d}{\|\boldsymbol{\xi}\|^{2+\alpha}} \boldsymbol{\xi} \cdot \mathbf{K}^{(1)}(\|\boldsymbol{\xi}\|) \boldsymbol{\xi} (u_1(\mathbf{x}') - u_1(\mathbf{x})) dV_{\mathbf{x}'} dV_{\mathbf{x}} \\ & + \frac{1}{2} \int_{\tilde{\Gamma}_{\delta_1}^{(1)}} \int_{\tilde{\Gamma}_{\delta_1}^{(1)}} (v(\mathbf{x}') - v(\mathbf{x})) \frac{\chi_{\delta_1}(\boldsymbol{\xi}) \gamma_{\delta_1}^d}{\|\boldsymbol{\xi}\|^{2+\alpha}} \boldsymbol{\xi} \cdot \mathbf{K}^{(1)}(\|\boldsymbol{\xi}\|) \boldsymbol{\xi} (u_1(\mathbf{x}') - u_1(\mathbf{x})) dV_{\mathbf{x}'} dV_{\mathbf{x}} \\ & + \frac{1}{2} \int_{\tilde{\Gamma}_{\delta_1}^{(1)}} \int_{\tilde{\Gamma}_{\delta_1}^{(2)}} (v(\mathbf{x}') - v(\mathbf{x})) \frac{\chi_{\delta_1}(\boldsymbol{\xi}) \gamma_{\delta_1}^d}{\|\boldsymbol{\xi}\|^{2+\alpha}} \boldsymbol{\xi} \cdot \mathbf{K}^{(1)}(\|\boldsymbol{\xi}\|) \boldsymbol{\xi} (u_2(\mathbf{x}') - u_1(\mathbf{x})) dV_{\mathbf{x}'} dV_{\mathbf{x}} \\ & + \int_{\Gamma_0} v(\mathbf{x}, t) (\mathbf{D}_2 \nabla u_2(\mathbf{x})) \cdot \mathbf{n}_2 dS_{\mathbf{x}} - \int_{\tilde{\Gamma}_{\delta_1}^{(2)}} v(\mathbf{x}) \nabla \cdot [\mathbf{D}_2 \nabla u_2(\mathbf{x})] dV_{\mathbf{x}} \\ & = \int_{\Gamma_\delta} v(\mathbf{x}) b(\mathbf{x}) dV_{\mathbf{x}}. \end{aligned} \end{aligned}$$

Local/Nonlocal Transmission Conditions

Transmission condition II for local/nonlocal system

We can also write the local/nonlocal transmission condition as

$$\begin{aligned}
 \text{Nonlocal interaction} & \left\{ - \int_{\Gamma_{\delta_1}^{(1)}} v(\mathbf{x}) \int_{\bar{\Omega}} \frac{\chi_{\delta}(\boldsymbol{\xi}) \gamma_{\delta}^d}{\|\boldsymbol{\xi}\|^{2+\alpha}} \boldsymbol{\xi} \cdot \mathbf{K}^{(1)}(\|\boldsymbol{\xi}\|) \boldsymbol{\xi} (u_1(\mathbf{x}') - u_1(\mathbf{x})) dV_{\mathbf{x}'} dV_{\mathbf{x}} \right. \\
 \text{Local interaction} & \left\{ - \int_{\tilde{\Gamma}_{\delta_1}^{(2)}} v(\mathbf{x}) \nabla \cdot [\mathbf{D}_2 \nabla u_2(\mathbf{x})] dV_{\mathbf{x}} \right. \\
 & + \int_{\tilde{\Gamma}_{\delta_1}^{(1)}} \int_{\tilde{\Gamma}_{\delta_1}^{(2)}} \left(\frac{v(\mathbf{x}') + v(\mathbf{x})}{2} \right) \frac{\chi_{\delta_1}(\boldsymbol{\xi}) \gamma_{\delta_1}^d}{\|\boldsymbol{\xi}\|^{2+\alpha}} \boldsymbol{\xi} \cdot \mathbf{K}^{(1)}(\|\boldsymbol{\xi}\|) \boldsymbol{\xi} (u_2(\mathbf{x}') - u_1(\mathbf{x})) dV_{\mathbf{x}'} dV_{\mathbf{x}} \\
 & + \int_{\Gamma_0} v(\mathbf{x}) (\mathbf{D}_2 \nabla u_2(\mathbf{x})) \cdot \mathbf{n}_2 dS_{\mathbf{x}} = \int_{\Gamma_{\delta}} v(\mathbf{x}) b(\mathbf{x}) dV_{\mathbf{x}}.
 \end{aligned}$$

↙
↘

Local flux
Nonlocal “flux-like”

A one dimensional example

Nonlocal continuum model

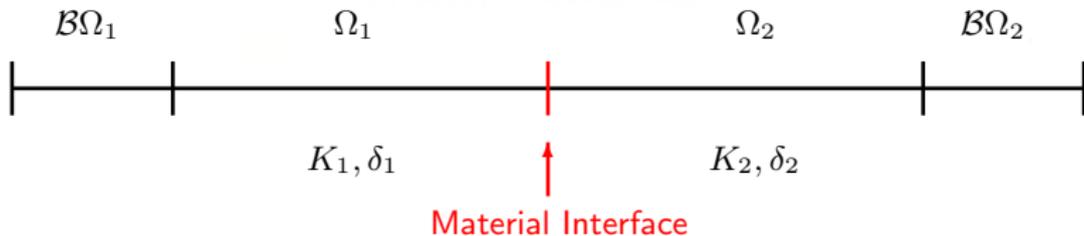
$$\begin{aligned}
 - \int_{\overline{\Omega}} c_{\text{sym}}(x', x) (u(x') - u(x)) dx' &= b(x) \\
 c(x', x) &= \begin{cases} \frac{2k_c}{\delta(x)^2 |x' - x|} & |x' - x| < \delta(x) \\ 0 & \text{otherwise} \end{cases}
 \end{aligned}$$

Local continuum model

$$-k_c \frac{d^2 u}{dx^2}(x) = b(x)$$

- How the nonlocal model differs from its local counterpart?
- Do we recover local model results for $\delta \rightarrow 0$?
- How two-scale nonlocal models behave for different conditions?
- Can we do a two-scale representation of a single material?

A one dimensional example



Discrete nonlocal system:

$$\mathbf{A} \mathbf{u}^h = \mathbf{b}$$

with

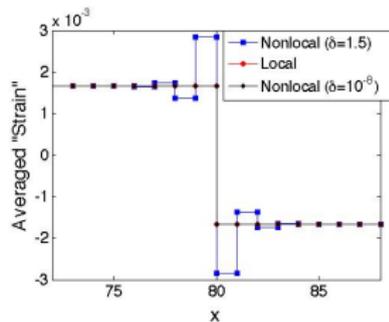
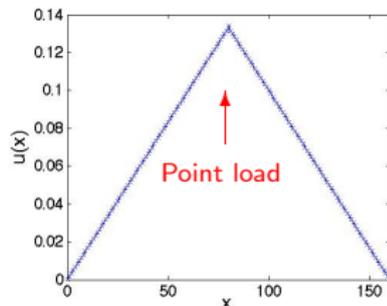
$$A_{ij} := \frac{1}{2} \int_{\Omega \cup B\Omega} \int_{\Omega \cup B\Omega} (\varphi_i(x') - \varphi_i(x)) c(x', x) (\varphi_j(x') - \varphi_j(x)) dx' dx,$$

$$b_i := \int_{\Omega \cup B\Omega} \varphi_i(x) b(x) dx.$$

$$A_{ij} = A_{ji}$$

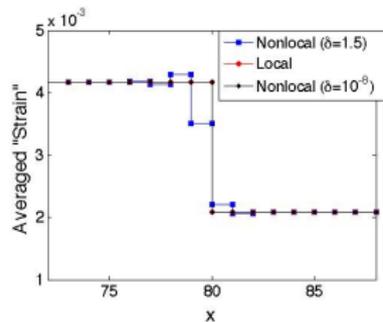
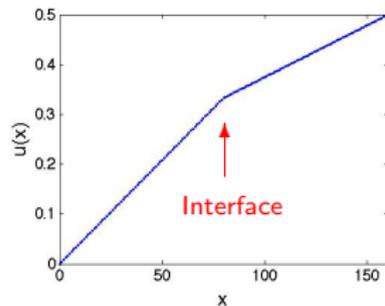
A one dimensional example (uniform δ)

Case 1 : point load



Local vs. nonlocal models

Case 2 : material interface ($k_2 = 2k_1$)

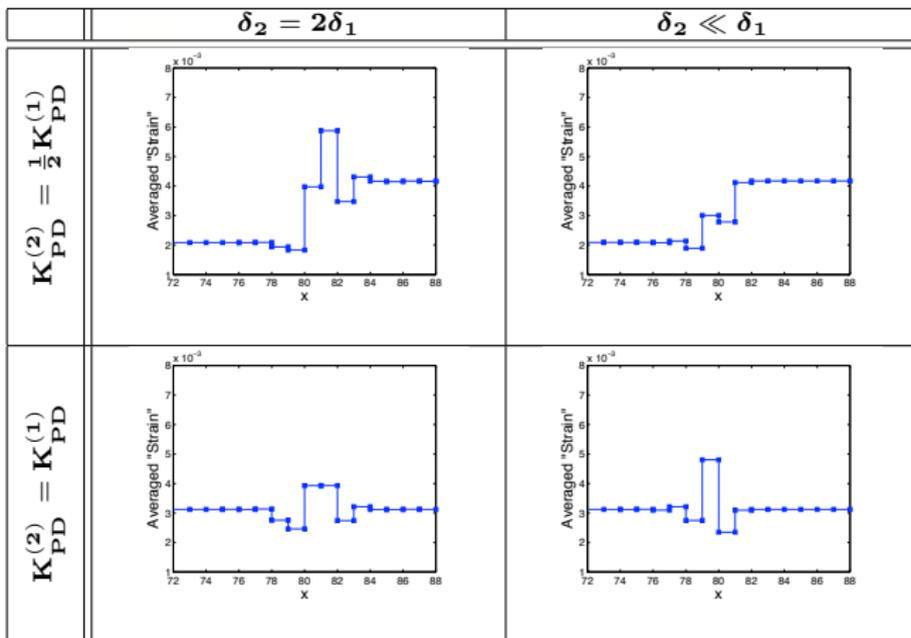


Local vs. nonlocal models

A one dimensional example

Case 3 : two materials/two horizons

No patch consistent!



A one dimensional example (patch consistency)

Can we have a local/nonlocal description of a single-material model?

Most methods do not satisfy Newton's 3rd law + "patch test" !



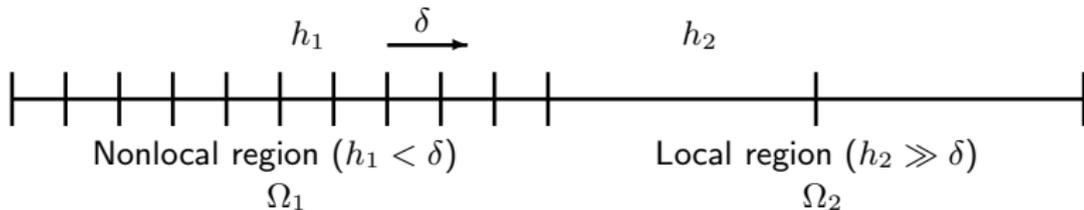
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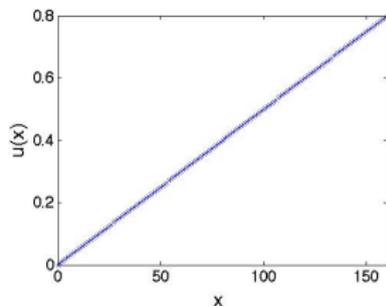


Coarsening the nonlocal model

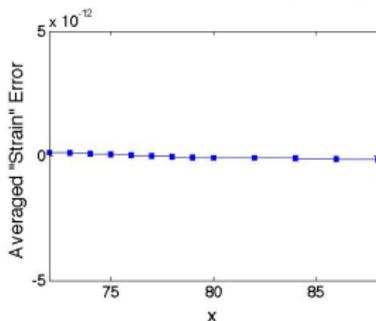


A one dimensional example (patch consistency)

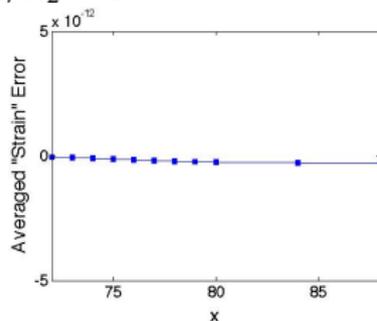
Case 4 : single material- linear displacement profile



$$\delta = 1.5, h_1 = 1, h_2 = 1$$



$$\delta = 1.5, h_1 = 1, h_2 = 2$$



$$\delta = 1.5, h_1 = 1, h_2 = 4$$

Summary of part IV

Presented a nonlocal formulation for interface problems:

- 1 The model allows:
 - different materials,
 - different interaction ranges.
- 2 Showed one-domain and two-domain convergence to local model for $\delta \rightarrow 0$.
- 3 Derived transmission conditions for local/nonlocal systems
- 4 Demonstrated numerically differences between local and nonlocal models, as well as the convergence of the nonlocal model results to its local counterpart for $\delta \rightarrow 0$.
- 5 Presented a coarsened approach for patch consistency

A few more questions ...

- Question 2: What is an appropriate patch test for two-interaction range systems? Do we have exact solutions? What are the right settings for these systems?
- Question 3: Which system are we solving when we coarsen the discretized PD equation requiring $h \gg \delta$ in certain region?
- Question 4: What does it mean to splits the state-based interaction in 2 contributions?
- Question 5: Which materials are non-ordinary?

What's next?

We are working on the implementation of peridynamics as a framework to **bridge between scales**. We investigate a simultaneous coupling of nonlocal **atomistic** and local **continuum** models through peridynamics.

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Thank you for your attention!