Consistent coupling of nonlocal and local diffusion problems

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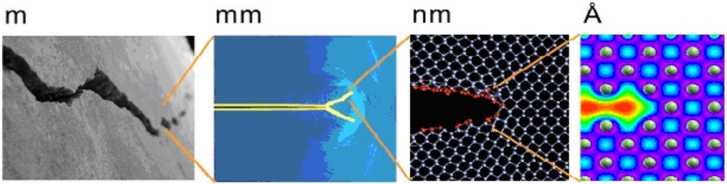
Modeling failure of materials

Computational goal: Efficiently and reliably predict failure of materials and design new materials. Need a fundamental level modeling.



Macroscale to **Mesoscale** to **Molecular scale** to **Atomistic scale**
Figure: Buehler group, MIT.

Approaches towards modeling material fracture

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- Top-down nonlocal modeling:
  e.g. Peridynamics (Hillerborg et al, 1976; Silling, 2000):
  - Replace PDEs by integral equations with parameter δ
  - Reduced to classical PDE with $\delta \to 0$

Local vs nonlocal models

Nonlocal Peridynamics model

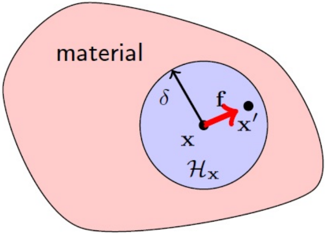
$$\rho \ddot{\mathbf{u}} = \int_{\mathcal{H}_x} \mathbf{f}\left(\mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x}, \mathbf{x} - \mathbf{x}')\right) d\mathbf{x}' + \mathbf{b}$$

Classical local continuum model

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

- Require certain regularity of displacement field.
- Additional equations need to be included when fracture (singularity) is involved.

- No spatial regularity required. Models continuous media and cracks within a single framework.
- Need special boundary treatments.



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- Efficiency purpose: reduce the computational costs by using local models.
- Application purpose: e.g. use variable horizon to model hierarchically structured materials and nonlocal heat conductors (Gao et al, 2007; Bobaru et al, 2010).
- Challenges near the boundary: how to impose classical boundary conditions.

Outline

- The linear nonlocal diffusion problem
- Consistent quasinonlocal coupling of nonlocal diffusions
- Properties of the coupling diffusion operator
- Numerical examples
- Conclusions

The linear nonlocal diffusion problem

- The (linear) nonlocal diffusion (integral) operator $\mathcal{L}_\delta$ is defined as

$$\mathcal{L}_\delta u_n(x) = \int_{\mathbb{R}^d} (u_n(y) - u_n(x))\, \gamma_\delta(x, y) dy, \quad \forall x \in \Omega,$$

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- The nonlocal diffusion problem is (Caffarelli et al, 2011)

$$\begin{cases} \frac{\partial u_n}{\partial t} = \mathcal{L}_\delta u_n(x) := \int (u_n(y) - u_n(x))\, \gamma_\delta(x,y) dy, \forall x \in \Omega, \\ u_n(x,t) = 0, \forall x \in \Omega_{\mathcal{I}}, \forall t \geq 0, \\ u_n(x,0) = u_n^0(x), \text{ on } \Omega, \end{cases}$$

where $\Omega_{\mathcal{I}}$ **has non-zero volume** and is disjoint from Ω.

The nonlocal diffusion kernel γ_δ (Du et al, 2012)

- The kernel $\gamma_\delta(x, y)$ is characterized by the horizon parameter δ (i.e. effective interaction range. For d-dim isotropic systems, it is assumed to be

$$s = |x - y|, \quad \gamma_\delta(s) = \frac{1}{\delta^{d+2}}\gamma(\frac{s}{\delta}).$$

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- Kernel function $\gamma(\cdot)$ satisfies
  - **Translational invariance and isotropy:** $\gamma(x, y) = \gamma(|y - x|) \geq 0$;
  - **Compact support:** $\gamma(x, y) = 0$ if $|x - y| \geq 1$;
  - **Finite second moment:** $\int s^2\gamma(s)ds < \infty$. Note that due to the scaling choice, the second moment is scale invariant.

Nonlocal energy space

- Define the Hilbert spaces associated with γ_δ to be

$$S_\delta := \Big\{ u \in L^2(\Omega \cup \Omega_{\mathcal{I}}) : \int_{\Omega \cup \Omega_{\mathcal{I}}} \int_{\Omega \cup \Omega_{\mathcal{I}}} \gamma_\delta(x,y)\,(u(y) - u(x))^2 \, dxdy < \infty,\ u\big|_{\Omega_{\mathcal{I}}} = 0 \Big\}.$$

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- More literatures about the properties of the nonlocal kernel and the nonlocal energy norms (Du et al 2013, E'Delia et al 2014, Tian et al 2013, 2016).

Recent developments in coupling nonlocal and local diffusions

An example list of reference papers:

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- The multiple layer-based coupling (Seamless coupling): Du & Tian 2016; ...

To the best of my knowledge, none of the above coupling is energy-based and consistent coupling.

Goal

Based on energy, we target to develop a consistent and stable coupling for γ_δ with local kernels, while keeps as much physical properties as possible.

Geometric reconstruction in 1D

- Assume $\Omega = (-1, 1)$ is decomposed into $\Omega_1 = (-1, 0)$ and $\Omega_2 = (0, 1)$ with interface at $x = 0$, and associated with kernels γ_{δ_1} and γ_{δ_2} with $\delta_1 = M\delta_2$.

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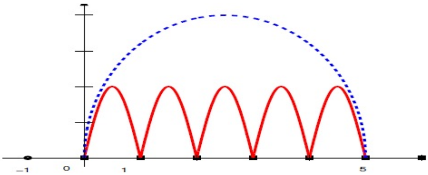
- Adopt the *geometric reconstruction* (Lu et al, 2006; Shapeev, 2012). For $0 \le j \le (M-1)$

$$u(y) - u(x) \to \left(u\big(x + \frac{j+1}{M}(y-x)\big) - u\big(x + \frac{j}{M}(y-x)\big) \right) M.$$

Reconstruct the longer interactions within δ_1 by shorter bonds within δ_2.



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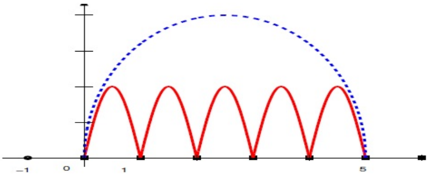

- Hence, approximate $\gamma_{\delta_2}(|y-x|)\,(u(y) - u(x))^2$ by

$$\gamma_{\delta_1}(|y-x|)\frac{1}{M}\sum_{j=0}^{M-1}\left(u\big(x + \frac{j+1}{M}(y-x)\big) - u\big(x + \frac{j}{M}(y-x)\big)\frac{\delta_1}{\delta_2} \right)^2.$$

Recover interactions of γ_{δ_2} by geometric reconstruction

Proposition. The energy functional defined on the entire domain $\Omega \cup \Omega_{\mathcal{I}}$ with geometric reconstruction

$$E^{\text{tot,gr}}(u) := \frac{1}{4} \int_{x,y\in\Omega\cup\Omega_{\mathcal{I}}} \gamma_{\delta_1}(|y-x|) \, dxdy$$
$$\frac{1}{M} \sum_{j=0}^{M-1} \left(u\left(x + \frac{j+1}{M}(y-x)\right) - u\left(x + \frac{j}{M}(y-x)\right)\right)^2 M^2$$

is equal to the total nonlocal energy with diffusion kernel γ_{δ_2}:

$$E^{\text{tot},\delta_2}(u) := \frac{1}{4} \int_{x,y\in\Omega\cup\Omega_{\mathcal{I}}} \gamma_{\delta_2}(|y-x|) \left(u(y) - u(x)\right)^2 \, dxdy.$$

The interactions of kernel γ_{δ_2} can be recast in terms of those of kernel γ_{δ_1} through geometric reconstruction .

Extend to couple γ_δ direct with local diffusions

- Let $M \to \infty$, then

$$\frac{1}{M}\sum_{j=0}^{M-1}\left(u\big(x+\frac{j+1}{M}(y-x)\big)-u\big(x+\frac{j}{M}(y-x)\big)\frac{\delta_1}{\delta_2}\right)^2$$

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$$\to \int_0^1 |\nabla u(x+t(y-x))|^2|y-x|^2 dt.$$

- Thus, we can replace local interactions $|\nabla u(x)|^2$ by

$$\gamma_\delta(|y-x|)\cdot\int_0^1 dt|\nabla u(x+t(y-x))|^2|y-x|^2.$$

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- **Apply the geometric reconstruction only when bond $\{x-y\}\in\Omega_2$.** The total coupling energy is defined as

$$E^{\text{tot,qnl}}(u) := \frac{1}{4}\int_{x<0 \text{ or } y<0}\gamma_\delta(|y-x|)\,(u(y)-u(x))^2\;dxdy$$

$$+\frac{1}{4}\int_{x>0 \text{ and } y>0} dxdy\,\gamma_\delta(|y-x|)\cdot\int_0^1 dt\left|\nabla u(x+t(y-x))\right|^2|y-x|^2.$$

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2. $0 < x < \delta$:

$$\mathcal{L}^{\mathrm{qnl}} u(x) = \int_{y<0} \gamma_\delta(|y - x|)\,(u(y) - u(x))\,dy$$
$$+ \left(\int_0^1 dt \int_0^{\frac{x}{t}} s^2 \gamma_\delta(s) ds\right) \Delta u(x) + \left(\int_x^\infty s\gamma_\delta(s) ds\right) \nabla u(x).$$

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3. $x > \delta$:

$$\begin{aligned}\mathcal{L}^{\mathrm{qnl}} u(x) =& \frac{1}{2}\nabla_x\left[\int_0^1 dt \int_{|y-x|<t\delta} dy\gamma_{t\delta}\left(|x-y|\right)\,|x-y|^2\nabla u(x)\right]\\ =& \frac{1}{2}\nabla_x\left[\int_0^1 dt 2C^*\nabla u(x)\right] = C^*\Delta u(x).\end{aligned}$$

Properties of $\mathcal{L}^{\mathrm{qnl}}$

- Symmetry (self-adjoint)

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- Symmetry (self-adjoint)
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- The maximum principle and the mass conservation
- $O(\delta)$ modeling errors

First order finite difference approximation

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- $\gamma_\delta(s)$ is fixed to be

$$\gamma_\delta(s) = \frac{2}{\delta^2 s}.$$

Numerical example: accuracy

- Consider the Dirichlet volume-constrained problem

$$u(x,0) = x^2\,(1-x^2), \quad f(x) = e^{-t}(12x^2-2) - e^{-t}x^2(1-x^2).$$

- The limiting local diffusion problem as $\delta \to 0$ is

$$\begin{cases} \frac{\partial u}{\partial t} - u_{xx} = f(x), \quad 0 < x < 1,\ \forall t > 0, \\ u(x,0) = x^2\,(1-x^2), \quad 0 < x < 1, \\ u(0,t) = u(1,t) \equiv 0, \forall t > 0, \end{cases}$$

The exact solution for the diffusion problem is

$$u_{\text{exact, limit}} = e^{-t}\,x^2\,(1-x^2).$$

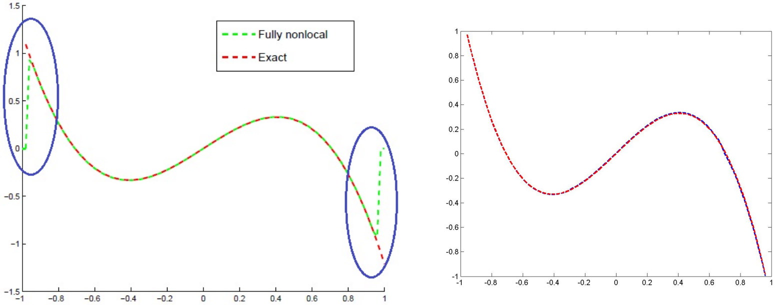
Numerical example: accuracy

h	$\|e_u\|_{L^\infty}$ of Case A	Order	$\|e_u\|_{L^\infty}$ of Case B	Order
$1/50$	$3.222e$-3	–	$2.334e$-2	–
$1/100$	$1.952e$-3	0.723	$5.935e$-3	1.98
$1/200$	$1.066e$-3	0.873	$1.464e$-3	2.02
$1/400$	$5.557e$-4	0.939	$3.510e$-4	2.06
$1/800$	$2.836e$-4	0.989	$7.961e$-5	2.14

Table: L^∞ differences of solution u with first order finite difference discretization to the local limiting solution.
Case A: $\delta = 3h$ and Case B: $\delta = 10h$.
The quasinonlocal local coupled with nonlocal, and then coupled with local with interfaces at $x_m^a = \frac{-1}{2}$ and $x_m^b = \frac{1}{2}$.

Artificial boundary layers vanished

Compute the $du(x)$ (strains) with Dirichlet boundary conditions.
The coupling method improves the issues of boundary layers.



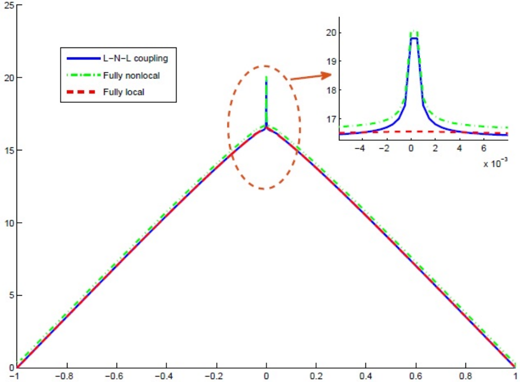
(a) Fully nonlocal (b) Coupling model

Numerical example: point defect for static problem

Consider a constant nonlocal kernel $\gamma_\delta^c(s) = \frac{3}{2\delta^3}$ for $|s| < \delta$.
Consider singular external forces at $x^* = -0.1 + h/2$: $h = 1/2000$, $\delta = 100h$.

$$f(x) = \frac{(1-x^2)(1+x^2)}{|x - x^*|}, \quad f(x) = 0.$$

Both quasinonlocal coupling and the fully nonlocal model capture the singularities near defects. The classical local model fails to capture the singularities.



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- A first order finite difference approximation is proposed based on a simple Riemann integral quadrature rule. This approximation keeps all the properties at the continuous levels.
- The coupling method resolve the issues of boundary layers.
- The coupled model agrees with that of the fully nonlocal one when there exists singularities.

Thank you for your attention!