Recent developments in peridynamic mechanics

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Why consider peridynamic balance laws?

Balance laws

- Balance of linear momentum
- Balances of angular momentum, energy
- Kinematics
- Thermomechanics
- Linear problems
- Volume constraints

Fracture nucleation and evolution

Why consider peridynamic balance laws?

- Classical balance laws assume the motion is sufficiently regular, e.g., differentiable—peridynamic balance laws are defined for discontinuous motion—same equations hold on and off of discontinuities
- Peridynamic mechanics is now 15 years old; much has been accomplished (but much) more work needs to be done
- My presentation reviews peridynamic mechanics and recent work on complex fracture nucleation and evolution (joint with Rob Lipton, Stewart Silling)

Applications/Software

- Google for a myriad of applications; brittle fracture has some interesting results
- Several three dimensional dynamic fracture codes (public domain)
- LS-DYNA has released an implementation

Balance law of linear momentum

- Let $\mathbf{y} = \mathbf{y}(\mathbf{x}, t)$ denote a motion; $\rho = \rho(\mathbf{x}, t)$ is the mass density; $\mathbf{b}(\mathbf{x}, t)$ is the body force density
- Classical balance of linear momentum

$$\frac{d}{dt}\int_{\Omega} \rho\,\dot{\mathbf{y}}\,dV = \int_{\partial\Omega} \mathbf{P}\,\mathbf{n}\,dA + \int_{\Omega} \mathbf{b}\,dV \qquad \forall\Omega$$

  where $\mathbf{P}$ is the stress tensor and $\mathbf{n}$ is the unit outward normal
- Peridynamic balance of linear momentum

$$\frac{d}{dt}\int_{\Omega} \rho\,\dot{\mathbf{y}}\,dV = \int_{\Omega}\int_{\mathbb{R}^3\setminus\Omega} \left(\mathbf{t} - \mathbf{t}'\right) dV'\,dV + \int_{\Omega} \mathbf{b}\,dV \qquad \forall\Omega$$

  where $\mathbf{t} := \mathbf{t}(\mathbf{x}', \mathbf{x}), \mathbf{t}' := \mathbf{t}(\mathbf{x}, \mathbf{x}')$ is the *bond force density*

Internal force interaction

- The difference between the balance laws are the terms

$$\int_{\partial\Omega} \mathbf{P}\,\mathbf{n}\,dA \quad \text{and} \quad \int_{\Omega}\int_{\mathbb{R}^3\setminus\Omega} \left(\mathbf{t} - \mathbf{t}'\right) dV'\,dV$$

  representing the internal forces within the body exerted upon Ω
- The nonlocal flux is associated with an alternate set of balance laws with significantly less regularity assumption results—no spatial derivatives are used

(Nonlocal) flux

The following conditions are equivalent

- Action-reaction:

$$\int_{\Omega_1}\int_{\Omega_2}\left(\mathbf{t}-\mathbf{t}'\right)dV'\,dV+\int_{\Omega_2}\int_{\Omega_1}\left(\mathbf{t}-\mathbf{t}'\right)dV'\,dV=\mathbf{0}\qquad\forall\Omega_1,\Omega_2$$

- Antisymmetry: $\mathbf{t}(\mathbf{x}',\mathbf{x})-\mathbf{t}(\mathbf{x},\mathbf{x}')=-\big(\mathbf{t}(\mathbf{x},\mathbf{x}')-\mathbf{t}(\mathbf{x}',\mathbf{x})\big)$
- Alternating: $\displaystyle\int_{\Omega}\int_{\Omega}\left(\mathbf{t}-\mathbf{t}'\right)dV'\,dV=0$ for all Ω (no self-interaction)
- The balance law is additive

$$\sum_{i=1}^{2}\frac{d}{dt}\int_{\Omega_i}\rho\dot{\mathbf{y}}\,dV=\sum_{i=1}^{2}\int_{\Omega_i}\int_{\mathbb{R}^3\setminus\Omega_i}\left(\mathbf{t}-\mathbf{t}'\right)dV'\,dV\qquad\forall\Omega_1,\Omega_2$$

Local, nonlocal fluxes compared

- Action-reaction: via surface interaction

$$\underbrace{\int_{\partial\Omega} \mathbf{P}\,\mathbf{n}\,dA}_{\text{force upon } \Omega} + \underbrace{\int_{\partial\Omega} \mathbf{P}(-\mathbf{n})\,dA}_{\text{force upon } \mathbb{R}^3\setminus\Omega} = \mathbf{0}$$

  or the (traction) force exerted upon Ω by $\mathbb{R}^3 \setminus \Omega$ is equal and opposite to that of the force exerted upon $\mathbb{R}^3 \setminus \Omega$ by Ω
- Action-reaction: via volume interaction

$$\underbrace{\int_{\Omega}\int_{\mathbb{R}^3\setminus\Omega} (\mathbf{t}-\mathbf{t}')\,dV'\,dV}_{\text{force upon } \Omega} + \underbrace{\int_{\mathbb{R}^3\setminus\Omega}\int_{\Omega} (\mathbf{t}-\mathbf{t}')\,dV'\,dV}_{\text{force upon } \mathbb{R}^3\setminus\Omega} = \mathbf{0}$$

Pointwise balance laws of linear momentum

- Use the divergence theorem $\int_{\Omega} \nabla \cdot \mathbf{P} \, dV = \int_{\partial\Omega} \mathbf{P}\,\mathbf{n} \, dA$ on the classical balance of linear momentum

$$\rho \, \ddot{\mathbf{y}} = \nabla \cdot \mathbf{P} + \mathbf{b}$$

  where $\mathbf{P}$ is the stress tensor
- The alternating principle implies a nonlocal divergence theorem $\int_{\Omega} \int_{\mathbb{R}^3} \left(\mathbf{t} - \mathbf{t}'\right) dV' \, dV = \int_{\Omega} \int_{\mathbb{R}^3 \setminus \Omega} \left(\mathbf{t} - \mathbf{t}'\right) dV' \, dV$
- Peridynamic balance of linear momentum

$$\rho \, \ddot{\mathbf{y}} = \int_{\mathbb{R}^3} \left(\mathbf{t} - \mathbf{t}'\right) dV' + \mathbf{b}$$

  where $\mathbf{t} := \mathbf{t}(\mathbf{x}', \mathbf{x}), \mathbf{t}' := \mathbf{t}(\mathbf{x}, \mathbf{x}')$

Nonlocality

- Local: $\nabla \cdot \mathbf{P}(\mathbf{x})$ only depends upon the value of the stress at $\mathbf{x}$
- Nonlocal: $\int_{\mathbb{R}^3} \left(\mathbf{t}(\mathbf{x}', \mathbf{x}) - \mathbf{t}(\mathbf{x}, \mathbf{x}')\right) dV'$ depends upon $\mathbf{x}' \neq \mathbf{x}$
- Be careful when speaking about a force acting across a finite distance because it's not clear what this means—how would you justify (or reject for that matter)?
- Nonlocal force interaction is picturesque language for a modeling assumption—the benefit is that regularity requirements can be lowered
- Principal of virtual work can be postulated (and be shown to be equivalent to the balance of linear momentum)

(Nonlocal) balances of angular momentum, energy

- Balance of angular momentum (global, pointwise)
- Balance of energy (global, pointwise); combined with the second law leads to thermodynamic restrictions (Coleman-Noll paradigm) for constitutive relations
- Satisfy analogous symmetries as the balance of linear momentum
- Do we have supporting evidence that the balances are valid?

Ensemble averaging in phase space

- Expressions for the peridynamic analogues of stress, heat flux, energy, and material velocity, i.e.,

$$\mathbf{t}, h, \epsilon, \text{ and } \dot{\mathbf{y}}$$

  (L. and Sears Phy. Rev. E 2011)
- Microscopic basis for the nonlocal balance laws in non-equilibrium statistical mechanics
- Builds upon the seminal paper by Irving & Kirkwood (J. Chem. Phys. 1950) derived approximate expressions for the stress, heat flux, energy, and material velocity as ensemble averages for the classical balances

Alternative derivation of nonlocal balance laws

- Frame indifference (invariant under rotations + translations) of the absorbed and supplied *power expenditures*

$$w_{\text{abs}}(\Omega) \stackrel{\text{def}}{=} \int_\Omega \int_{\mathbb{R}^3} \mathbf{t} \cdot (\mathbf{v}' - \mathbf{v})\, dV' dV \quad \text{“absorbed power”}$$

$$w_{\text{sup}}(\Omega) \stackrel{\text{def}}{=} \int_\Omega \int_{\mathbb{R}^3 \setminus \Omega} (\mathbf{t} \cdot \mathbf{v}' - \mathbf{t}' \cdot \mathbf{v})\, dV' dV + \int_\Omega \mathbf{b} \cdot \mathbf{v}\, dV$$

“supplied power”

$$\mathbf{v}' = \mathbf{v}(\mathbf{x}', t) = \dot{\mathbf{u}}(\mathbf{x}', t)$$

- Resulting power expenditures satisfy analogous symmetries as the previous balances
- Balances of angular, linear momentum and energy result

Nonlocal Kinematics

$$\tilde{\nabla}\,\mathbf{y}(\mathbf{x}) \stackrel{\text{def}}{=} -\int_{\mathbb{R}^3} \mathbf{y}(\mathbf{x}') \otimes \boldsymbol{\alpha}_\epsilon(\mathbf{x}' - \mathbf{x})\,\mathrm{d}\mathbf{x}'$$

where

$$\int_{\mathbb{R}^3} \boldsymbol{\alpha}_\epsilon(\mathbf{x}' - \mathbf{x})\,\mathrm{d}\mathbf{x}' = \mathbf{0} \qquad \Big(\boldsymbol{\alpha}_\epsilon(\mathbf{x}' - \mathbf{x}) = -\boldsymbol{\alpha}_\epsilon(\mathbf{x} - \mathbf{x}')\Big)$$

- $\tilde{\nabla}\,\mathbf{y}$ is dimensional-less when $\mathbf{y}$ has dimensions of length
- $\tilde{\nabla}\,(\mathbf{A}\,\mathbf{x} + \mathbf{c}) = \mathbf{A}\tilde{\nabla}\,\mathbf{x} = \mathbf{A}$ when $\mathbf{A}$ and $\mathbf{c}$ are a matrix and a vector
- Select $\boldsymbol{\alpha}_\epsilon(\mathbf{x}' - \mathbf{x}) = \dfrac{\partial}{\partial \mathbf{x}'}\delta(\mathbf{x}' - \mathbf{x})$ to recover $\nabla\,\mathbf{y}$

Nonlocal strain

- Deformation $\mathbf{y}(\mathbf{x}, t) = \mathbf{x} + \mathbf{u}(\mathbf{x}, t)$
- Nonlocal deformation gradient $\tilde{\mathbf{F}} \stackrel{\text{def}}{=} \mathbf{I} + \tilde{\nabla}\mathbf{u}$
- Nonlocal strain $\tilde{\mathbf{E}} \stackrel{\text{def}}{=} \frac{1}{2}\left(\tilde{\mathbf{F}}^T\tilde{\mathbf{F}} - \mathbf{I}\right)$
- Rigid body modes have zero nonlocal strain (elastic and plastic)

A bit of thermomechanics

- Nonlocal Coleman-Noll
- Free energy ψ

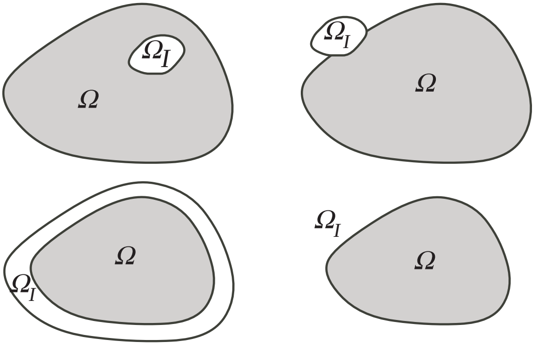
$$\frac{\mathrm{d}}{\mathrm{d}t}\psi(\tilde{\mathbf{F}}) = \frac{\partial \psi}{\partial \tilde{\mathbf{F}}} : \dot{\tilde{\mathbf{F}}}$$

- Energy imbalance for nonlocal elasticity

$$\int_\Omega \frac{1}{\theta} \underbrace{\rho \frac{\partial \psi}{\partial \tilde{\mathbf{F}}} : \dot{\tilde{\mathbf{F}}}}_{\text{power}} \, dV - \underbrace{w_{\mathrm{abs}}(\Omega)}_{\text{absorbed power}} \leq 0$$

- Leads to restrictions on constitutive relations

Interaction region $\Omega_{\mathcal{I}}$



- Four of the possible configurations for $\Omega_{\mathcal{I}}$, the nonlocal analogue of the boundary $\partial\Omega$
- $\Omega_{\mathcal{I}}$ is (typically) the union of spheres about $\mathbf{x} \in \Omega$; peridynamic horizon $\mathcal{H}_{\varepsilon}(\mathbf{x})$

Well-posed volume constrained problems

- Dirichlet volume constrained nonlocal diffusion and peridynamic Navier problems

$$\begin{cases} -\mathcal{L}u = b & \text{on } \Omega \\ u = 0 & \text{on } \Omega_{\mathcal{I}}, \end{cases} \qquad \begin{cases} -\boldsymbol{\mathcal{L}}\mathbf{u} = \mathbf{b} & \text{on } \Omega \\ \mathbf{u} = \mathbf{h} & \text{on } \Omega_{\mathcal{I}} \end{cases}$$

- Variational formulation and the Lax-Milgram theorem to demonstrate that the equations are well-posed
- Volume constraint is crucial to establish coercivity on Hilbert spaces without a trace operator—such as fractional Sobolev spaces $H^s(\Omega \cup \Omega_{\mathcal{I}}), 0 < s < 1/2$ and $L^2(\Omega \cup \Omega_{\mathcal{I}})$
- Discontinuous Galerkin FEM are conforming (LS-DYNA implementation)

Nonlocal diffusion and Navier operators

- Nonlocal diffusion equation

$$\mathcal{L}u(\mathbf{x}) = -\mathcal{D}(\Phi\,\mathcal{D}^* u)(\mathbf{x}) = 2\int_{\Omega\cup\Omega_\mathcal{I}} \gamma(\mathbf{x},\mathbf{y})\big(u(\mathbf{y}) - u(\mathbf{x})\big)\, d\mathbf{y}$$

- Peridynamic Navier equation

$$\begin{aligned}\boldsymbol{\mathcal{L}}\mathbf{u}(\mathbf{x}) &= -\mathcal{D}\Big(\eta\varpi\big(\mathcal{D}^*\mathbf{u}\big)^T\Big)(\mathbf{x}) - \mathcal{D}_\omega\Big(\sigma \mathrm{Tr}\big(\mathcal{D}_\omega^*\mathbf{u}\big)\mathbf{I}\Big)(\mathbf{x}) \\ &= \int_{\Omega\cup\Omega_\mathcal{I}} \boldsymbol{\Gamma}(\mathbf{x},\mathbf{y})\big(\mathbf{u}(\mathbf{y}) - \mathbf{u}(\mathbf{x})\big)\, d\mathbf{y}\end{aligned}$$

- The kernels $\gamma(\mathbf{x},\mathbf{y})$ and $\boldsymbol{\Gamma}(\mathbf{x},\mathbf{y})$ determine whether $\mathcal{L}$ and $\boldsymbol{\mathcal{L}}$ smooth the data—kernels must be non-integrable otherwise $L^2(\Omega\cup\Omega_\mathcal{I})$ is mapped to $L^2(\Omega\cup\Omega_\mathcal{I})$

Nonconvex Material Model

- Strain

$$\mathcal{S}_u(\mathbf{y},\mathbf{x}) = \frac{u(\mathbf{y},t) - u(\mathbf{x},t)}{|\mathbf{y}-\mathbf{x}|} \cdot \frac{\mathbf{y}-\mathbf{x}}{|\mathbf{y}-\mathbf{x}|}$$

- Internal force density

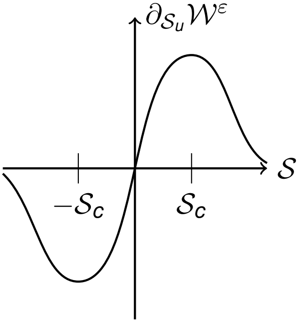
$$\frac{4}{|\mathcal{H}_\varepsilon(\mathbf{x})|} \int_{\mathcal{H}_\varepsilon(\mathbf{x})} \partial_{\mathcal{S}_u} \mathcal{W}^\varepsilon \left(\mathcal{S}_u(\mathbf{y},\mathbf{x}), \mathbf{y}-\mathbf{x}\right) \frac{\mathbf{y}-\mathbf{x}}{|\mathbf{y}-\mathbf{x}|} \, d\mathbf{y}$$

where

$$\mathcal{W}^\varepsilon\left(\mathcal{S}_u(\mathbf{y},\mathbf{x}), \mathbf{y}-\mathbf{x}\right) = \frac{2}{\varepsilon} \Psi\left(|\mathbf{y}-\mathbf{x}| \mathcal{S}_u^2(\mathbf{y},\mathbf{x})\right) J\left(\frac{|\mathbf{y}-\mathbf{x}|}{\varepsilon}\right)$$

J is a positive weighting function, Ψ is a C^1 scalar function $\Psi(0) = 0 < \Psi(0)$

Nonconvex $\partial_{\mathcal{S}_u}\mathcal{W}^\varepsilon$



- Equation of motion is well-posed (given initial conditions, volume constraint) in $C^2([0,T];L^2_0(\Omega))$ (Lipton 2014, 2015)

Complex fracture nucleation and evolution

- Linear stability analysis for a small jump discontinuity given the nonconvex material model
- If the stability matrix is indefinite (positive, negative eigenvalues) then exponential growth of jump may occur
- Significance is that cracks may nucleate spontaneously—no supplemental kinetic relation or explicit damage evolution law
- As the horizon $\varepsilon \to 0$, the solution of the peridynamic equation
  1. is that of the Navier equation away from the crack set, and
  2. on the crack set, the solution has bounded Griffith surface energy with critical energy release rate
- Numerical examples support theoretical findings

Summary

- Peridynamic balance laws are defined for discontinuous motion—same equations hold on and off of discontinuities, minimal supplementary relations
- Much has been accomplished (but much) more work needs to be done—development of constitutive relations and improving usability of codes are a priority
- LS-DYNA entry is a welcome addition

Data driven mechanics

- DIC (digital image correlation) generates a tremendous amount of data that is largely unused
- Can we exploit this technology for material identification and model fit?
- Determine objective measures for accessing and comparing models