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A Mathematical Theory for Peridynamics: Force Flux and the Peridynamic Stress Tensor

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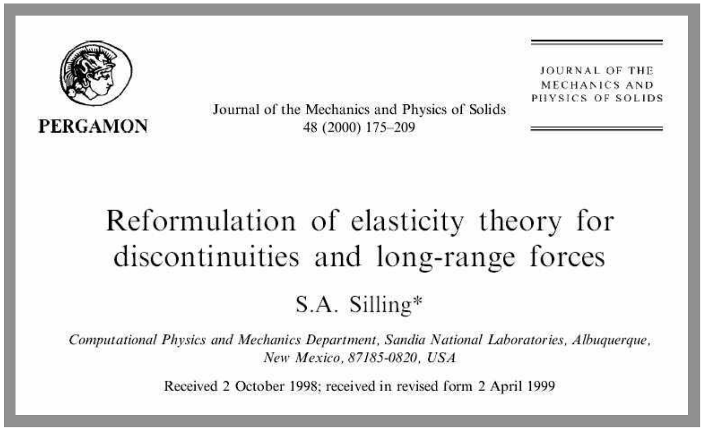
Peridynamics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Reformulation of elasticity theory for discontinuities and long-range forces

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- Original motivation: continuum theory for cracks and fragmentation
- Peridynamics (PD)
  - Uses a *nonlocal* model of force
  - No assumption on the displacement field

- Micro-continuum theories defined by embedding a continuum model with *non-locality* to describe long-range material interaction
- These theories are certainly not new, eg
  - Cosserat brothers(1909)
  - Micromorphic (Eringen 1960’s)

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Three types of non-local micro-continuum theories

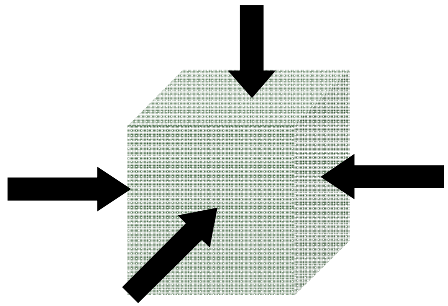
- Augment the displacement field with supplementary fields to provide information on fine-scale kinematics
- Augment the gradient of the displacement field with higher order gradients
- Use an integral operator (local average)

Average the strain

$$\boldsymbol{\sigma}(\mathbf{x}) = \int_V \mathbf{D}_e \alpha(\mathbf{x}, \boldsymbol{\xi}) \boldsymbol{\epsilon}(\boldsymbol{\xi}) \, d\boldsymbol{\xi} = \mathbf{D}_e \int_V \alpha(\mathbf{x}, \boldsymbol{\xi}) \boldsymbol{\epsilon}(\boldsymbol{\xi}) \, d\boldsymbol{\xi} = \mathbf{D}_e \overline{\boldsymbol{\epsilon}}(\mathbf{x}) \qquad (12)$$

Our view is that assuming a strain (gradient of a displacement) is problematic. Can we postulate a micro-continuum theory without assumptions on the displacement?

Local and nonlocal force models

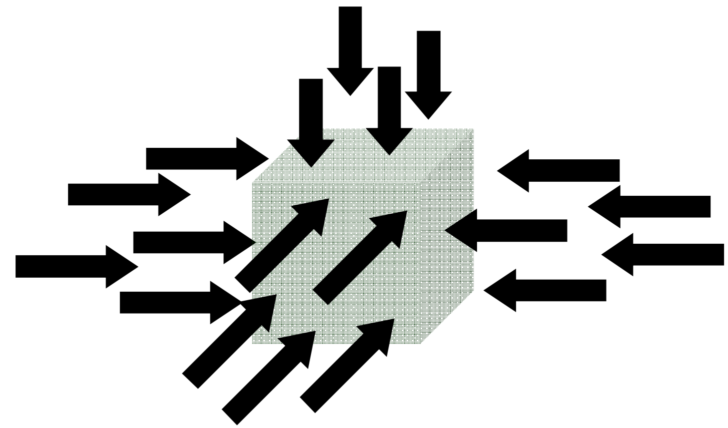


Classical model (Cauchy): Exterior of cube imparts force to the interior via the surface

$$\int \mathbf{t}(x,\mathbf{n})dS$$

Force is local because the postulate is that the force between the interior and exterior can be confined to the surface

Classical continuum particles cannot exert force on each other when NOT in contact



Non-local model:
Exterior of cube imparts force to the interior—***not just at the surface***

Nearly all classical continuum discretizations (EFG, SPH, MPM, XFEM) assume a local force model, and differentiability of the displacement field

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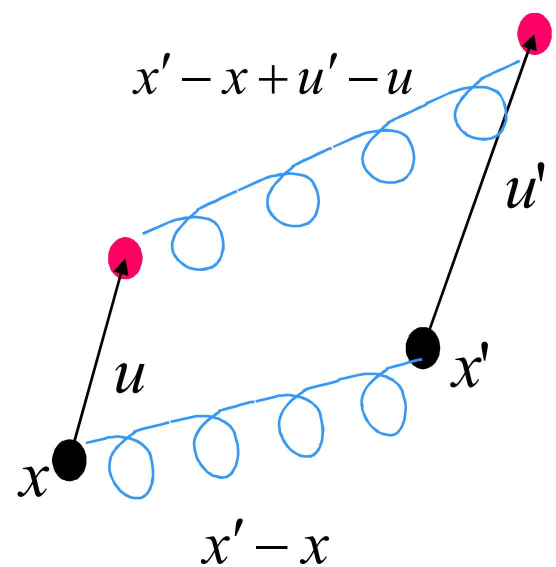
PD (peridynamics) equation of motion

- PD equation of motion (Silling 2000)

$$\rho \ddot{u} = \int_R f(u' - u, x' - x)\,dV' + b$$

$$u = u(x,t)$$
$$u' = u(x',t)$$
$$b = b(x,t)$$

- $f(\cdot,\cdot)$ is the force density per unit volume that x' exerts on *x*, given



- material-specific behavior is contained in $f(\cdot,\cdot)$ and is a function of displacement
  - Classical continuum mechanics assumes a stress-strain relationship

Equivalent PD Equation of Motion

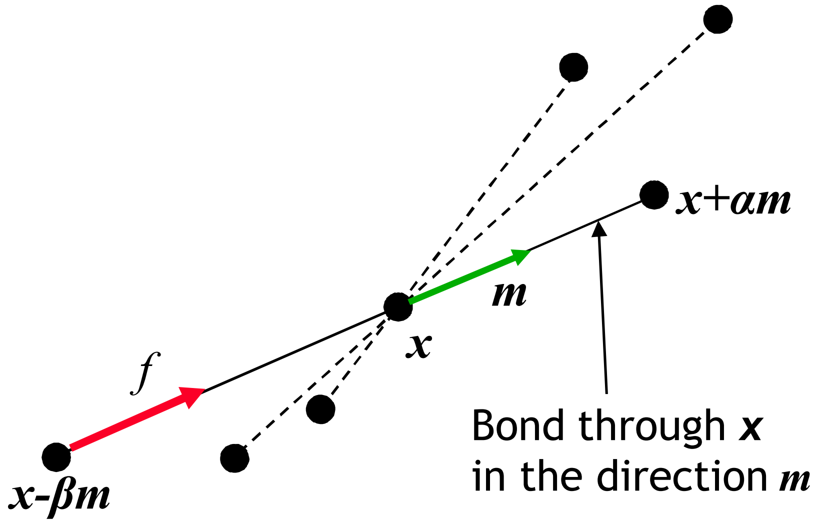
$$\rho \ddot{u} = \int_R f(u' - u, x' - x)\, dV' + b$$

• As originally presented, stress (force per unit area) is not a primary quantity (or even a well-defined one) for PD

• Can we formulate PD in a more conventional fashion?

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

PD stress tensor



$$\nu(x) = \frac{1}{2}\int_S \int_0^\infty \int_0^\infty (\alpha+\beta)^2 f(u'-u, (\alpha+\beta)\mathbf{m}) \otimes \mathbf{m} \; d\alpha \, d\beta \, d\Omega_m$$

$$f \in C^1 \Rightarrow \nabla \cdot \nu(x) = \int_R f(u'-u, x'-x)\, dV'$$

Variational formulation for the PD Stress tensor

$$\inf \frac{1}{2}\int |v_i|^2 \quad \text{subject to} \quad \nabla \cdot v_i = \int_B f_i(u'-u, x'-x)\,dV'$$

$$v_i \in H_0(div, B)$$

$$v(x) = \frac{1}{2}\int_S \int_0^\infty \int_0^\infty (\alpha+\beta)^2 f(u'-u, (\alpha+\beta)\mathbf{m}) \otimes \mathbf{m}\, d\alpha\, d\beta\, d\Omega_m$$

solves the above minimization problem!

$$H_0(div, B) = \left\{ u \mid u \in L^2(B)^3, \nabla \cdot u \in L^2(B), u \cdot n\,|_{\partial B} = 0 \right\}$$

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Let's step back in time

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.

- See Timoshenko, History of the strength of materials, pages 108-109
- Loose translation of a definition due to St. Venant that was accepted by Cauchy (See Todhunter and Pearson for the definition in French)
- Substitute peridynamic particle for molecule

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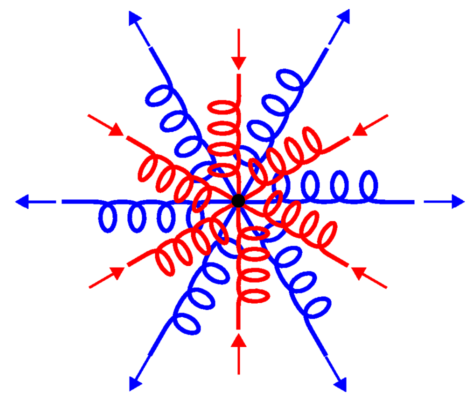
Unstressed configurations

- Forces between particles can be nonzero even when the stress vanishes
  - Newton's second law implies that the sum of forces is zero—not that any of the forces is zero
  - Typically some pairs of particles are repelling while others are attracting
  - Peridynamic model can account for much more complex "force structure"
  - Reminiscent of atomistics
- Unless there is direct contact, the classical theory implies that the forces are zero

$$\nabla \cdot \nu = 0 = \int_R f(u' - u, x' - x)\,dV'$$

$$\not\Rightarrow \quad f(u' - u, x' - x) = 0 \;\; \forall x'$$



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PD Force Flux

$$\int_B \big(\rho\ddot{u}(x,t) - b\big)dV, \quad B \subset R$$

$$= \int_B \int_R f(u' - u, x' - x)\,dV'dV$$

$$= \int_B \nabla \cdot \nu(x)\,dV = \int_{\partial B} \nu(x)\mathbf{n}\,dA$$

- We define $\tau(x,n)$ to be the peridynamic *force flux*

$$\equiv \int_{\partial B} \tau(x,\mathbf{n})\,dA$$

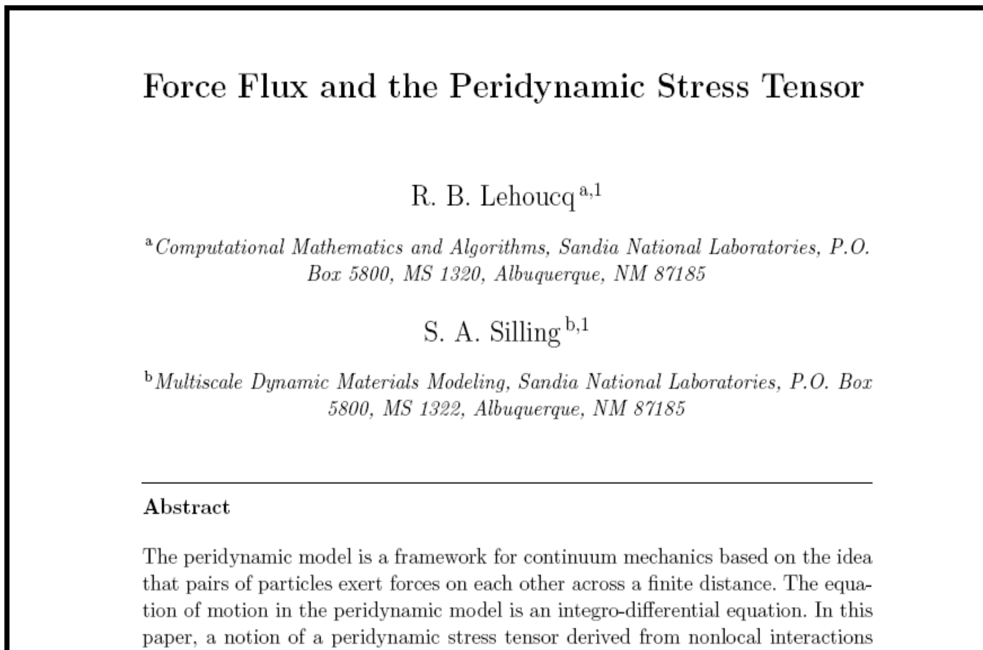
- Represents the force per unit area exerted on the interior of B

Force Flux and the PD stress tensor

$$\rho\ddot{u} = \int_R f(u' - u, x' - x)dV' + b$$

$$\rho\ddot{u} = \nabla \cdot \nu(x) + b$$

Well posed PD traction vector (force flux) can be handed over to classical continuum mechanics (say FEM) so that PD to FEM coupling is enabled



Force Flux and the Peridynamic Stress Tensor

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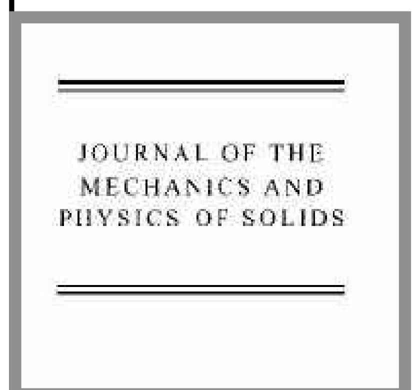
Abstract

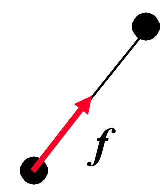
The peridynamic model is a framework for continuum mechanics based on the idea that pairs of particles exert forces on each other across a finite distance. The equation of motion in the peridynamic model is an integro-differential equation. In this paper, a notion of a peridynamic stress tensor derived from nonlocal interactions

Accepted in



PD for non-pairwise forces

Force function $f(\cdot,\cdot)$ acting along a line between **x** and **x**´ not necessary for deriving a more general PD



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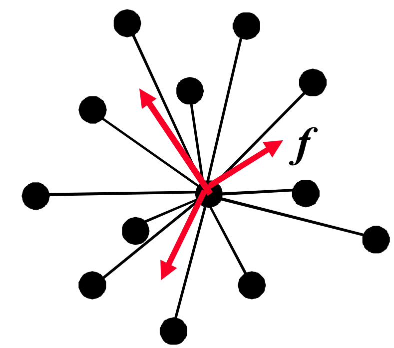

State

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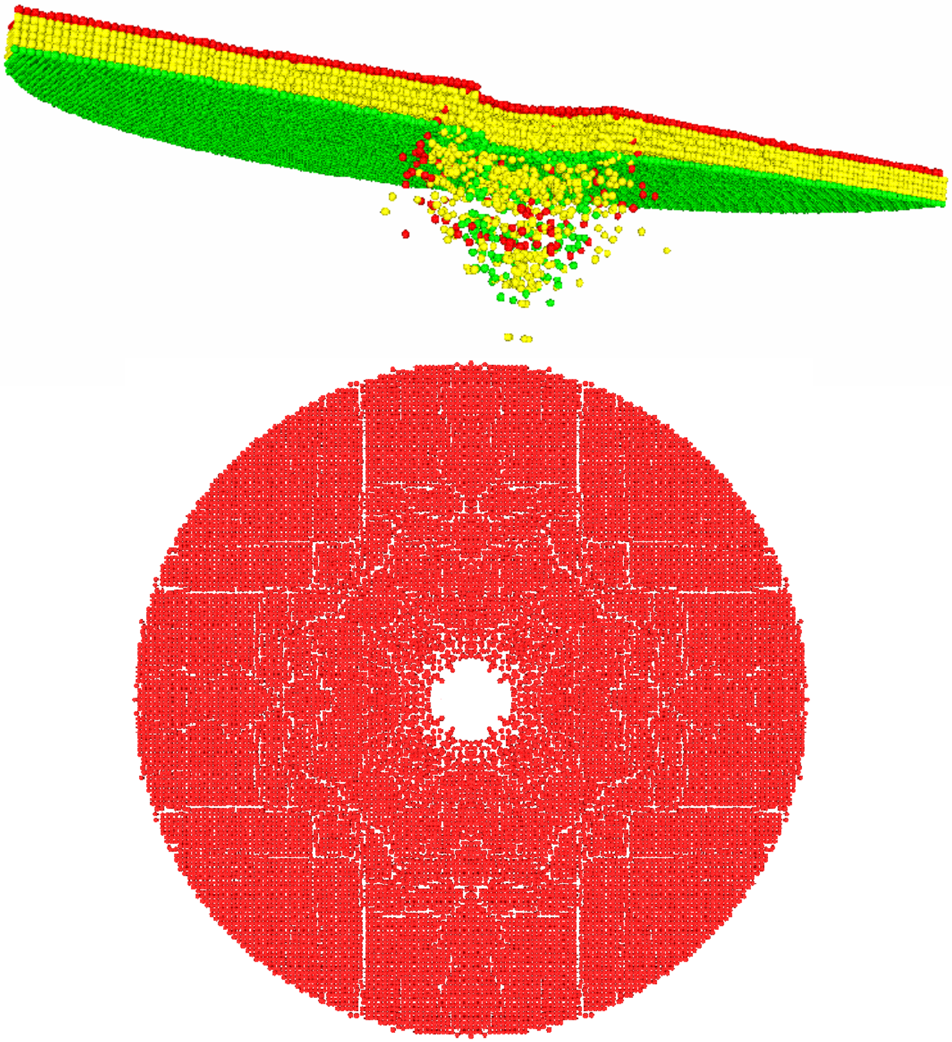
Peridynamic States and Constitutive Modeling

S. A. Silling · M. Epton · O. Weckner · J. Xu · E. Askari

PD implementation within LAMMPS

- LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) open source C++ software for MD
- Provide MD users a computational microcontinuum mechanics capability
- Provide PD users the ability to use interatomic potentials
- Silling has a Fortran 90 code EMU for PD



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