Mathematical and numerical analysis of peridynamics for multiscale materials modeling

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INTRODUCTION

- Silling proposes the peridynamic nonlocal continuum theory

PERGAMON — Journal of the Mechanics and Physics of Solids 48 (2000) 175–209

Reformulation of elasticity theory for discontinuities and long-range forces

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✓ *Motivation:* materials undergoing discontinuous deformation

✓ *Goal:* Dynamic material failure simulations

✓ *Key:* Nonlocal model of force via integral operators

✓ Generalization to "State-based" theory proposed in 2007

- A statistical mechanical basis for nonlocality appears in

PHYSICAL REVIEW E 84, 031112 (2011)

Statistical mechanical foundation of the peridynamic nonlocal continuum theory: Energy and momentum conservation laws

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✓ Important conclusion is that nonlocality is intrinsic to continuum balance laws

- Recent review

Advances in Applied Mechanics, Volume 44, 2010, Pages 73–168

Peridynamic Theory of Solid Mechanics

S.A. Silling and R.B. Lehoucq

✓ Balance of energy; second law of thermodynamics

OBJECTIVES

- Mathematical analysis for the peridynamic continuum theory; preliminary theory given in

ESAIM: Mathematical Modelling and Numerical Analysis

MATHEMATICAL ANALYSIS FOR THE PERIDYNAMIC NONLOCAL CONTINUUM THEORY

Qiang Du and Kun Zhou

SIAM J. Numer. Anal. — © 2010 Society for Industrial and Applied Mathematics

MATHEMATICAL AND NUMERICAL ANALYSIS OF LINEAR PERIDYNAMIC MODELS WITH NONLOCAL BOUNDARY CONDITIONS

Kun Zhou and Qiang Du

✓ In particular, provide a mathematical analysis for the state-based theory

- Describe *volume-constraints*, the nonlocal analogue of boundary conditions
- Analysis facilitated by the development of a *nonlocal vector calculus*; preliminary development given in

Multiscale Model. Simul. — © 2010 Society for Industrial and Applied Mathematics

A NONLOCAL VECTOR CALCULUS WITH APPLICATION TO NONLOCAL BOUNDARY VALUE PROBLEMS

Max Gunzburger and R. B. Lehoucq

- Short-term goal: linear peridynamic materials, diffusion, numerical analysis
- Long-term goal: nonlinear peridynamic materials, coupling with the classic theory and molecular dynamics

OVERVIEW

- Balance of linear momentum

$$\rho(x,t)\ddot{y}(x,t) = \int_{\mathbb{R}^3} \big(\mathbf{t}(x',x,t) - \mathbf{t}(x,x',t)\big)dx' + b(x,t)$$

- Balance of linear momentum is equivalent to or action-reaction.

$$\int_{\Omega_1}\int_{\Omega_2} \big(\mathbf{t}(x',x,t) - \mathbf{t}(x,x',t)\big)dx'dx + \int_{\Omega_2}\int_{\Omega_1} \big(\mathbf{t}(x',x,t) - \mathbf{t}(x,x',t)\big)dx'dx = 0$$

$$\forall \Omega_1 \,\&\, \Omega_2, \Omega_1 \cap \Omega_2 = \varnothing$$

- Nonlocal because force may be nonzero even when Ω_1 and Ω_2 are not in contact

$$\underbrace{\int_{\Omega} \rho(x,t)\ddot{y}(x,t)dx}_{\text{Rate of change of momentum}} = \underbrace{\int_{\Omega}\int_{\mathbb{R}^3\setminus\Omega} \big(\mathbf{t}(x',x,t) - \mathbf{t}(x,x',t)\big)dx'dx}_{\text{Force exerted upon }\Omega} + \underbrace{\int_{\Omega} b(x,t)dx}_{\text{External force upon }\Omega}$$

- Balance of energy

$$\underbrace{\frac{d}{dt}\int_{\Omega}\varepsilon(x,t)dx}_{\text{Internal energy}} + \underbrace{\frac{1}{2}\frac{d}{dt}\int_{\Omega}\dot{y}(x,t)\bullet\dot{y}(x,t)dx}_{\text{Kinetic energy over }\Omega} = \underbrace{\int_{\Omega}\int_{\mathbb{R}^3\setminus\Omega} \big(\mathbf{t}(x',x)\bullet\dot{y}(x',t) - \mathbf{t}(x,x')\bullet\dot{y}(x,t)\big)dx'dx}_{\text{Supplied power to }\Omega}$$

$$+ \underbrace{\int_{\Omega}\int_{\mathbb{R}^3\setminus\Omega} q(x',x)dx'dx}_{\text{Supplied thermal power to }\Omega}$$

$$\dot{\varepsilon}(x,t) = \underbrace{\int_{\mathbb{R}^3} \mathbf{t}(x',x)\bullet\big(\dot{y}(x',t) - \dot{y}(x,t)\big)dx'}_{\text{Absorbed power density}} + \underbrace{\int_{\mathbb{R}^3} q(x',x)dx'}_{\text{Thermal power}}$$

- Constitutive relations

Define the deformation state $\underline{\mathbf{Y}}[x,t]\langle x'-x\rangle := y(x',t) - y(x,t) \;\; \forall x'$ so that the *Force State* $\underline{\mathbf{T}}[x,t] = \hat{\underline{\mathbf{T}}}\big(\underline{\mathbf{Y}}[x,t]\big)$ depends collective motion

The needed relations can be written as

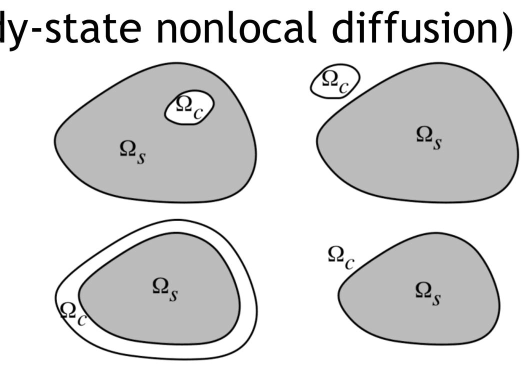
$$\mathbf{t}(x',x,t) = \underline{\mathbf{T}}[x,t]\langle x'-x\rangle = \hat{\underline{\mathbf{T}}}\big(\underline{\mathbf{Y}}[x,t]\big)\langle x'-x\rangle$$
$$q(x',x,t) = \underline{Q}[x,t]\langle x'-x\rangle = \hat{\underline{Q}}\big(\underline{\mathbf{Y}}[x,t]\big)\langle x'-x\rangle$$

- Can now discuss the well-posedness of the balance laws; in particular for linear materials
- Can also show that the second law of thermodynamic is not violated for classes of materials

CASE STUDY: NONLOCAL DIFFUSION

- Special case of the balance of energy of linear diffusion (modeling anomalous diffusion) serves to introduce the nonlocal vector calculus and provide well-posedness
- Consider the nonlocal Dirichlet problem (steady-state nonlocal diffusion)

$$\mathcal{D}\big(\Theta\mathcal{D}^*\big)u = f \;\text{ on } \Omega_s$$
$$u = g \;\text{ on } \Omega_c$$



- The solution constrained over the volume Ω_c
- A volume-constrained problem is the nonlocal analogue of a boundary value problem

$$\big(\mathcal{D}f\big)(x) := \int_{\mathbb{R}^n} \big(f(x,y) + f(y,x)\big)\cdot\boldsymbol{\alpha}(x,y)dy, \quad \boldsymbol{\alpha}(x,y) = -\boldsymbol{\alpha}(y,x)$$

$$\big(\mathcal{D}^*u\big)(x,y) := -\big(u(y,t) - u(x,t)\big)\boldsymbol{\alpha}(x,y)$$

$$\mathcal{D}\big(\Theta\mathcal{D}^*u\big)(x) = 2\int_{\mathbb{R}^n} \big(u(y,t) - u(x,t)\big)\boldsymbol{\alpha}(x,y)\cdot\Theta(x,y)\boldsymbol{\alpha}(x,y)dy$$

- $\mathcal{D}$ and $\mathcal{D}^*$ are the nonlocal divergence and it's adjoint; the operator $\mathcal{D}\mathcal{D}^*$ is the nonlocal Laplacian
- The kernel $\alpha\Theta\alpha$ determines the regularity for the volume-constrained problem; an integrable kernel implies that $\mathcal{D}\Theta\mathcal{D}^*u : L^2(\Omega_s\cup\Omega_c) \rightarrow L^2(\Omega_s\cup\Omega_c)$; no smoothing of the data
- Fractional smoothing occurs for $\alpha(x,y)\Theta(x,y)\alpha(x,y) \sim |x-y|^{-n-2s}, 0<s<1$ because then $\mathcal{D}\Theta\mathcal{D}^*u : H^s(\Omega_s\cup\Omega_c) \rightarrow H^s(\Omega_s\cup\Omega_c)$
- Can extend to nonlocal Neumann, Robin problems; also consider peridynamic linear elastic volume-constrained problems

SUMMARY

- Peridynamic continuum theory reformulated using a nonlocal vector calculus
- Variational formulation leads to the well-posedness of the
  - ✓ peridynamic equilibrium equation for linear isotropic solids
  - ✓ nonlocal linear diffusion
- Deformation can be discontinuous
- Volume-constraints, the nonlocal analogue of boundary conditions, are crucial

Related work

- Probabilistic interpretation for nonlocal linear diffusion
- Nonlocal, nonlinear advection
- Finite element formulation; see

Comput. Methods Appl. Mech. Engrg.

Continuous and discontinuous finite element methods for a peridynamics model of mechanics

X. Chen, Max Gunzburger

- Two Ph.d theses; Pablo Seleson (FSU) and Nate Burch (CSU)

PUBLICATIONS

1. *A nonlocal vector calculus, nonlocal volume-constrained problems, and nonlocal balance laws* SAND 2010-8353J (Q. Du, M. Gunzburger, R. Lehoucq, K. Zhou).
2. *An approach to nonlocal, nonlinear advection* SAND 2011-3164J (Q. Du, J. Kamm, R. Lehoucq, M. Parks).
3. *Analysis and approximation of nonlocal diffusion problems with volume constraints* SAND 2011-3168J (Q. Du, M. Gunzburger, R. Lehoucq, K. Zhou)
4. *Application of a nonlocal vector calculus to the analysis of linear peridynamic materials* SAND 2011-3870J (Q. Du, M. Gunzburger, R. Lehoucq, K. Zhou)
5. *A posteriori error analysis of finite element method for linear nonlocal diffusion and peridynamic models* (Q. Du, L. Ju. L. Tian, K. Zhou)

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