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

Rich Lehoucq and Mark P. Sears, Phys Rev E **84** 2011
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Outline

- Provide a basis for the peridynamic balance laws using the principles of non-equilibrium statistical mechanics
- Integral operators replace the classical divergence operators
- The classical balance laws can be derived by subsequent assumptions, e.g., contact force and power expenditures

Statistical Mechanics

- The macroscopic world is comprised of atoms, or particles
- The motion of atoms subject to forces dictates the behavior of bodies
- Given the enormous number of atoms (10^{23}) comprising the macroscopic world, consider instead their averaged behavior using the principles of probability
- Such averaged behavior is exemplified by continuum mechanics, a phenomenological description
- Let's explain *a* link between the world of particles and continuum mechanics using the principles of statistical mechanics

The balance laws of classical continuum mechanics

Mass: $$\frac{\partial}{\partial t}\rho + div\left(\rho \mathbf{v}\right) = 0$$

Momentum: $$\frac{\partial}{\partial t}\left(\rho \mathbf{v}\right) + div\left(\rho \mathbf{v} \otimes \mathbf{v}\right) = div\left(\boldsymbol{\sigma}_K + \boldsymbol{\sigma}_U\right)$$

Energy: $$\frac{\partial}{\partial t}\varepsilon + div\left(\varepsilon \mathbf{v}\right) = div\left((\boldsymbol{\sigma}_K + \boldsymbol{\sigma}_U)\mathbf{v} - (\mathbf{q}_K + \mathbf{q}_U)\right)$$

$\boldsymbol{\sigma}_K, \mathbf{q}_K$ are the kinetic molecular contributions to the stress and heat flux

$\boldsymbol{\sigma}_U, \mathbf{q}_U$ are the contributions due to molecular forces to the stress and heat flux

The peridynamic balance of linear momentum

$$\frac{\partial}{\partial t}\left(\rho v\right)+div\left(\rho v\otimes v\right)=div\boldsymbol{\sigma}_K+\underbrace{\int_{\mathbb{R}^3}\left(T(x,x')-T(x',x)\right)dx'}_{\text{internal force, analogue of } div\,\boldsymbol{\sigma}_U}$$

Classical: $\frac{\partial}{\partial t}\left(\rho v\right)+div\left(\rho v\otimes v\right)=div\left(\boldsymbol{\sigma}_K+\boldsymbol{\sigma}_U\right)$

The peridynamic balance of energy

$$\frac{\partial}{\partial t}\varepsilon + div\left(\varepsilon v\right) = div\left(\boldsymbol{\sigma}_K v - q_K\right)$$

$$+ \underbrace{\int_{\mathbb{R}^3} \left(T(x,x')\bullet v(x) - T(x',x)\bullet v(x')\right) dx'}_{\text{internal power (analogue of div } \boldsymbol{\sigma}_U v\text{)}}$$

$$+ \underbrace{\int_{\mathbb{R}^3} \left(h(x,x',t) - h(x',x,t)\right) dx'}_{\text{internal heating (analogue of div } q_U\text{)}}$$

Classical: $$\frac{\partial}{\partial t}\varepsilon + div\left(\varepsilon v\right) = div\left(\boldsymbol{\sigma}_K v - q_K\right) + div\left(\boldsymbol{\sigma}_U v - q_U\right)$$

The plot

- Classical, peridynamic balance laws
- Particle mechanics
- Expected values in phases, or ensemble averages in phase space
- Peridynamic balance of linear momentum
- Peridynamic balance of energy

Hamiltonian and conservative particle forces

- Energy for the particle system is given by the Hamiltonian

$$H = \underbrace{\sum_{i=1}^{N} \frac{1}{2m_i} p_i \bullet p_i}_{\text{Kinetic energy}} + \underbrace{U(x_1, \ldots, x_N)}_{\text{Potential energy}}$$

- Force on particle i is given by

$$-\frac{\partial}{\partial x_i} H = -\frac{\partial}{\partial x_i} U = -\nabla_{x_i} U$$

is by definition a conservative force

Potential U

- The force exerted on particle i by the remaining particles is $-\nabla_{x_i} U$

- Assume U is invariant under translation, rotation, and reflection

$$U(Qx_1 + c, \ldots, Qx_N + c) = U(x_1, \ldots, x_N)$$

where Q and c are an orthogonal matrix and constant vector, respectively

- Pair potential is a special case; we consider general multibody potentials

Resulting force interaction

$$U = \hat{U}(\underbrace{\xi_{1,2}, \xi_{1,3}, \ldots, \xi_{N-1,N}}_{\frac{N(N-1)}{2} \text{ distances}}), \quad \xi_{ij} = \frac{1}{2}\left|x_i - x_j\right|^2$$

$$-\nabla_{x_i} U = \sum_j \mathbf{f}_{ij}, \quad \mathbf{f}_{ij} = \underbrace{(x_i - x_j)}_{\text{elongation}} \underbrace{\frac{\partial U}{\partial \xi_{ij}}}_{\text{stiffness}}$$

1. $\mathbf{f}_{ij} = -\mathbf{f}_{ji}$ (action-reaction)
2. $\mathbf{f}_{ij} \times (x_i - x_j) = \mathbf{0}$ (colinearity)

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Phase space

$$\Pi_N := \mathcal{E}_1 \times \mathcal{V}_1 \times \cdots \times \mathcal{E}_N \times \mathcal{V}_N$$ is "phase space"

$x_i \in \mathcal{E}_i$ point space for particle *i*

$p_i \in \mathcal{V}_i$ vector space for the momentum of particle *i*

Phase space density

$\Pi_N := \mathcal{E}_1 \times \mathcal{V}_1 \times \cdots \times \mathcal{E}_N \times \mathcal{V}_N$ is "phase space"

$f : \Pi_N \times \mathbb{R} \to \mathbb{R}$ is phase space density

$$f \geq 0, \int_{\Pi_N} f = 1$$

$$f(x_1,\ldots,x_N,p_1,\ldots,p_N,t)dx_1 \cdots dx_N dp_1 \cdots dp_N$$

is the probability that the i-th particle has position and velocity between (x_i, p_i) and $(x_i + dx_i, p_i + dp_i)$

Liouville's equation

$$\frac{\partial}{\partial t} f + \mathrm{div}(f\dot{\pi}) = 0,\ \dot{\pi} = \frac{d}{dt}\pi,\ \pi \in \Pi_N$$

Conservative particle forces imply

$$\mathrm{div}(\dot{\pi}) = 0$$

and results in Liouville's equation:

$$\frac{\partial}{\partial t} f + \dot{\pi}\cdot\mathrm{grad}(f) = 0$$

Expectation in phase space

$$\langle \alpha ; f \rangle := \int_{\Pi_N} \alpha(\pi) f(\pi, t)\, dV_\pi, \quad \pi \in \Pi_N$$

is the expected value of $\alpha : \Pi_N \to \mathbb{R}$

$$\frac{\partial}{\partial t} \langle \alpha ; f \rangle = -\langle \alpha ; \dot{\pi} \cdot \mathrm{grad}_\pi (f) \rangle \quad \text{(Liouville's eqn)}$$

$$= \langle \dot{\pi} \cdot \mathrm{grad}_\pi (\alpha) ; f \rangle \quad \text{(Divergence thm)}$$

Related work

- Deriving balance laws using the principles of statistical mechanics started with the seminal paper by Irving and Kirkwood JCP 1950; many approximations and a pair potential
- Noll 1955 removed the above approximations
  - Noll introduced two amazing Lemmas that provide closed form expressions for the stress, heat fluxes
- Related approach by Hardy, JCP 1982, worked in real space and also removed approximations (unaware of Noll's work)
  - Another set of closed form expressions for the stress, heat fluxes
- Murdoch & Bedeaux, Proc. Roy. Soc. London A. 1994, (unaware of Hardy's work), similar in scope used Noll's two Lemmas

Related work

- Much recent work on understanding microscopic stress (see Admal & Tadmor, J. Elasticity 2010);
  - Admal & Tadmor JCP 2011 for the balance of energy
  - used a multibody potential
- See also very recent book by Murdoch *Physical Foundations of Continuum Mechanics*

We avoid determining expressions for the stress, heat flux given a multibody potential

Avoid the divergence operator and use the integral expressions

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Momentum density

$$\alpha(\pi) = \sum_{i=1}^{N} p_i \phi(x - x_i), \quad \phi : \mathbb{R}^3 \to \mathbb{R}, \phi \geq 0, \int \phi = 1$$

$\rho v := \langle \alpha; f \rangle = \langle \sum_{i=1}^{N} p_i \phi(x - x_i); f \rangle$ is momentum density in phase space

$\phi(x - x_i)dx$ is the probability of locating x_i about the volume dx

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After the dust settles

$$\frac{\partial}{\partial t}(\rho v) + \mathrm{div}(\rho v \otimes v) =$$

$$\overbrace{\mathrm{div}\boldsymbol{\sigma}_K}^{\text{Internal kinetic force}} \quad \overbrace{-\langle \sum_{i,j}^{N} \frac{\partial U}{\partial \xi_{ij}} (x_i - x_j)\phi(x - x_i) \rangle}^{\text{Internal force density}}$$

$$v(x,t) := \frac{\langle \sum_{j=1}^{N} p_j \phi(x - x_j); f \rangle}{\langle \sum_{j=1}^{N} m_j \phi(x - x_j); f \rangle}$$ is the mean velocity of the N particles

kinetic stress is $\boldsymbol{\sigma}_K(x,t) := -\langle \sum_{i=1}^{N} m_i (\dot{x}_i - v) \otimes (\dot{x}_i - v)\phi(x - x_i); f \rangle$

Statistical basis for the peridynamic balance of linear momentum derived

$$\frac{\partial}{\partial t}(\rho v) + \mathrm{div}(\rho v \otimes v)$$
$$= \mathrm{div}\boldsymbol{\sigma}_k + \int \left(T(x, x') - T(x', x) \right) dx'$$

$$T(x, x') = \frac{1}{4} \langle \sum_{i,j}^{N} \frac{\partial U}{\partial \xi_{ij}} \left(x_j - x_i \right) \phi(x - x_i) \phi(x' - x_j); f \rangle$$
$$- \frac{1}{4} \langle \sum_{i,j}^{N} \frac{\partial U}{\partial \xi_{ij}} \left(x_j - x_i \right) \phi(x' - x_i) \phi(x - x_j); f \rangle$$

- $T(x, x')$ is a field quantity representing force
- The difference $T(x, x')dxdx' - T(x', x)dx'dx$ is the force between dx and dx'

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Force interaction and the force state

1. $\mathbf{f}_{ij} = -\mathbf{f}_{ji}$ (action-reaction)
2. $\mathbf{f}_{ij} \times (x_i - x_j) = \mathbf{0}$ (colinearity)

1. $T(x,x') - T(x',x) = -\left(T(x',x) - T(x,x')\right)$ (action-reaction)
2. $\left(T(x,x') - T(x',x)\right) \times \left(x' - x\right) \neq 0$ in general; justifies non-ordinary peridynamic materials

Necessary and sufficient condition for the balance of angular momentum is

$$\int_{\mathbb{R}^3} \left(x' - x\right) \times T(x,x')dx' = 0 \text{ for all } x$$

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Energy density

$$\alpha(\pi) = \sum_{i=1}^{N} e_i \phi(x - x_i), \quad \phi : \mathbb{R}^3 \to \mathbb{R}, \phi \geq 0, \int \phi = 1$$

$$e_i = \frac{m_i}{2} v_i \bullet v_i + U^{(i)}$$

$\varepsilon_i := \langle \sum_{i=1}^{N} e_i \phi(x - x_i); f \rangle$ is energy density in phase space

$U^{(i)}$ is a partition of the potential energy among the N particles

Peridynamic balance of energy

$$\frac{\partial}{\partial t}\varepsilon + div\left(\varepsilon v\right) = div\left(\boldsymbol{\sigma}_K v - q_K\right)$$

$$+ \underbrace{\int_{\mathbb{R}^3} \left(T(x,x')\bullet v(x,t) - T(x',x)\bullet v(x',t)\right) dx'}_{\text{internal power (analogue of div } \boldsymbol{\sigma}_U v)}$$

$$+ \underbrace{\int_{\mathbb{R}^3} \left(h(x,x',t) - h(x',x,t)\right) dx'}_{\text{internal heating (analogue of div } q_U)}$$

$$h(x,x',t) := \frac{1}{2}\langle \sum_{i,j}^{N} \frac{\partial U^{(j)}}{\partial \xi_{ij}} \bullet v_i \phi(x - x_i)\phi(x' - x_j); f \rangle$$

$$- \frac{1}{2}\langle \sum_{i,j}^{N} \frac{\partial U^{(j)}}{\partial \xi_{ij}} \bullet v_i \phi(x' - x_i)\phi(x - x_j); f \rangle - T(x,x') \cdot v(x,t)$$

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The peridynamic balance of internal energy

$$\frac{\partial}{\partial t}\varepsilon_{\text{int}} + div\left(\varepsilon_{\text{int}} v\right) = \boldsymbol{\sigma}_K : grad\, v - div\, q_K$$

$$+ \underbrace{\int_{\mathbb{R}^3} T(x',x)\bullet\left(v(x',t) - v(x,t)\right)dx'}_{\text{absorbed power (analogue of stress power)}}$$

$$+ \underbrace{\int_{\mathbb{R}^3} \left(p(x,x',t) - p(x',x,t)\right)dx'}_{\text{internal heating (analogue of the div } q_U\text{)}}$$

$$\varepsilon = \varepsilon_{\text{int}} + \frac{\rho}{2} v\bullet v; \quad p(x,x',t) = h(x,x',t) + T(x,x')\bullet v(x,t)$$

Comments

- Integral expressions avoid the effort devoted to determining stress tensor and heat flux

- Can determine expressions for heat flux and stress via Noll's Lemmas, assuming these fields sufficiently regular, e.g., are differentiable

- Where is the traction force, heat flux in the integral expressions? In other words, are the nonlocal equations we derived balance laws?

Nonlocal flux

$$\underbrace{\int_{\Omega_1}\int_{\Omega_2}\Big(T(x,x') - T(x',x)\Big)dx'dx}_{\text{force upon }\Omega_2\text{ by }\Omega_1} + \underbrace{\int_{\Omega_2}\int_{\Omega_1}\Big(T(x,x') - T(x',x)\Big)dx'dx}_{\text{force upon }\Omega_2\text{ by }\Omega_1} = 0$$

- This is action-reaction; also holds for the internal power and heating
- Equivalent conditions
    - resulting balance laws are additive over disjoint regions
    - antisymmetry of the integrand
    - no self-interaction
- The above regions need not be in contact and give rise to a nonlocal interaction

Comments

- Integral expressions make no assumptions on the differentiability of the fields (nor of any kinematic quantities)
- Given that we can determine expressions for heat flux and stress via Noll's Lemmas (assuming these fields are differentiable),
- Precisely in what sense the fields are "weak" is the subject of current research
  - the integral operators can be seen as "weak" divergence operators acting on spaces functions containing jump discontinuities

Kinematics

- But we've said nothing about kinematics
  - Silling postulated the deformation state representing collective motion

- Discontinuous deformation allowed—jump discontinuities are allowable and require no special treatment

- See recent J. Elasticity paper where the peridynamic Navier equation is demonstrated to be well-posed in the space of square integrable functions