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

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The statistical mechanical foundation of the peridynamic nonlocal continuum theory: energy and momentum conservation laws

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Abstract

The purpose of this paper is to derive the energy and momentum conservation laws of the peridynamic nonlocal continuum theory using the principles of classical statistical mechanics. The peridynamic laws allow the consideration of discontinuous motion, or deformation, by relying on integral operators. These operators sum forces and power expenditures separated by a finite distance and so represent nonlocal interaction. The integral operators replace the differential divergence operators conventionally used so obviating special treatment at points of discontinuity.

The derivation presented employs a general multibody interatomic potential avoiding the standard assumption of a pairwise decomposition. The integral operators are also expressed in terms of a stress tensor and heat flux vector under the assumption that these fields are differentiable demonstrating that the classical continuum energy and momentum conservation laws are consequences of the more general peridynamic laws. An important conclusion is that nonlocal interaction is intrinsic to continuum conservation laws when derived using the principles of statistical mechanics.

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1. INTRODUCTION

Dynamics in continuum mechanics is established by the phenomenological balance laws describing conservation of mass, momentum, and energy. In Eulerian form, the classical balance laws for conservation of mass, linear momentum and energy are

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial \mathbf{x}^{\mu}}\big(\mathbf{v}^{\mu}\rho\big) = 0, \tag{1a}$$

$$\frac{\partial}{\partial t}\boldsymbol{\pi}^{\nu} + \frac{\partial}{\partial \mathbf{x}^{\mu}}\big(\mathbf{v}^{\mu}\boldsymbol{\pi}^{\nu}\big) = \frac{\partial}{\partial \mathbf{x}^{\mu}}\boldsymbol{\sigma}^{\mu\nu}, \tag{1b}$$

$$\frac{\partial}{\partial t}\epsilon + \frac{\partial}{\partial \mathbf{x}^{\mu}}\big(\mathbf{v}^{\mu}\epsilon\big) = \frac{\partial}{\partial \mathbf{x}^{\mu}}\big(\boldsymbol{\sigma}^{\mu\nu}\mathbf{v}^{\mu} - \mathbf{q}^{\mu}\big), \tag{1c}$$

respectively, where ρ, $\boldsymbol{\pi}$, ϵ denote the mass, momentum and energies densities, respectively, $\mathbf{v}$ is the material velocity field, and $\boldsymbol{\sigma}$ and $\mathbf{q}$ denote the Cauchy stress tensor and heat flux, respectively. The balance law for the conservation of angular momentum follows from the symmetry of the Cauchy stress tensor. The balance laws (1) use lower-case Greek letters, to denote the components of vector and tensor fields over the range $1, 2, 3$ with an implied summation. This notation is adopted in the remainder of the paper.

The corresponding peridynamic nonlocal balance laws for the conservation of linear momentum and energy are given by

$$\frac{\partial}{\partial t}\boldsymbol{\pi}^{\nu} + \frac{\partial}{\partial \mathbf{x}^{\mu}}\big(\mathbf{v}^{\mu}\boldsymbol{\pi}^{\nu}\big) = \frac{\partial}{\partial \mathbf{x}^{\mu}}\boldsymbol{\sigma}_{\mathrm{K}}^{\mu\nu} + \int_{\mathbb{R}^3}\big(\mathbf{T}^{\nu}(\mathbf{x},\mathbf{x}') - \mathbf{T}^{\nu}(\mathbf{x}',\mathbf{x})\big)\,d\mathbf{x}' \tag{2a}$$

$$\frac{\partial}{\partial t}\epsilon + \frac{\partial}{\partial \mathbf{x}^{\mu}}\big(\mathbf{v}^{\mu}\epsilon\big) = \frac{\partial}{\partial \mathbf{x}^{\mu}}\big(\boldsymbol{\sigma}_{\mathrm{K}}^{\mu\nu}\mathbf{v}^{\nu} - \mathbf{q}_{\mathrm{K}}^{\mu}\big) + \int_{\mathbb{R}^3}\big(p(\mathbf{x},\mathbf{x}') - p(\mathbf{x}',\mathbf{x})\big)\,d\mathbf{x}'. \tag{2b}$$

where $\boldsymbol{\sigma}_{\mathrm{K}}^{\mu\nu}$ and $\mathbf{q}_{\mathrm{K}}^{\mu}$ are the kinetic stress tensor and kinetic heat flux, respectively. The kinetic term represents the underlying momentum exchange and potential energy of the molecules, respectively. The vector $\mathbf{T}$ and scalar p fields represent the *force* and *power* states, respectively, and have units of force and power per unit volume squared, respectively. These two fields represent nonlocal force interaction and nonlocal power expenditure due to force interaction among the molecules, or particles. The integrands of (2) are antisymmetric in the variables $\mathbf{x}$ and $\mathbf{x}'$ and so lead to a nonlocal flux.

The purpose of this paper is to derive the nonlocal energy and momentum conservation laws (2) using the principles of classical statistical mechanics given a multibody interatomic potential. The potential is assumed to be not only invariant under rotation and translation but also reflection of the particles. Our derivations are not limited to particle systems interacting via a pair-potential and so include, in principle, sophisticated molecular dynamic multibody potentials. The analysis in this paper demonstrates that the force and power states correspond naturally to microscopic notions of molecules interacting by way of an interatomic potential. We also derive a microscopic Cauchy stress tensor and heat flux fields associated with force interaction and the mechanical power expenditure among the particles. Therefore, the classical balance laws (1) follow from the peridynamic balance laws under the additional assumption that these fields are differentiable.

The peridynamic[15] continuum theory was proposed in [1] by Silling, and subsequently generalized in [2]. The recent review [3] also introduced a first law of thermodynamics and provides many citations to the peridynamic literature. The balance (2a) is the spatial or Eulerian description of the conservation of linear momentum, in contrast to the reference or Lagrangian description associated with [1, 2]. The peridynamic laws allow the consideration of discontinuous motion, or deformation, by relying on integral operators embodying nonlocal interaction. The integral operators replace the differential divergence operators conventionally used so obviating special treatment at points of discontinuity.

The first derivation of the conservation laws for continuum mechanics (1) using the principles of statistical mechanics was presented in the seminal paper by Irving and Kirkwood [4]. A difficulty encountered by Irving and Kirkwood was in the use of Dirac delta functions, which results in an inelegant set of expressions for the microscopic stress and heat flux involving an infinite expansion. Moreover, their derivation only considered particles interacting under a pair-potential.

Further progress was made by Noll [5][16]. The use of Dirac delta functions was avoided, and closed-form expressions for a stress tensor and heat flux are derived so avoiding the infinite expansion of [4] by use of a mathematically rigorous result; see Lemma I in [5] or the translation [6]. However, Noll only applied his Lemma I in the case of a pair-potential.

Hardy [7] avoided expectation in phase space and instead replaced the use of Dirac delta functions with localization functions. Hardy did not invoke Noll's Lemma, and derived another closed-form expression for a stress tensor and heat flux. However, the restriction to a pair-potential was retained. The related paper by Murdoch and Bedeaux [8] also avoids phase space expectation, employs weighting functions and exploits Noll's Lemma I for yet more closed-form expressions a stress tensor. See also the recent papers [9, 10] by Admal and Tadmor building upon and extending the aforementioned work including the consideration of a general multibody potential.

A central tenant of the current study is that the peridynamic balance laws (2) arise directly from averaging in phase space—nonlocal interaction is an intrinsic aspect. The classical balance laws (1) are derived under further assumptions, e.g., the hypotheses needed by Lemma I in [5]. As we will demonstrate, the balance laws (2) embody a notion of nonlocal flux and correspond to a continuum version of particle mechanics remaining valid under a discontinuous deformation.

The paper is organized as follows. Section 2 introduces the microscopic model employed, including the presentation of the multibody interatomic potential, a brief overview of expectation in phase space, and a listing of the mass, momentum energy densities including a derivation of mass conservation (1a) and material velocity $\mathbf{v}$ in Subsection 2.3. Sections 3 and 4 derive the peridynamic balance laws (2). The latter section also derives the related balance of internal energy. The latter two sections also derive the corresponding classical balance laws (1b) and (1b) given the peridynamic balance laws. Section 5 summarizes the results of the paper.

2. PRELIMINARIES

The procedure used to derive the peridynamic balance laws (2) parallels the approach pioneered by Irving and Kirkwood. A microscopic model is proposed and we assume that observables are given by expectation values of physical quantities in an ensemble defined by a phase space probability density. Therefore Liouville's equation and Green's theorem are used to convert the time derivative of an ensemble average into ensemble averages of quantities involving derivatives with respect to the particle momenta and position.

2.1. Microscopic Model

The Hamiltonian of an atomic system is assumed to be

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m_i} + U$$

where the mass and momenta associated with each of the N particles are denoted by m_i and $\mathbf{p}_i$, respectively, and U is the potential given as a function of possibly all the particle positions $\mathbf{x}_i$. In contrast to the lower-case Greek letters used for the balance laws (1), lower-case Roman letters i, j, k are used for the particle index over the range $1, \ldots, N$ with no implied summation in the remainder of the paper.

The interatomic potential U is invariant under translation, rotation, and reflection (parity) if

$$U(\mathbf{Q}\mathbf{x}_1 + \mathbf{c}, \ldots, \mathbf{Q}\mathbf{x}_N + \mathbf{c}) = U(\mathbf{x}_1, \ldots, \mathbf{x}_N), \tag{3}$$

where $\mathbf{Q}$ is an orthogonal matrix , and $\mathbf{c}$ is a constant vector. Invariance under reflection occurs when the determinant of $\mathbf{Q}$ is equal to negative one (so that $\mathbf{Q}$ is not assumed to be a rotation). Under the assumption that the interatomic potential satisfies (3), U can be re-expressed as a function of the $N(N-1)/2$ inter-particle distances $|\mathbf{x}_j - \mathbf{x}_k|$; see the discussion in [9]. Although the distance representation may not be the most convenient in practice, it is easily established, for example, that dependence on bond angles and torsions can be replaced with a distance representation. Thus U is not restricted to a pair-potential, but is valid for a multibody potential that satisfies (3) that includes those commonly used in molecular dynamics simulations.

Define the *distance parameters*

$$\xi_{jk} := \frac{1}{2} |\mathbf{x}_j - \mathbf{x}_k|^2 , \tag{4}$$

for each pair of atoms j and k. These distance parameters are more convenient in use than the distances themselves and are equivalent. For instance, the gradient of a distance parameter with respect to particle position i is

$$\nabla_{\mathbf{x}_i} \xi_{jk} = (\mathbf{x}_j - \mathbf{x}_k)(\delta_{ij} - \delta_{ik}), \tag{5}$$

using Kronecker delta notation. The chain rule implies that

$$\nabla_{\mathbf{x}_i} U = \sum_j (\mathbf{x}_i - \mathbf{x}_j) G_{ij}, \tag{6}$$

where the pair function G_{ij} is defined

$$G_{ij} := \frac{\partial U}{\partial \xi_{ij}}. \tag{7}$$

Although G_{ij} references atoms i and j, G_{ij} does in principle depend on all the distance pairs. It will be important in what follows to remember that G_{ij} is symmetric in the indices

i, j, and that each of the terms in (6) are antisymmetric. The G_{ij} can be thought of as a generalized force, e.g., stiffness, with dimensions of force per unit length.

The force exerted on atom i by the remainder of the atoms can be decomposed as $-\nabla_{\mathbf{x}_i} U = \sum_j \mathbf{f}_{ij}$, where the pairwise forces are given by $\mathbf{f}_{ij} := -(\mathbf{x}_i - \mathbf{x}_j)G_{ij}$. This decomposition also satisfies the strong form of Newton's third law, e.g., $\mathbf{f}_{ij} = -\mathbf{f}_{ji}$ where $\mathbf{f}_{ij}$ is collinear with the line between $\mathbf{x}_i$ and $\mathbf{x}_j$.

2.2. Expectation in Phase Space

The continuum balance laws (2) are derived as expectation in phase using the following well-known procedure (see [4, eq. (2.4)], and [11, Chapter 3] for a more extended discussion). Given a time-independent function α of all the particle momenta, positions and the real space position $\mathbf{x}$, then Liouville's equation and Green's theorem implies the well-known formula

$$\frac{\partial}{\partial t}\langle \alpha \rangle = \left\langle \sum_i \frac{\partial \alpha}{\partial \mathbf{x}_i^\mu} \mathbf{v}_i^\mu \right\rangle - \left\langle \sum_i \frac{\partial \alpha}{\partial \mathbf{p}_i^\mu} \frac{\partial U}{\partial \mathbf{x}_i^\mu} \right\rangle, \tag{8}$$

where $\mathbf{v}_i = \mathbf{p}_i / m_i$ is the velocity of particle i. The brackets denote an ensemble average, or phase space expectation, with respect to phase space density, which otherwise does not appear in any expressions.

By selecting α equal to a real space density, the righthand side of (8) is manipulated to obtain the desired continuum balance law. Examples for α representing the mass, momentum and energy densities at a point $\mathbf{x}$, respectively, are defined as

$$\rho := \left\langle \sum_i m_i \phi_i \right\rangle \tag{9a}$$

$$\boldsymbol{\pi} := \left\langle \sum_i \mathbf{p}_i \phi_i \right\rangle \tag{9b}$$

$$\epsilon := \left\langle \sum_i e_i \phi_i \right\rangle \tag{9c}$$

where $\phi_i := \phi(\mathbf{x} - \mathbf{x}_i)$ is the Hardy localization function and

$$e_i := \frac{m_i}{2} \mathbf{v}_i \cdot \mathbf{v}_i + U^{(i)} \tag{9d}$$

represents the energy per particle and $U^{(i)}$ is a partition of the potential energy U among the particles that satisfies

$$\int_{\mathbb{R}^3} \epsilon \, d\mathbf{x} = \sum_i \frac{m_i}{2} \mathbf{v}_i \cdot \mathbf{v}_i + U. \tag{9e}$$

We also assume that the $U^{(i)}$ are invariant under reflections, rotations and translations. Irving and Kirkwood employed the choice of a Dirac delta function for the localization function, but this is unnecessary, as was demonstrated by Noll [5]. Hardy [7] restricted the choice of ϕ by the requirements that ϕ be nonnegative and integrate to one over real space, and be well-localized, e.g., be peaked about the particle position. The units of this function must therefore be per unit volume (of real space).

2.3. Conservation of mass

Given (9a) and (9b), the conservation of mass (1a) results, for instance, see section IV of [4]. In the continuum mechanics literature, the primary variables are often mass density and material velocity. A microscopic point of view explains that mass and momentum densities are the primary variables. Evidently material velocity must be *defined* in terms of mass and momentum densities. That is

$$\mathbf{v} := \frac{\boldsymbol{\pi}}{\rho} \tag{10}$$

defines the material velocity field $\mathbf{v}$ that is invariant under a constant translation of the particle velocities.

3. CONSERVATION OF LINEAR MOMENTUM

Inserting the momentum density (9b) into (8) followed by use of the relations (6) and (10) imply the balance of linear momentum

$$\frac{\partial}{\partial t} \boldsymbol{\pi}^{\nu} + \frac{\partial}{\partial \mathbf{x}^{\mu}} \mathbf{v}^{\mu} \boldsymbol{\pi}^{\nu} = \frac{\partial}{\partial \mathbf{x}^{\mu}} \boldsymbol{\sigma}_{\mathrm{K}}^{\mu\nu} + \Big\langle \sum_{i,j} (\mathbf{x}_j^{\nu} - \mathbf{x}_i^{\nu}) G_{ij} \phi_i \Big\rangle, \tag{11a}$$

where the kinetic stress $\boldsymbol{\sigma}_{\mathrm{K}}$ is defined by

$$\boldsymbol{\sigma}_{\mathrm{K}}^{\mu\nu} := -\Big\langle \sum_i m_i (\mathbf{v}_i - \mathbf{v})^{\mu} (\mathbf{v}_i - \mathbf{v})^{\nu} \phi_i \Big\rangle. \tag{11b}$$

The tensor $\boldsymbol{\sigma}_{\mathrm{K}}$ represents stress due to the momentum of the particles relative to the material velocity (10) and corresponds, for example, to pressure in an ideal gas.

Since $\phi'_j := \phi(\mathbf{x}' - \mathbf{x}_j)$ integrates to one over real space, the antisymmetry in the indices i and j of $(\mathbf{x}_j - \mathbf{x}_i)G_{ij}$ implies that the rightmost term of (11a) may be rewritten as

$$\begin{aligned}\int_{\mathbb{R}^3} \Big\langle \sum_{i,j} (\mathbf{x}_j^\nu - \mathbf{x}_i^\nu) G_{ij} \phi_i \phi'_j \Big\rangle \, d\mathbf{x}' &= \frac{1}{2} \int_{\mathbb{R}^3} \Big\langle \sum_{i,j} (\mathbf{x}_j^\nu - \mathbf{x}_i^\nu) G_{ij} \big(\phi_i \phi'_j - \phi'_i \phi_j\big) \Big\rangle \, d\mathbf{x}' \\ &= \int_{\mathbb{R}^3} \big(\mathbf{T}^\nu(\mathbf{x}, \mathbf{x}') - \mathbf{T}^\nu(\mathbf{x}', \mathbf{x})\big) \, d\mathbf{x}'\end{aligned} \tag{12a}$$

where a microscopic force state is given by

$$\mathbf{T}(\mathbf{x}, \mathbf{x}') := \frac{1}{4} \Big\langle \sum_{i,j} (\mathbf{x}_j^\nu - \mathbf{x}_i^\nu) G_{ij} \left(\phi_i \phi'_j - \phi'_i \phi_j\right) \Big\rangle. \tag{12b}$$

Substitution of (12b) into (11a) results in the peridynamic balance of linear momentum (2a).

The decomposition of the integrand in the first term of (12a) into a difference of force states is not unique. For instance, if the vector field $\mathbf{S}(\mathbf{x}, \mathbf{x}')$, symmetric under an exchange in $\mathbf{x}$ and $\mathbf{x}'$, is added to the force state (12b), then the last equality of (12a) is also satisfied. The special choice of force state (12b) satisfies $\mathbf{T}(\mathbf{x}', \mathbf{x}) = -\mathbf{T}(\mathbf{x}, \mathbf{x}')$ for all $\mathbf{x}$ and $\mathbf{x}'$ so that only $\mathbf{S} = \mathbf{0}$ is possible. To underscore the indeterminacy of the force state, the difference of force states is employed even though the special choice (12b) implies that $\mathbf{T}(\mathbf{x}, \mathbf{x}') - \mathbf{T}(\mathbf{x}', \mathbf{x}) = 2\mathbf{T}(\mathbf{x}, \mathbf{x}')$.

The force state is invariant under a translation of the particles. The vector $\big(\mathbf{T}(\mathbf{x}, \mathbf{x}') - \mathbf{T}(\mathbf{x}', \mathbf{x})\big) \, d\mathbf{x}' \, d\mathbf{x}$ represents the force exerted on the ensemble average of the particles in $d\mathbf{x}$ by the ensemble average of the particles in $d\mathbf{x}'$, and is the negative of the force that the particles in $d\mathbf{x}'$ exert upon the particles in $d\mathbf{x}$ because $\big(\mathbf{T}(\mathbf{x}', \mathbf{x}) - \mathbf{T}(\mathbf{x}, \mathbf{x}')\big) = -\big(\mathbf{T}(\mathbf{x}, \mathbf{x}') - \mathbf{T}(\mathbf{x}', \mathbf{x})\big)$.

The idea of rewriting the internal force density, the rightmost term of (11a), as the integral of a force density per unit volume is due to Noll [5]. This is a crucial step not taken by Irving and Kirkwood, and leads to a closed form expression for the potential stress given by Lemma I of [5]. A property associated with the difference of force states is that, in general,

$$\big(\mathbf{T}(\mathbf{x}, \mathbf{x}') - \mathbf{T}(\mathbf{x}', \mathbf{x})\big) \times \big(\mathbf{x}' - \mathbf{x}\big) \neq \mathbf{0}, \tag{13}$$

although $\big(\mathbf{x}_i - \mathbf{x}_j\big) G_{ij} \times \big(\mathbf{x}_i - \mathbf{x}_j\big) = \mathbf{0}$. Evidently, the indeterminacy in the localization function ϕ is manifest in (13). This indeterminacy provides a microscopic basis for the necessity of the more general peridynamic state theory postulated in [2] over than originally given in [1]. The force state (12b) may be decomposed into two force states $\mathbf{T}_{\|}$ and $\mathbf{T}_{\perp}$ collinear and perpendicular with $\mathbf{x}' - \mathbf{x}$, respectively. The difference $\mathbf{T}_{\perp}(\mathbf{x}, \mathbf{x}') - \mathbf{T}_{\perp}(\mathbf{x}', \mathbf{x})$ explains that the force density (12a) gives rise to a non-zero couple when (13) holds.

Let $\Omega \subset \mathbb{R}^3$ be a region in real space. Because $\mathbf{T}(\mathbf{x}, \mathbf{x}') - \mathbf{T}(\mathbf{x}', \mathbf{x})$ is antisymmetric with respect to $\mathbf{x}$ and $\mathbf{x}'$, then

$$\int_{\Omega} \int_{\mathbb{R}^3} \big(\mathbf{T}^{\nu}(\mathbf{x}, \mathbf{x}') - \mathbf{T}^{\nu}(\mathbf{x}', \mathbf{x})\big)\, d\mathbf{x}'\, d\mathbf{x} = \int_{\Omega} \int_{\mathbb{R}^3 \setminus \Omega} \big(\mathbf{T}^{\nu}(\mathbf{x}, \mathbf{x}') - \mathbf{T}^{\nu}(\mathbf{x}', \mathbf{x})\big)\, d\mathbf{x}'\, d\mathbf{x} \tag{14a}$$

because

$$\int_{\Omega} \int_{\Omega} \big(\mathbf{T}^{\nu}(\mathbf{x}, \mathbf{x}') - \mathbf{T}^{\nu}(\mathbf{x}', \mathbf{x})\big)\, d\mathbf{x}'\, d\mathbf{x} = \mathbf{0}, \tag{14b}$$

or equivalently, the force of region Ω on itself is zero. This observation is also due to Noll; see Lemma II of [5]. This result explains that the righthand side of (14a) denotes momentum flux between Ω and $\mathbb{R}^3 \setminus \Omega$.

Integrating the balance of linear momentum (2a) over the region τ results in

$$\begin{aligned} \int_{\Omega} \Big(\frac{\partial}{\partial t}\boldsymbol{\pi}^{\nu} + \frac{\partial}{\partial \Omega}(\mathbf{v}^{\mu}\boldsymbol{\pi}^{\nu})\Big)\, d\mathbf{x} &= \int_{\partial\Omega} \boldsymbol{\sigma}_{\mathrm{K}}^{\mu\nu}\mathbf{n}^{\mu}\, dA \\ &\quad + \int_{\Omega} \int_{\mathbb{R}^3 \setminus \Omega} \big(\mathbf{T}^{\nu}(\mathbf{x}, \mathbf{x}') - \mathbf{T}^{\nu}(\mathbf{x}', \mathbf{x})\big)\, d\mathbf{x}'\, d\mathbf{x}, \end{aligned} \tag{15a}$$

where $\mathbf{n}$ is the unit normal to the surface $\partial\Omega$ of Ω. In words, the rate of change of linear momentum is balanced by the sum of forces external to Ω. The rightmost term of (15a) represents the internal force on the region Ω exerted by the region external to Ω. This force is nonlocal because points $\mathbf{x}' \neq \mathbf{x}$ are involved in the interaction.

Suppose $\Omega = \Omega_1 \cup \Omega_2$ where the nonzero regions Ω_1 and Ω_2 are disjoint. Then (15a) leads to

$$\begin{aligned} &\sum_{i=1}^{2} \int_{\Omega_i} \Big(\frac{\partial}{\partial t}\boldsymbol{\pi}^{\nu} + \frac{\partial}{\partial \Omega}(\mathbf{v}^{\mu}\boldsymbol{\pi}^{\nu})\Big)\, d\mathbf{x} \\ &\qquad = \int_{\partial(\Omega_1 \cup \Omega_2)} \boldsymbol{\sigma}_{\mathrm{K}}^{\mu\nu}\mathbf{n}^{\mu}\, dA + \int_{\Omega_1 \cup \Omega_2} \int_{\mathbb{R}^3 \setminus (\Omega_1 \cup \Omega_2)} \big(\mathbf{T}^{\nu}(\mathbf{x}, \mathbf{x}') - \mathbf{T}^{\nu}(\mathbf{x}', \mathbf{x})\big)\, d\mathbf{x}'\, d\mathbf{x} \\ &\qquad = \sum_{i=1}^{2} \Big(\int_{\partial\Omega_i} \boldsymbol{\sigma}_{\mathrm{K}}^{\mu\nu}\mathbf{n}^{\mu}\, dA + \int_{\Omega_i} \int_{\mathbb{R}^3 \setminus \Omega_i} \big(\mathbf{T}^{\nu}(\mathbf{x}, \mathbf{x}') - \mathbf{T}^{\nu}(\mathbf{x}', \mathbf{x})\big)\, d\mathbf{x}'\, d\mathbf{x} \Big), \end{aligned} \tag{15b}$$

where the last equality follows because antisymmetry of the integrand with respect to the arguments $\mathbf{x}$ and $\mathbf{x}'$ is equivalent to the relationship

$$\int_{\Omega_1} \int_{\Omega_2} \big(\mathbf{T}^{\nu}(\mathbf{x}, \mathbf{x}') - \mathbf{T}^{\nu}(\mathbf{x}', \mathbf{x})\big)\, d\mathbf{x}'\, d\mathbf{x} + \int_{\Omega_2} \int_{\Omega_1} \big(\mathbf{T}^{\nu}(\mathbf{x}, \mathbf{x}') - \mathbf{T}^{\nu}(\mathbf{x}', \mathbf{x})\big)\, d\mathbf{x}'\, d\mathbf{x} = \mathbf{0} \tag{15c}$$

for all disjoint regions Ω_1 and Ω_2 or Newton's third law. This establishes that the balance of linear momentum (2a) is additive over disjoint subregions if and only if the difference of force states is antisymmetric.

3.1. Classical conservation of linear momentum

The righthand of (11a) may be recast as the divergence of a microscopic symmetric stress tensor field, or a Cauchy stress. This results in a microscopic interpretation for the balance of linear momentum (1b) that *follows* from the microscopic peridynamic balance law of linear momentum (2a). A Cauchy stress tensor $\boldsymbol{\sigma}$ is derived by first rewriting (12a) as

$$\frac{1}{2}\Big\langle \sum_{i,j} \big(\mathbf{x}_i^{\nu} - \mathbf{x}_j^{\nu}\big)\big(\phi_i - \phi_j\big) G_{ij} \Big\rangle = \frac{\partial}{\partial \mathbf{x}^{\mu}} \boldsymbol{\sigma}_{\mathrm{U}}^{\mu\nu}$$

where the potential stress tensor and the Hardy bond function β are given by

$$\boldsymbol{\sigma}_{\mathrm{U}} := \frac{1}{2}\Big\langle \sum_{i,j} \big(\mathbf{x}_i^{\mu} - \mathbf{x}_j^{\mu}\big)\big(\mathbf{x}_i^{\nu} - \mathbf{x}_j^{\nu}\big)\, \beta_{ij}\, G_{ij} \Big\rangle, \tag{16a}$$

$$\beta_{ij}(\mathbf{x}) := -\int_0^1 \phi\big(\mathbf{x} - \lambda \mathbf{x}_i - (1-\lambda)\mathbf{x}_j\big)\, d\lambda, \tag{16b}$$

respectively. The Hardy bond function is strictly a function of the localization function.

A desired Cauchy stress is therefore the sum of the kinetic (11b) and potential (16a) stress tensors

$$\boldsymbol{\sigma} := \boldsymbol{\sigma}_{\mathrm{K}} + \boldsymbol{\sigma}_{\mathrm{U}}. \tag{17}$$

The peridynamic balance law of linear momentum (2a) is then re-expressed as the classical balance (1b). The former balance law, though, is more general because by (12a) the first equality of

$$\frac{\partial}{\partial \mathbf{x}^{\mu}} \boldsymbol{\sigma}_{\mathrm{U}}^{\mu\nu} = \Big\langle \sum_{i,j} \big(\mathbf{x}_i^{\nu} - \mathbf{x}_j^{\nu}\big) \phi_i G_{ij} \Big\rangle = \int_{\mathbb{R}^3} \big(\mathbf{T}^{\nu}(\mathbf{x}, \mathbf{x}') - \mathbf{T}^{\nu}(\mathbf{x}', \mathbf{x})\big)\, d\mathbf{x}'$$

holds under the additional assumption that the potential stress is differentiable, or equivalently that ϕ is differentiable. In contrast, the nonlocal internal force density is valid for discontinuous ϕ. This explains why the peridynamic internal force density remains defined under a discontinuous deformation.

The symmetry of the stress tensor $\boldsymbol{\sigma}$, in particular the component $\boldsymbol{\sigma}_{\mathrm{U}}$, is a consequence of the derivation in terms of distance parameters that in turn is a consequence of the invariance

(3). The pair functions G_{ij} are defined in terms of the total potential energy U without the need to partition U among the particles. This generalizes the result of Hardy and may be compared, for example, with the corresponding expression in [12] that is only carried out for the Tersoff [13, 14] potential.

4. CONSERVATION OF ENERGY

Inserting the energy density (9c) into (8) followed by use of the relation (10) implies the balance of energy

$$\frac{\partial}{\partial t}\epsilon + \frac{\partial}{\partial \mathbf{x}^{\mu}}\big(\mathbf{v}^{\mu}\epsilon\big) = \frac{\partial}{\partial \mathbf{x}^{\mu}}\big(\boldsymbol{\sigma}_{\mathrm{K}}^{\mu\nu}\mathbf{v}^{\nu} - \mathbf{q}_{\mathrm{K}}^{\mu}\big) + \Big\langle \sum_{i,j} \frac{\partial U^{(j)}}{\partial \mathbf{x}_i^{\mu}}\mathbf{v}_i^{\mu}\big(\phi_j - \phi_i\big)\Big\rangle \tag{18a}$$

where

$$\mathbf{q}_{\mathrm{K}} = \Big\langle \sum_i \big(\frac{m_i}{2}|\mathbf{v}_i - \mathbf{v}|^2 + U^{(i)}\big)\big(\mathbf{v}_i - \mathbf{v}\big)\phi_i\Big\rangle, \tag{18b}$$

accounts for the heat flux due to particle kinetic and potential energies, respectively.

Since $\phi_j' := \phi(\mathbf{x}' - \mathbf{x}_j)$ integrates to one over real space, the rightmost term of (18a) may be rewritten as

$$\begin{aligned}\Big\langle \sum_{i,j} \frac{\partial U^{(j)}}{\partial \mathbf{x}_i^{\mu}}\mathbf{v}_i^{\mu}\big(\phi_j - \phi_i\big)\Big\rangle &= \int_{\mathbb{R}^3} \Big\langle \sum_{i,j} \frac{\partial U^{(j)}}{\partial \mathbf{x}_i^{\mu}}\mathbf{v}_i^{\mu}\big(\phi_i'\phi_j - \phi_i\phi_j'\big)\Big\rangle\, d\mathbf{x}' \\ &= \int_{\mathbb{R}^3} \big(p(\mathbf{x},\mathbf{x}') - p(\mathbf{x}',\mathbf{x})\big)\, d\mathbf{x}'\end{aligned} \tag{19a}$$

where a microscopic power state is given by

$$p(\mathbf{x},\mathbf{x}') := \frac{1}{2}\Big\langle \sum_{i,j} \frac{\partial U^{(j)}}{\partial \mathbf{x}_i^{\mu}}\mathbf{v}_i^{\mu}\big(\phi_i'\phi_j - \phi_i\phi_j'\big)\Big\rangle. \tag{19b}$$

Substitution of (19b) into (18a) yields the balance of energy (2b).

The decomposition of the integrand in the first term of (19a) into a difference of power states is not unique. For instance, if the scalar field $\mathbf{s}(\mathbf{x},\mathbf{x}')$, symmetric under an exchange in $\mathbf{x}$ and $\mathbf{x}'$, is added to the power state (19b), then the last equality of (19a) is also satisfied. The special choice of power state (19b) satisfies $p(\mathbf{x}',\mathbf{x}) = -p(\mathbf{x},\mathbf{x}')$ for all $\mathbf{x}$ and $\mathbf{x}'$ so that only $\mathbf{s} = \mathbf{0}$ is possible. To underscore the indeterminacy of the power state, the difference of power states is employed even though the special choice (19b) implies that $p(\mathbf{x},\mathbf{x}') - p(\mathbf{x}',\mathbf{x}) = 2p(\mathbf{x},\mathbf{x}')$.

The expression $\big(p(\mathbf{x},\mathbf{x}') - p(\mathbf{x}',\mathbf{x})\big)\,d\mathbf{x}'\,d\mathbf{x}$ represents the power exerted by the ensemble average of the particles in $d\mathbf{x}$ upon the ensemble average of the particles in $d\mathbf{x}'$, and is the negative of the power exerted by the particles in $d\mathbf{x}'$ upon the particles in $d\mathbf{x}$ because $\big(p(\mathbf{x}',\mathbf{x}) - p(\mathbf{x},\mathbf{x}')\big) = -\big(p(\mathbf{x},\mathbf{x}') - p(\mathbf{x}',\mathbf{x})\big)$. Evidently the power density (19a) is the nonlocal analogue of

$$\frac{\partial}{\partial \mathbf{x}^\mu}\big(\boldsymbol{\sigma}_{\mathrm{U}}^{\mu\nu}\mathbf{v}^\mu - \mathbf{q}_{\mathrm{U}}^\mu\big)$$

for a potential heat flux $\mathbf{q}_{\mathrm{U}}$ and so represents both mechanical and thermal power among the particles. A relationship between the thermal power density $\partial \mathbf{q}_{\mathrm{U}}^\mu/\partial \mathbf{x}^\mu$ as the difference of the power density from the stress power is given in Section 4.1.

An analogous derivation leading to (15a) grants that integrating the balance of energy (2b) over the region Ω results in

$$\int_\Omega \big(\frac{\partial}{\partial t}\epsilon + \frac{\partial}{\partial \mathbf{x}^\mu}(\mathbf{v}^\mu \epsilon)\big)\,d\mathbf{x} = \int_{\partial\Omega}\big(\boldsymbol{\sigma}_{\mathrm{K}}^{\mu\nu}\mathbf{v}^\nu - \mathbf{q}_{\mathrm{K}}^\mu\big)\mathbf{n}^\mu\,dA + \int_\Omega\int_{\mathbb{R}^3\setminus\Omega}\big(p(\mathbf{x},\mathbf{x}') - p(\mathbf{x}',\mathbf{x})\big)\,d\mathbf{x}'\,d\mathbf{x}. \tag{20}$$

In words, the rate of change of energy is balanced by the sum of forces external to Ω. The rightmost term of (20) represents the internal power on the region Ω exerted by the region external to Ω; the power exerted upon Ω by Ω is zero. This power is nonlocal because points $\mathbf{x}' \neq \mathbf{x}$ are involved in the interaction.

The analysis leading to (15b) can also be reproduced since the integrand of the power density is antisymmetric under an interchange of the arguments $\mathbf{x}$ and $\mathbf{x}'$. Such an analysis leads to the conclusion the balance of energy (2b) is additive over disjoint regions Ω_1 and Ω_2, e.g.,

$$\sum_{i=1}^{2}\int_{\Omega_i}\big(\frac{\partial}{\partial t}\epsilon + \frac{\partial}{\partial \mathbf{x}^\mu}(\mathbf{v}^\mu \epsilon)\big)\,d\mathbf{x} = \sum_{i=1}^{2}\Big(\int_{\partial\Omega_i}\big(\boldsymbol{\sigma}_{\mathrm{K}}^{\mu\nu}\mathbf{v}^\nu - \mathbf{q}_{\mathrm{K}}^\mu\big)\mathbf{n}^\mu\,dA + \int_{\Omega_i}\int_{\mathbb{R}^3\setminus\Omega_i}\big(p(\mathbf{x},\mathbf{x}') - p(\mathbf{x}',\mathbf{x})\big)\,d\mathbf{x}'\,d\mathbf{x}\Big).$$

Define the internal energy

$$\epsilon_{\text{int}} := \Big\langle \sum_j \Big(\frac{m_j}{2}\big(\mathbf{v}_j - \mathbf{v}\big)\cdot\big(\mathbf{v}_j - \mathbf{v}\big) + U^{(j)}\Big)\phi_j\Big\rangle \tag{21}$$

so that

$$\epsilon = \epsilon_{\text{int}} + \frac{\rho}{2}\mathbf{v}\cdot\mathbf{v}.$$

Multiplication of the balance of linear momentum (2a) by the material velocity $\mathbf{v}$ and then subtracting the resulting equation from the balance of energy (2b) results in

$$\begin{aligned}\frac{\partial}{\partial t}\epsilon_{\text{int}} + \frac{\partial}{\partial \mathbf{x}^\mu}\big(\mathbf{v}^\mu \epsilon_{\text{int}}\big) = \boldsymbol{\sigma}_{\mathrm{K}}^{\mu\nu}\frac{\partial}{\partial \mathbf{x}^\nu}\mathbf{v}^\mu - \frac{\partial}{\partial \mathbf{x}^\mu}\mathbf{q}_{\mathrm{K}}^\mu + \int_{\mathbb{R}^3}\big(p(\mathbf{x},\mathbf{x}') - p(\mathbf{x}',\mathbf{x})\big)\,d\mathbf{x}' \\ - \int_{\mathbb{R}^3}\big(\mathbf{T}^\mu(\mathbf{x},\mathbf{x}') - \mathbf{T}^\mu(\mathbf{x}',\mathbf{x})\big)\mathbf{v}^\mu(\mathbf{x},t)\,d\mathbf{x}'.\end{aligned} \tag{22a}$$

Define the quantity

$$\widehat{p}(\mathbf{x},\mathbf{x}',t) := p(\mathbf{x},\mathbf{x}') - \mathbf{T}(\mathbf{x},\mathbf{x}')\cdot\mathbf{v}(\mathbf{x},t). \tag{22b}$$

so that (22a) becomes the peridynamic balance of internal energy

$$\begin{aligned}\frac{\partial}{\partial t}\epsilon_{\text{int}} + \frac{\partial}{\partial \mathbf{x}^\mu}\big(\mathbf{v}^\mu \epsilon_{\text{int}}\big) = \boldsymbol{\sigma}_{\mathrm{K}}^{\mu\nu}\frac{\partial}{\partial \mathbf{x}^\nu}\mathbf{v}^\mu + \int_{\mathbb{R}^3}\mathbf{T}^\mu(\mathbf{x}',\mathbf{x})\big(\mathbf{v}^\mu(\mathbf{x},t) - \mathbf{v}^\mu(\mathbf{x}',t)\big)\,d\mathbf{x}' \\ - \frac{\partial}{\partial \mathbf{x}^\mu}\mathbf{q}_{\mathrm{K}}^\mu + \int_{\mathbb{R}^3}\big(\widehat{p}(\mathbf{x},\mathbf{x}',t) - \widehat{p}(\mathbf{x}',\mathbf{x},t)\big)\,d\mathbf{x}'.\end{aligned} \tag{22c}$$

The term

$$\int_{\mathbb{R}^3}\mathbf{T}^\mu(\mathbf{x}',\mathbf{x})\big(\mathbf{v}^\mu(\mathbf{x},t) - \mathbf{v}^\mu(\mathbf{x}',t)\big)\,d\mathbf{x}' \tag{22d}$$

represents the absorbed power density and is the peridynamic analogue of the classical stress power

$$\boldsymbol{\sigma}_{\mathrm{U}}^{\mu\nu}\frac{\partial}{\partial \mathbf{x}^\nu}\mathbf{v}^\mu.$$

The absorbed power is invariant under the addition of a constant velocity field to $\mathbf{v}$ and a constant translation of the particle velocities. The term

$$\int_{\mathbb{R}^3}\big(\widehat{p}(\mathbf{x},\mathbf{x}',t) - \widehat{p}(\mathbf{x}',\mathbf{x},t)\big)\,d\mathbf{x}'$$

represents nonlocal heating due to inter-particle forces and is also invariant under a translation of the particle velocities.

4.1. Classical conservation of energy

The decomposition

$$\frac{\partial}{\partial \mathbf{x}^\mu}\mathbf{q}_{\mathrm{U}}^\mu := \frac{\partial}{\partial \mathbf{x}^\mu}\big(\boldsymbol{\sigma}_{\mathrm{U}}^{\mu\nu}\mathbf{v}^\mu\big) - \int_{\mathbb{R}^3}\big(p(\mathbf{x},\mathbf{x}') - p(\mathbf{x}',\mathbf{x})\big)\,d\mathbf{x}' \tag{23}$$

defines the divergence of the potential heat flux as the difference of the rate of work per volume of the potential stress and the power due to inter-particle forces. The nonlocal balance of energy (2b) results in the classical balance of energy (1c) by defining the heat flux $\mathbf{q} := \mathbf{q}_{\mathrm{U}} + \mathbf{q}_{\mathrm{K}}$. An explicit expression for the potential heat flux is determined by invoking Lemma I in [5] to obtain a vector field $\mathbf{f}$ satisfying

$$\frac{\partial}{\partial \mathbf{x}^{\mu}} \mathbf{f}^{\mu}(\mathbf{x}) = \int_{\mathbb{R}^3} \big(p(\mathbf{x}, \mathbf{x}') - p(\mathbf{x}', \mathbf{x})\big)\, d\mathbf{x}'$$

so that a choice for $\mathbf{q}_{\mathrm{U}}$ is given by $\boldsymbol{\sigma}_{\mathrm{U}} \mathbf{v} - \mathbf{f}$. The decomposition (23) and an expression for the potential heat flux necessitate that the potential stress and the vector field $\mathbf{f}$ are differentiable. In contrast, the internal power density (19a) is not required to be differentiable and so is defined under a discontinuous deformation.

A relationship with the classical balance of internal energy

$$\frac{\partial}{\partial t} \epsilon_{\mathrm{int}} + \frac{\partial}{\partial \mathbf{x}^{\mu}} \big(\mathbf{v}^{\mu} \epsilon_{\mathrm{int}}\big) = \boldsymbol{\sigma}^{\mu\nu} \frac{\partial}{\partial \mathbf{x}^{\nu}} \mathbf{v}^{\mu} - \frac{\partial}{\partial \mathbf{x}^{\mu}} \mathbf{q}^{\mu} \tag{24}$$

is achieved by exploiting the decomposition (23) rewritten as

$$\begin{aligned} &\boldsymbol{\sigma}_{\mathrm{U}}^{\mu\nu} \frac{\partial}{\partial \mathbf{x}^{\nu}} \mathbf{v}^{\mu} - \frac{\partial}{\partial \mathbf{x}^{\mu}} \mathbf{q}_{\mathrm{U}}^{\mu} \\ &\qquad = \int_{\mathbb{R}^3} \mathbf{T}^{\mu}(\mathbf{x}', \mathbf{x}) \big(\mathbf{v}^{\mu}(\mathbf{x}, t) - \mathbf{v}^{\mu}(\mathbf{x}', t)\big)\, d\mathbf{x}' + \int_{\mathbb{R}^3} \big(\widehat{p}(\mathbf{x}, \mathbf{x}', t) - \widehat{p}(\mathbf{x}', \mathbf{x}, t)\big)\, d\mathbf{x}'. \end{aligned}$$

Inserting this expression into (22c) results in the classical balance of internal energy (24) where $\boldsymbol{\sigma} = \boldsymbol{\sigma}_{\mathrm{U}} + \boldsymbol{\sigma}_{\mathrm{K}}$ and $\mathbf{q} = \mathbf{q}_{\mathrm{U}} + \mathbf{q}_{\mathrm{K}}$.

5. SUMMARY OF RESULTS

The peridynamic balance laws for the conservation of linear momentum and energy (2) were derived using the principles of statistical mechanics. In addition, the peridynamic balance of internal energy (22c) was derived. This provides the first microscopic basis for the peridynamic balance laws. The given derivations of the peridynamic conservation laws avoided the standard limitation of a pairwise decomposition of the interatomic potential U. Instead U was assumed to not only be invariant under translation and rotation, but also reflection.

The derivation of the force and power states $\mathbf{T}$ and p, respectively, lead to expressions for the internal force and power densities (12a) and (19a), respectively. The absorbed power density (22d) was demonstrated to be the nonlocal analogue of the classical stress power.

The two integral operators for the peridynamic conservation laws were also re-expressed as the classical continuum energy and momentum conservation laws (1). This was accomplished by determining closed-form expressions for the potential stress and potential heat flux fields, respectively, by assuming these fields were differentiable. The derivation of a stress tensor and heat flux demonstrated that the classical continuum energy and momentum conservation laws are consequences of the more general peridynamic laws holding under discontinuous deformation. An important conclusion is that nonlocal interaction is intrinsic to continuum conservation laws.

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[15] Peridynamic is comprised from the Greek roots for “near” and “force”.

[16] See the translation [6]