A material frame approach for evaluating continuum variables in atomistic simulations

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ABSTRACT

We present a material frame formulation analogous to the spatial frame formulation developed by Hardy, whereby expressions for continuum mechanical variables such as stress and heat flux are derived from atomic-scale quantities intrinsic to molecular simulation. This formulation is ideally suited for developing an atomistic-to-continuum correspondence for solid mechanics problems. We derive expressions for the first Piola–Kirchhoff (P–K) stress tensor and the material frame heat flux vector directly from the momentum and energy balances using localization functions in a reference configuration. The resulting P–K stress tensor, unlike the Cauchy expression, has no explicit kinetic contribution. The referential heat flux vector likewise lacks the kinetic contribution appearing in its spatial frame counterpart. Using a proof for a special case and molecular dynamics simulations, we show that our P–K stress expression nonetheless represents a full measure of stress that is consistent with both the system virial and the Cauchy stress expression developed by Hardy. We also present an expanded formulation to define continuum variables from micromorphic continuum theory, which is suitable for the analysis of materials represented by directional bonding at the atomic scale.

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1. Introduction

Continuum theory has been used for decades to analyze and predict the mechanics of materials and structures. However, as technologies shrink to the nanometer range, quantities such as stress and strain become ill-defined and the application of continuum mechanics in nanomechanical frameworks becomes suspect. This brings into question whether the traditional design tools used for manufacturing can be applied to micro or nano electro-mechanical systems. And while atomic-scale modeling and simulation methods, e.g. molecular dynamics, have provided a wealth of information for such systems, the use of such methods has not been standardized. Certainly, the use of continuum mechanics methods would be invaluable provided that clear connections between nanoscale mechanics and engineering-scale analysis can be made.

The development of definitions for continuum variables that are calculable within an atomic system has a long and rich history. In the late 19th century, Clausius [1] and Maxwell [2,3] simultaneously developed the virial theorem (VT) to define the stress applied to the surface of a fixed volume containing interacting particles and a non-zero temperature. Since these initial efforts, there have been many subsequent works to improve on this definition [4–19], most of which have occurred in the last quarter of the 20th century and have continued into the 21st century. The articles cited here have addressed important issues such as the consistency of stress expressions with the mechanical concept of a force acting on a unit area, the validity of an atomic stress based on the VT, and the role of both spatial and time averaging. For brevity, we refer the reader to the discussions in [16,19] for more information.

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Among these efforts is the notable work by Hardy and colleagues [8,20,21]. Hardy's formalism uses a finite-valued and finite-ranged localization function in lieu of the Dirac delta function [4] to establish a self-consistent manner of distributing discrete atomic contributions to thermomechanical fields. While the range and form of the localization function can be selected arbitrarily, the resulting expression for, say, the stress has a certain amount of regularity with varying sized support regions given reasonable choices for the form. Hardy's original formulation is based on the Eulerian or spatial configuration where localization volumes are essentially control volumes fixed in space that matter occupies at a particular time. Hence, Hardy's expressions for stress and heat flux contain both potential (based on derivatives of potential energy) and kinetic (based on the flux of momentum or energy through the localization volume) terms. The validity of kinetic contributions to stress has been an issue of some contention, and has been examined in detail by such authors as Zhou [17] and Murdoch [18].

An alternative approach that obviates the separation of potential and kinetic contributions to stress is to construct a similar formulation to Hardy's in the Lagrangian or material frame. In the material frame, an appropriate stress measure is the 1st Piola–Kirchhoff tensor **P**, which represents the amount of current force exerted on a unit area as measured in the reference configuration. Expressions to calculate **P** have been developed by Andia et al. [22–25]; however, their definition is constructed as a system average, i.e. a single value representative of the average stress state for a cell with periodic boundary conditions. In addition, Andia et al. make the distinction between internal and external forces, separating the interactions between atoms within the cell and the interactions between atoms with "ghost" atoms located across the periodic boundaries. This distinction is not made in many of the approaches mentioned earlier, and application of this concept is not straightforward for the localization volume framework of Hardy.

In this paper, we present a material frame formulation analogous to the one developed by Hardy for the spatial frame. This formulation relies on a mapping from reference to current positions of material points. It is ideally suited for developing an atomistic-to-continuum correspondence for solid mechanics problems as it contains atom-to-material point mapping functions that need only be calculated once for a given simulation. Also, it easily links to concepts and variables used within continuum constitutive models such as the deformation gradient. In Section 2, we derive an expression for P–K stress and the referential heat flux directly from the momentum and energy balances using localization functions in a zero temperature reference configuration. Neither the P–K stress nor the referential heat flux vector have explicit dependence on kinetic energy. Nevertheless, we demonstrate that the derived P–K stress is consistent with the Hardy expression for Cauchy stress using a proof based on a system average in Section 2.4.2, as well as pointing out the obvious connection between the continuum versions of these two quantities which are derived directly from the appropriate balance laws. Furthermore, we employ molecular dynamics simulations discussed in Section 3 to verify that our stress expression is consistent even for systems where the kinetic portion of the Cauchy stress is a significant fraction of the total value. As a further extension of this work, we also present an expanded formulation to define continuum variables from micromorphic continuum theory in Section 4. This extension relies crucially on the Lagrangian framework we develop and shows that our formulation is useful for the analysis of materials represented by directional bonding at the atomic scale.

2. Formulation for standard continuum mechanics

Before we begin our formulation, we define the notation for spatial and temporal derivatives and operators used in this paper. Letting the notations $\tilde{\mathbf{g}}$ and $\hat{\mathbf{g}}$ refer to **g** as a function of the spatial coordinate **x** or the material coordinate **X**, respectively, we can write $\mathbf{g} = \tilde{\mathbf{g}}(\mathbf{x}, t) = \tilde{\mathbf{g}}(\hat{\mathbf{x}}(\mathbf{X}, t), t) = \hat{\mathbf{g}}(\mathbf{X}, t)$, for any scalar, vector or tensor function **g**. With this notation we can define the spatial frame and material frame divergences to be $\nabla_{\mathbf{x}} \cdot \tilde{\mathbf{g}}$ and $\nabla_{\mathbf{X}} \cdot \hat{\mathbf{g}}$, and likewise define the spatial frame and material frame gradients as $\nabla_{\mathbf{x}}\tilde{\mathbf{g}}$ and $\nabla_{\mathbf{X}}\hat{\mathbf{g}}$. In the following, this explicit notation will not be used; rather, it will be clear from context whether the field referred to is a function of the spatial configuration or the material configuration, as is customary in the continuum mechanics literature, e.g. [26,27]. Also, it is understood that if $\mathbf{g}(\mathbf{X}, t)$ is a tensor of "mixed" character, e.g. the 1st Piola–Kirchhoff stress tensor, then the expression $\nabla_{\mathbf{X}} \cdot \mathbf{g}$ is defined to be consistent with the index notation $g_{iJ,J}$, where lower-case Roman letters denote spatial frame indices and upper-case Roman letters denote material frame indices, with both types of subscripts referring to the Cartesian coordinate components of vector or tensor quantities. Regarding derivatives in time, we express the partial time derivative of $\tilde{\mathbf{g}}(\mathbf{x}, t)$ as $\frac{\partial \mathbf{g}}{\partial t} \equiv \frac{\partial \mathbf{g}}{\partial t}|_{\mathbf{x}}$ and the full or material time derivative as $\frac{d\mathbf{g}}{dt} \equiv \frac{\partial \mathbf{g}}{\partial t}|_{\mathbf{X}}$. As usual, these two time derivatives are related through the expression $\frac{d\mathbf{g}}{dt} = \frac{\partial \mathbf{g}}{\partial t} + \nabla_{\mathbf{x}}\mathbf{g} \cdot \mathbf{v}$.

2.1. Balance laws

We begin by modifying Hardy's formulation for the Lagrangian or material frame. Hardy's work uses the balance equations for mass, linear momentum and energy. These are expressed in a spatial configuration as follows:

$$\frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{v}) = 0 \tag{1}$$

$$\frac{\partial (\rho \mathbf{v})}{\partial t} = \nabla_{\mathbf{x}} \cdot (\boldsymbol{\sigma} - \rho \mathbf{v} \otimes \mathbf{v}) + \rho \mathbf{b} \tag{2}$$

$$\frac{\partial (\rho e)}{\partial t} = \nabla_{\mathbf{x}} \cdot (\boldsymbol{\sigma} \cdot \mathbf{v} - \rho e \mathbf{v} - \mathbf{q}) + \rho \mathbf{b} \cdot \mathbf{v} + \rho h \tag{3}$$

These expressions can be manipulated to use the full or material time derivative $\frac{d}{dt}$ instead of the partial time derivative $\frac{\partial}{\partial t}$:

$$\frac{d\rho}{dt} + \rho \nabla_{\mathbf{x}} \cdot \mathbf{v} = 0 \tag{4}$$

$$\rho \frac{d\mathbf{v}}{dt} = \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} + \rho \mathbf{b} \tag{5}$$

$$\rho \frac{d\epsilon}{dt} = \boldsymbol{\sigma} : \nabla_{\mathbf{x}} \mathbf{v} - \nabla_{\mathbf{x}} \cdot \mathbf{q} + \rho h \tag{6}$$

In Eqs. (1)–(6) ρ is mass density, $\mathbf{v}$ is velocity, $\boldsymbol{\sigma}$ is Cauchy stress, $\mathbf{b}$ is body force per unit mass, e is total energy per unit mass, ϵ is internal energy per unit mass (total energy contains contributions from both internal energy and continuum kinetic energy: $e = \epsilon + \frac{1}{2} v^2$), $\mathbf{q}$ is heat flux and h is energy generation per unit mass. Eqs. (1)–(3) are commonly used in fluid dynamics analyses whereas Eqs. (4)–(6) are typically used to solve solid mechanics problems. Nevertheless, the variables used within all of these equations are defined with respect to the current/spatial configuration, i.e. variables are functions of spatial coordinate $\mathbf{x}$ and time t.

These variables and equations can also be expressed with respect to the reference/material configuration:

$$\frac{d\rho_0}{dt} = 0 \tag{7}$$

$$\rho_0 \frac{d\mathbf{v}}{dt} = \nabla_{\mathbf{X}} \cdot \mathbf{P} + \rho_0 \mathbf{b} \tag{8}$$

$$\rho_0 \frac{d\epsilon}{dt} = \mathbf{P} : \frac{d\mathbf{F}}{dt} - \nabla_{\mathbf{X}} \cdot \mathbf{Q} + \rho_0 h \tag{9}$$

In these equations, ρ_0 is reference mass density (mass per unit reference volume), $\mathbf{P}$ is 1st Piola–Kirchhoff stress (force per unit reference area), $\mathbf{F}$ is the deformation gradient ($\frac{\partial \mathbf{x}}{\partial \mathbf{X}}$), and $\mathbf{Q}$ is the reference heat flux (energy per unit reference area per unit time). These variables in Eqs. (7)–(9) are all functions of the reference coordinate $\mathbf{X}$ and time t, with the material time derivative retaining its earlier definition, $\frac{d\mathbf{g}(\mathbf{X},t)}{dt} = \frac{\partial \mathbf{g}}{\partial t}|_{\mathbf{X}}$. Although different in form and functional dependencies, all three sets of Eqs. (1)–(9), represent the same fundamental balance laws and are derivable from one another as shown in standard texts on continuum mechanics, e.g. [26,27].

2.2. Densities and localization

We consider a body to be a system of N atoms which are interacting with each other through some inter-atomic potential energy formulation. Each atom α is characterized by its mass m^α, its position in the reference configuration $\mathbf{X}^\alpha$, its position in the current configuration $\mathbf{x}^\alpha(t)$, its velocity $\mathbf{v}^\alpha(t) = \frac{d\mathbf{x}^\alpha}{dt}$, and a displacement $\mathbf{u}^\alpha(t) \equiv \mathbf{x}^\alpha(t) - \mathbf{X}^\alpha$. Herein, any superscripted, lower-case Greek letter will be used to refer to a particular atom.

In Hardy's formulation, two views of the material system are considered. One perspective is the continuum, where quantities are point-wise functions of time and position. These quantities include mass density $\rho_0(\mathbf{X}, t)$, momentum density $\mathbf{p}_0(\mathbf{X}, t)$, and energy density $\rho_0 e(\mathbf{X}, t)$. The other perspective is that the material system contains atoms, each of which has its own mass, momentum, potential energy and kinetic energy. In order to connect the two views, Hardy uses a localization function ψ which spatially averages the properties of the atoms, and allows many atoms to contribute to a continuum property at a specific position and time. In his original formulation, Hardy expressed ψ as a function of current position. In our derivation, we instead choose it to be a function of reference position. The three key relations analogous to Hardy's spatial forms are:

$$\rho_0(\mathbf{X}) = \sum_{\alpha=1}^{N} m^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X}) \tag{10}$$

$$\mathbf{p}_0(\mathbf{X}, t) = \sum_{\alpha=1}^{N} m^\alpha \mathbf{v}^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X}) \tag{11}$$

$$\rho_0(\mathbf{X}) e(\mathbf{X}, t) = \sum_{\alpha=1}^{N} \left\{ \frac{1}{2} m^\alpha (v^\alpha)^2 + \phi^\alpha \right\} \psi(\mathbf{X}^\alpha - \mathbf{X}). \tag{12}$$

A few important things to note:

- The localization function $\psi(\mathbf{r})$ is non-negative,[1] i.e. $\psi(\mathbf{r}) \geqslant 0$.
- $\psi(\mathbf{r})$ has dimensions of inverse volume.
- $\psi(\mathbf{r})$ is a normalized function, thus

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[1] While it is possible to choose localization functions that are not non-negative (as discussed on p. 77 of [28]), in practice this is rarely done as it contains the potential to admit unbounded values for the extremum. In such instances, additional regularity requirements are needed.
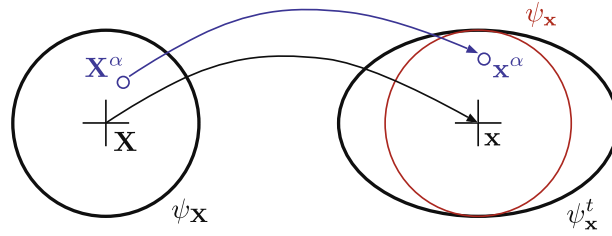
Fig. 1. Schematic showing the motion of atom $\alpha: \mathbf{X}^\alpha \to \mathbf{x}^\alpha$ and a nearby point $\mathbf{X} \to \mathbf{x}$. Also shown are the support of the localization function in the reference configuration $\psi_{\mathbf{x}}$ and its image in the current $\psi_{\mathbf{x}}^t$ which is subject to deformation. For comparison the undeformed kernel $\psi_{\mathbf{x}}$ identical to $\psi_{\mathbf{X}}$ but centered at $\mathbf{x}$ in the current configuration is also shown.

$$\int_\Omega \psi(\mathbf{r})d^3 r = 1, \tag{13}$$

where $\Omega \subset R^3$ is the domain of interest containing the collection of atoms.

- In Eq. (12), the total potential energy density of the system is expressed as the summation of individual atomic potential energies, ϕ^α.
- The velocity field $\mathbf{v}$ is defined by the expression

$$\mathbf{v}(\mathbf{X}, t) \equiv \frac{\mathbf{p}_0(\mathbf{X}, t)}{\rho_0(\mathbf{X})} = \frac{\sum_{\alpha=1}^N m^\alpha \mathbf{v}^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X})}{\sum_{\alpha=1}^N m^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X})}. \tag{14}$$

which is effectively a mass weighted average. With velocity defined in this manner, the displacement field $\mathbf{u}$ can be defined as

$$\mathbf{u}(\mathbf{X}, t) = \frac{\sum_{\alpha=1}^N m^\alpha \mathbf{u}^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X})}{\sum_{\alpha=1}^N m^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X})}, \tag{15}$$

which is consistent with the velocity field defined in (14), i.e. $\mathbf{v} = \frac{d\mathbf{u}}{dt}$. With a displacement field we can construct the motion of material points $\mathbf{X}$ from reference to current configuration as a function of time in the usual way $\mathbf{x}(\mathbf{X}, t) = \mathbf{X} + \mathbf{u}(\mathbf{X}, t)$. Furthermore, we can apply the differential operator $\nabla_{\mathbf{X}}$ to (15) to define a displacement gradient,

$$\nabla_{\mathbf{X}}\mathbf{u} = \frac{\sum_{\alpha=1}^N m^\alpha (\mathbf{u}^\alpha - \mathbf{u}(\mathbf{X}, t)) \otimes \nabla_{\mathbf{X}}\psi(\mathbf{X}^\alpha - \mathbf{X})}{\sum_{\alpha=1}^N m^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X})}, \tag{16}$$

which then can be used to form a locally defined deformation gradient $\mathbf{F}(\mathbf{X}, t) = \mathbf{1} + \nabla_{\mathbf{X}}\mathbf{u}$. However, this use of Hardy localization places additional requirements on the smoothness and exact form of ψ. For example, a so-called "top hat" or radial Heaviside function that is constant and non-zero only in compact region would not produce smooth, continuous displacement gradients.

The question arises: can one relate a Lagrangian/referential field $\hat{g}(\mathbf{X}, t)$ derived from atomic data to an Eulerian/spatial field $\tilde{g}(\mathbf{x}, t)$ derived from the same data? First, let us examine the mass density starting with the referential definition (10). To map this referential function into a spatial one we need to transform the localization function ψ and its base point $\mathbf{X}$ to the current configuration. Given a reference configuration for the atoms $\{\mathbf{X}^\alpha\}$, which defines the atomic displacements $\mathbf{u}^\alpha(t) = \mathbf{x}^\alpha(t) - \mathbf{X}^\alpha$, we can construct the continuum/coarse-scale motion $\mathbf{x}(\mathbf{X}, t) = \mathbf{u}(\mathbf{X}, t) + \mathbf{X}$ from the field $\mathbf{u}$ defined by Eq. (15). Then

$$\psi_{\mathbf{X}} = \psi_{\mathbf{X}(\mathbf{x}, t)} \equiv \psi_{\mathbf{x}}^t \tag{17}$$

where $\psi_{\mathbf{x}}^t$ is the deformed version of $\psi_{\mathbf{X}}$ which is not equivalent to $\psi_{\mathbf{x}}$ in general, please refer to the schematic in Fig. 1. Here, we have introduced new notation, e.g. $\psi_{\mathbf{X}}(\mathbf{X}^\alpha) = \psi(\mathbf{X}^\alpha - \mathbf{X})$, to make clear that the function ψ on $\mathbb{R}^3$ transforms differently than its argument $\mathbf{X}^\alpha$ in going from reference to current configuration, i.e. the kernel transforms with the displacement field and the atoms follow their particular trajectories. To first order, i.e. where the kernel radius is small enough relative to the spatial gradient of the motion $\mathbf{F}$,

$$\int_{\Omega_0} \psi_{\mathbf{X}}(\mathbf{Y}) \ d^3 Y = \int_\Omega \psi_{\mathbf{x}}^t(\mathbf{y}) \frac{1}{\det \mathbf{F}} \ d^3 y \approx \frac{1}{\det \mathbf{F}} \int_\Omega \psi_{\mathbf{x}}^t(\mathbf{y}) \ d^3 y \tag{18}$$

and $(\det \mathbf{F})\psi_{\mathbf{x}} \approx \psi_{\mathbf{x}}^t$ since $\int_{\Omega_0} \psi_{\mathbf{X}}(\mathbf{X}) \ d^3 X = \int_\Omega \psi_{\mathbf{x}}(\mathbf{x}) \ d^3 x = 1$. With this in hand, we have the usual relation between referential and spatial mass density

$$\rho_0(\mathbf{X}) = \sum_{\alpha=1}^N m^\alpha \psi_{\mathbf{X}}(\mathbf{X}^\alpha) = \sum_{\alpha=1}^N m^\alpha \psi_{\mathbf{x}}^t(\mathbf{x}^\alpha) \approx \det \mathbf{F} \sum_{\alpha=1}^N m^\alpha \psi_{\mathbf{x}}(\mathbf{x}^\alpha) = \det \mathbf{F}(\mathbf{X}, t) \ \rho(\mathbf{X}, t) \tag{19}$$

This derivation can also be directly applied to the momentum and energy densities which were defined as primary fields in (11) and (12). Please note that, despite the mapping of $\psi_{\mathbf{X}}$ to $\psi_{\mathbf{x}}^t$ by the coarse-scale motion, the same atoms may not contribute to the density of corresponding points $\mathbf{X}$ and $\mathbf{x}$. For solids, [2] where the discrepancies in coarse motion $\mathbf{x}(\mathbf{X}^\alpha, t)$ and the atomic trajectory $\mathbf{x}^\alpha(t)$ are small and of a thermal nature, there should not be significant changes in the set of atoms that contribute the densities calculated with $\psi_{\mathbf{X}}$ or $\psi_{\mathbf{x}}^t$.[3] Now turning to the derived velocity (14) and displacement (15) fields, we see that they are simply ratios of the momentum to mass density and hence the determinant factors $\det \mathbf{F}$ drop out so that

$$\hat{\mathbf{u}}(\mathbf{X},t) = \frac{\sum_{\alpha=1}^N m^\alpha \mathbf{u}^\alpha \psi_{\mathbf{X}}(\mathbf{X}^\alpha)}{\sum_{\alpha=1}^N m^\alpha \psi_{\mathbf{X}}(\mathbf{X}^\alpha)} = \frac{\sum_{\alpha=1}^N m^\alpha \mathbf{u}^\alpha \psi_{\mathbf{x}}^t(\mathbf{x}^\alpha)}{\sum_{\alpha=1}^N m^\alpha \psi_{\mathbf{x}}^t(\mathbf{x}^\alpha)} \approx \frac{\det \mathbf{F} \sum_{\alpha=1}^N m^\alpha \mathbf{u}^\alpha \psi_{\mathbf{x}}(\mathbf{x}^\alpha)}{\det \mathbf{F} \sum_{\alpha=1}^N m^\alpha \psi_{\mathbf{x}}(\mathbf{x}^\alpha)} = \tilde{\mathbf{u}}(\mathbf{x},t) \tag{20}$$

for instance. As will be made clear in Section 2.4.2, the connection between Lagrangian and Eulerian fluxes such as stress, is made through the correspondence between continuum balance laws (1)–(3), and (7)–(9).

On closing this section, we note that in his earlier works [8,21], Hardy established an important property of the localization function ψ. Given regularity of ψ, a bond function $B^{\alpha\beta}(\mathbf{X})$ between atoms α and β can be defined by the expression

$$B^{\alpha\beta}(\mathbf{X}) \equiv \int_0^1 \psi(\lambda \mathbf{X}^{\alpha\beta} + \mathbf{X}^\beta - \mathbf{X})d\lambda, \tag{21}$$

where $\mathbf{X}^{\alpha\beta} = \mathbf{X}^\alpha - \mathbf{X}^\beta$. By taking the derivative of $\psi(\lambda \mathbf{X}^{\alpha\beta} + \mathbf{X}^\beta - \mathbf{X})$ with respect to λ,

$$\frac{\partial \psi(\lambda \mathbf{X}^{\alpha\beta} + \mathbf{X}^\beta - \mathbf{X})}{\partial \lambda} = -\mathbf{X}^{\alpha\beta} \cdot \nabla_{\mathbf{X}} \psi(\lambda \mathbf{X}^{\alpha\beta} + \mathbf{X}^\beta - \mathbf{X}), \tag{22}$$

and then integrating from $\lambda = 0$ to $\lambda = 1$, one obtains the identity:

$$\psi(\mathbf{X}^\alpha - \mathbf{X}) - \psi(\mathbf{X}^\beta - \mathbf{X}) = -\mathbf{X}^{\alpha\beta} \cdot \nabla_{\mathbf{X}} B^{\alpha\beta}(\mathbf{X}). \tag{23}$$

We will revisit the connection between the bond function in the reference and current configuration in Section 2.4.2.

2.3. Energy and force assumptions

Hardy makes four key assumptions about the forms of the energies of, and forces on, the atoms in the system. The first is that the total potential energy of the system, Φ, can be considered to be the summation of individual potential energies of each atom within the system,

$$\Phi = \sum_{\alpha=1}^N \phi^\alpha. \tag{24}$$

The usual procedure for constructing ϕ^α is to partition the energies per bond to each of the constituent atoms such that the partition factors add to one.

The second assumption is that the force on any atom can be expressed by the summation

$$\mathbf{f}^\alpha \equiv -\frac{\partial \Phi}{\partial \mathbf{x}^\alpha} = \sum_{\beta \neq \alpha}^N \mathbf{f}^{\alpha\beta}. \tag{25}$$

Although it is not always clear what the physical meaning of $\mathbf{f}^{\alpha\beta}$ is, this partition can always be made. When Φ is the summation of pair potentials, $\phi^\alpha = \frac{1}{2} \sum_{\beta \neq \alpha}^N \phi^{\alpha\beta}(x^{\alpha\beta})$ where $x^{\alpha\beta} = \|\mathbf{x}^{\alpha\beta}\|$ and $\mathbf{x}^{\alpha\beta} \equiv \mathbf{x}^\alpha - \mathbf{x}^\beta$, or for the embedded atom method (EAM) [29], $\mathbf{f}^{\alpha\beta}$ obviously means the force exerted on atom α by atom β. However, for some multi-body potentials, such as the 3-body term in the Stillinger–Weber potential [30], the meaning is not so straightforward; nevertheless, the force partition (25) can be constructed. This partition is not unique; more discussion of this fact will be given in Sections 2.4.3 and 4.3.4.

The third assumption Hardy makes is that the atomic potential energies depend only on the relative inter-atomic distances, $\phi^\alpha = \phi^\alpha(x^{\alpha\beta}, x^{\alpha\gamma}, \ldots, x^{\beta\gamma})$, so

$$\mathbf{f}^\alpha = -\sum_{\beta \neq \alpha}^N \frac{\partial \Phi}{\partial x^{\alpha\beta}} \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} = -\sum_{\beta \neq \alpha}^N \sum_{\gamma=1}^N \frac{\partial \phi^\gamma}{\partial x^{\alpha\beta}} \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}. \tag{26}$$

This expression includes the possibility that $\alpha = \gamma$. While it is clear that radially-symmetric potentials such as Lennard-Jones [31,32] and EAM satisfy this assumption, it is also true that potential energies that depend on bond orientations satisfy this as well. For the 3-body term in the Stillinger–Weber potential [30], it can be shown by way of the law of cosines, which relates the bond angles to relative inter-atomic distances, that this third assumption is valid.

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[2] Fluids and granular materials will be touched on in Section 5 at the end of the paper.

[3] An alternate viewpoint considering only the transformation of discrete values of the localization function following the trajectories of the relevant atoms $\psi_{\mathbf{X}}(\mathbf{X}_\alpha)$ from the reference to current, would not lead to any change in the set of atoms but says nothing about points in space not occupied by atoms nor provides a simple route to (18).

Finally, the fourth assumption made is that each atomic potential energy depends only on the distances between the atom under consideration and all other atoms, $\phi^\alpha = \phi^\alpha(x^{\alpha\beta}, x^{\alpha\gamma}, \ldots, x^{\alpha N})$. Thus, the force between atoms α and β can be expressed as

$$\mathbf{f}^{\alpha\beta} = -\left\{\frac{\partial\phi^\alpha}{\partial x^{\alpha\beta}} + \frac{\partial\phi^\beta}{\partial x^{\alpha\beta}}\right\}\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} = -\mathbf{f}^{\beta\alpha}. \tag{27}$$

Clearly, while pair potentials and EAM qualify for this assumption, the potential of Stillinger–Weber does not since the angle between atoms α, β, γ depends on all three relative distances including $x^{\beta\gamma}$. This should in no-way imply that the quantity $\mathbf{f}^{\alpha\beta}$ cannot be defined. Rather, we merely note that for some choices of inter-atomic potential Hardy's fourth assumption does not appear to be applicable. This point will be further addressed in Section 4.

2.4. Derivation of continuum expressions

Here we apply the kinematic definitions (10)–(12) to the balance laws (7)–(9) in order to define the referential fluxes of stress and heat. We also make connections between these fluxes and their spatial counterparts through the well-known Piola transform which is ultimately derived from the relations between the respective balance laws, (7)–(9) and (1)–(3), respectively.

2.4.1. Balance of mass
Inspection of Eq. (10) reveals that

$$\frac{d\rho_0}{dt} = 0,$$

since locations of atoms in the reference configuration, $\{\mathbf{X}^\alpha\}$, are fixed.

2.4.2. Balance of linear momentum
Starting with Hardy's expression for momentum density (11),

$$\rho_0\frac{d\mathbf{v}}{dt} = \frac{d\mathbf{p}_0}{dt} = \frac{d}{dt}\left\{\sum_{\alpha=1}^N m^\alpha\mathbf{v}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X})\right\} = \sum_{\alpha=1}^N m^\alpha\frac{d\mathbf{v}^\alpha}{dt}\psi(\mathbf{X}^\alpha - \mathbf{X}) = \sum_{\alpha=1}^N(\mathbf{f}^\alpha + m^\alpha\mathbf{b}^\alpha)\psi(\mathbf{X}^\alpha - \mathbf{X}),$$

where we have applied Newton's 2nd law for each atom and divided the total force on atom α into the sum of total internal force $\mathbf{f}^\alpha$ and the body force $m^\alpha\mathbf{b}^\alpha$. The internal force term on the RHS of the above expression can be combined with Hardy's second force assumption to obtain,

$$\sum_{\alpha=1}^N\mathbf{f}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X}) = \sum_{\alpha=1}^N\sum_{\beta\neq\alpha}^N\mathbf{f}^{\alpha\beta}\psi(\mathbf{X}^\alpha - \mathbf{X}).$$

Since α and β run over all atoms in the system, they are considered dummy indices and can be switched. By doing this, and using the symmetry condition, (27), one obtains

$$\sum_{\alpha=1}^N\mathbf{f}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X}) = \frac{1}{2}\sum_{\alpha=1}^N\sum_{\beta\neq\alpha}^N\mathbf{f}^{\alpha\beta}(\psi(\mathbf{X}^\alpha - \mathbf{X}) - \psi(\mathbf{X}^\beta - \mathbf{X})).$$

Using this with expression (23), the time derivative of the momentum density becomes

$$\rho_0\frac{d\mathbf{v}}{dt} = \sum_{\alpha=1}^N(\frac{1}{2}\sum_{\beta\neq\alpha}^N\mathbf{f}^{\alpha\beta}(-\mathbf{X}^{\alpha\beta}\cdot\nabla_\mathbf{X}B^{\alpha\beta}(\mathbf{X})) + m^\alpha\mathbf{b}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X})) \tag{28}$$

$$= \nabla_\mathbf{X}\cdot(-\frac{1}{2}\sum_{\alpha=1}^N\sum_{\beta\neq\alpha}^N\mathbf{f}^{\alpha\beta}\otimes\mathbf{X}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X})) + \sum_{\alpha=1}^N m^\alpha\mathbf{b}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X}). \tag{29}$$

Comparing Eq. (29) with the continuum balance of momentum (8), we observe that in order for these expressions to be consistent with one another,

$$\mathbf{P}(\mathbf{X}, t) = -\frac{1}{2}\sum_{\alpha=1}^N\sum_{\beta\neq\alpha}^N\mathbf{f}^{\alpha\beta}\otimes\mathbf{X}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X}), \tag{30}$$

and

$$\mathbf{b}(\mathbf{X}, t) = \frac{1}{\rho_0(\mathbf{X})}\sum_{\alpha=1}^N m^\alpha\mathbf{b}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X}) = \frac{\sum_{\alpha=1}^N m^\alpha\mathbf{b}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X})}{\sum_{\alpha=1}^N m^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X})}. \tag{31}$$

For pair and other central force potentials (e.g. EAM),

$$\mathbf{P} = \frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \left\{ \frac{\partial \phi^{\alpha}}{\partial x^{\alpha\beta}} + \frac{\partial \phi^{\beta}}{\partial x^{\alpha\beta}} \right\} \frac{\mathbf{x}^{\alpha\beta} \otimes \mathbf{X}^{\alpha\beta}}{x^{\alpha\beta}} B^{\alpha\beta}(\mathbf{X}). \tag{32}$$

This expression can be further simplified by splitting this expression into two terms, switching the dummy indices used in one of the terms, and using the relations $x^{\beta\alpha} = x^{\alpha\beta}, \mathbf{x}^{\beta\alpha} = -\mathbf{x}^{\alpha\beta}, \mathbf{X}^{\beta\alpha} = -\mathbf{X}^{\alpha\beta}$ and $B^{\beta\alpha} = B^{\alpha\beta}$ to obtain

$$\mathbf{P} = \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \frac{\partial \phi^{\beta}}{\partial x^{\alpha\beta}} \frac{\mathbf{x}^{\alpha\beta} \otimes \mathbf{X}^{\alpha\beta}}{x^{\alpha\beta}} B^{\alpha\beta}(\mathbf{X}). \tag{33}$$

It is interesting to note that Eq. (30) shows that $\mathbf{P}$ is connected to the underlying atomic displacements through the inter-atomic forces $\mathbf{f}^{\alpha\beta}$. It is also through this connection that $\mathbf{P}$ is implicitly dependent on thermal motion of the atomic system. Our expression defines stress without the need to necessarily define a deformation gradient field or a hyperelastic stored energy function.

Also note that Eq. (30) contains only force terms on the right-hand side; no explicit dependence on velocity is present, [4] unlike the Cauchy stress expression

$$\boldsymbol{\sigma}(\mathbf{x}, t) = -\frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \mathbf{x}^{\alpha\beta} \widetilde{B}^{\alpha\beta}(\mathbf{x}) - \sum_{\alpha=1}^{N} m^{\alpha} \mathbf{w}^{\alpha} \otimes \mathbf{w}^{\alpha} \tilde{\psi}(\mathbf{x}^{\alpha} - \mathbf{x}) \tag{34}$$

from the Eulerian analysis [8,21]. The relative velocity $\mathbf{w}^{\alpha}$ is defined

$$\mathbf{w}^{\alpha}(\mathbf{x}, t) \equiv \mathbf{v}^{\alpha} - \mathbf{v}(\mathbf{x}, t). \tag{35}$$

and has the property

$$\sum_{\alpha=1}^{N} m^{\alpha} \mathbf{w}^{\alpha} \tilde{\psi}(\mathbf{x}^{\alpha} - \mathbf{x}) = \mathbf{0} \tag{36}$$

by virtue of the Eulerian analogue of the definition (14). Note that $\tilde{\psi}$ and $\widetilde{B}$ are the localization and bond functions expressed in units of inverse current/deformed volume rather than units of inverse reference/undeformed volume.

In addition to the well-known connection between the continuum measures of stress, $\mathbf{P}$ and $\boldsymbol{\sigma}$, we now show that our expression for $\mathbf{P}$ given in Eq. (30) can be directly related to Hardy's Cauchy stress expression (34) in a manner consistent with this connection. Given the continuum Piola transformation[5] from 1st P–K stress to Cauchy stress, $\boldsymbol{\sigma} = \frac{1}{J} \mathbf{P} \cdot \mathbf{F}^{T}$ where $J \equiv \det \mathbf{F}$, we produce

$$\frac{1}{J} \mathbf{P} \cdot \mathbf{F}^{T} = -\frac{1}{J} \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \frac{1}{2} \mathbf{f}^{\alpha\beta} \otimes \mathbf{X}^{\alpha\beta} B^{\alpha\beta}(\mathbf{X}) \cdot \mathbf{F}^{T}. \tag{37}$$

In order to simplify this equation, we assert that the position of each atom can be decomposed into a rigid body translation, $\mathbf{r}(t)$, a homogeneous deformation $\mathbf{F}$ relative to the material point $\mathbf{X}$, plus a perturbation due to thermal fluctuations and/or inhomogeneities in the deformation field,

$$\mathbf{x}^{\alpha} = \mathbf{r}(t) + \mathbf{F}(\mathbf{X}, t) \cdot \mathbf{X}^{\alpha} + \mathbf{z}^{\alpha}(\mathbf{X}, t), \tag{38}$$

where $\mathbf{z}^{\alpha}$ is merely the remainder of $\mathbf{x}^{\alpha}$ with respect to the expansion of $\mathbf{x}^{\alpha}$ to first order in $\mathbf{X}^{\alpha}$. We define $\boldsymbol{\Xi}^{\alpha} = \mathbf{X}^{\alpha} - \mathbf{X}$ where now $\mathbf{X}$ satisfies the relation

$$\mathbf{X} = \frac{1}{\rho_0(\mathbf{X})} \sum_{\alpha=1}^{N} m^{\alpha} \mathbf{X}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X}). \tag{39}$$

This relation enforces the restriction that material points $\mathbf{X}$ coincide with the centers of mass of the localization volumes they are associated with. This restriction apparently makes the selection of material points $\mathbf{X}$ non-trivial since (39) is an implicit relationship. However, since most crystal structures possess a high degree of symmetry, especially if an undeformed, defect-free configuration is used as a reference state, immediate selection of the appropriate locations of material points is possible and can be as dense as the lattice itself. Eq. (39) allows us to write

$$\mathbf{v}^{\alpha} = \frac{d\mathbf{r}}{dt} + \frac{d\mathbf{F}}{dt} \cdot \mathbf{X}^{\alpha} + \frac{d\mathbf{z}^{\alpha}}{dt} = \frac{d\mathbf{r}}{dt} + \frac{d\mathbf{F}}{dt} \cdot \mathbf{X} + \frac{d\mathbf{F}}{dt} \cdot \boldsymbol{\Xi}^{\alpha} + \frac{d\mathbf{z}^{\alpha}}{dt} \tag{40}$$

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[4] The P–K expression (30) also differs from the Cauchy expression (34) in that it gives a zero value for the somewhat degenerate case of a non-interacting gas regardless of temperature.

[5] The Piola transform comes directly from Nanson's formula $d\mathbf{a} = \det(\mathbf{F})\mathbf{F}^{-T} d\mathbf{A}$ which relates the change in directed area elements from reference to current configuration by way of the deformation gradient.

and then to identify

$$\mathbf{w}^{\alpha} = \frac{d\mathbf{F}}{dt}\mathbf{\Xi}^{\alpha} + \frac{d\mathbf{z}^{\alpha}}{dt} \tag{41}$$

with the part of the velocity $\mathbf{v}^{\alpha}$ that satisfies (36). Since $\mathbf{x}^{\alpha\beta} = \mathbf{F} \cdot \mathbf{X}^{\alpha\beta} + \mathbf{z}^{\alpha\beta}$, we can recast (37) as

$$\frac{1}{J}\mathbf{P} \cdot \mathbf{F}^{T} = -\frac{1}{2J}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta} \otimes (\mathbf{x}^{\alpha\beta} - \mathbf{z}^{\alpha\beta})B^{\alpha\beta}(\mathbf{X}) = -\frac{1}{2J}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta} \otimes \mathbf{x}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X}) + \frac{1}{2J}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta} \otimes \mathbf{z}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X}). \tag{42}$$

If we now examine the special case of a full system average such that $\frac{1}{J}B^{\alpha\beta} = 1/V$ for all points in a system with finite volume V, the Piola transformed $\mathbf{P}$ from (42) becomes

$$\frac{1}{J}\mathbf{P} \cdot \mathbf{F}^{T} = -\frac{1}{2V}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta} \otimes \mathbf{x}^{\alpha\beta} + \frac{1}{2V}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta} \otimes \mathbf{z}^{\alpha\beta}, \tag{43}$$

and the Cauchy stress (34) becomes

$$\boldsymbol{\sigma} = -\frac{1}{2V}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta} \otimes \mathbf{x}^{\alpha\beta} - \frac{1}{V}\sum_{\alpha=1}^{N}m^{\alpha}\mathbf{w}^{\alpha} \otimes \mathbf{w}^{\alpha}. \tag{44}$$

The difference between these two expressions, (43) and (44), is

$$\frac{1}{J}\mathbf{P} \cdot \mathbf{F}^{T} - \boldsymbol{\sigma} = \frac{1}{V}\sum_{\alpha=1}^{N}\frac{1}{2}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta} \otimes \mathbf{z}^{\alpha\beta} + \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{w}^{\alpha} \otimes \mathbf{w}^{\alpha} = \frac{1}{V}\sum_{\alpha=1}^{N}(\mathbf{f}^{\alpha} \otimes \mathbf{z}^{\alpha} + m^{\alpha}\mathbf{w}^{\alpha} \otimes \mathbf{w}^{\alpha}) \tag{45}$$

after using the identity

$$\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta} \otimes \mathbf{z}^{\alpha\beta} = \frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta} \otimes (\mathbf{z}^{\alpha} - \mathbf{z}^{\beta}) = \frac{1}{2}\left(\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta} \otimes \mathbf{z}^{\alpha} + \sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\beta\alpha} \otimes \mathbf{z}^{\beta}\right) = \sum_{\alpha=1}^{N}\mathbf{f}^{\alpha} \otimes \mathbf{z}^{\alpha} \tag{46}$$

which results simply from the manipulation of dummy indices, the definition (25) and the symmetry condition (27). In the absence of a body force ($\mathbf{f}^{\alpha} = m^{\alpha}\frac{d\mathbf{v}^{\alpha}}{dt}$),

$$\left\langle \sum_{\alpha=1}^{N}\mathbf{f}^{\alpha} \otimes \mathbf{z}^{\alpha} \right\rangle = \left\langle \frac{d}{dt}\sum_{\alpha=1}^{N}m^{\alpha}\mathbf{v}^{\alpha} \otimes \mathbf{z}^{\alpha} \right\rangle - \left\langle \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{v}^{\alpha} \otimes \frac{d\mathbf{z}^{\alpha}}{dt} \right\rangle = -\left\langle \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{v}^{\alpha} \otimes \frac{d\mathbf{z}^{\alpha}}{dt} \right\rangle$$

$$= -\left\langle \sum_{\alpha=1}^{N}m^{\alpha}(\mathbf{v} + \mathbf{w}^{\alpha}) \otimes \left(\mathbf{w}^{\alpha} - \frac{d\mathbf{F}}{dt}\mathbf{\Xi}^{\alpha}\right) \right\rangle$$

$$= -\left\langle \mathbf{v} \otimes \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{w}^{\alpha} \right\rangle + \left\langle \mathbf{v} \otimes \frac{d\mathbf{F}}{dt}\sum_{\alpha=1}^{N}m^{\alpha}\mathbf{\Xi}^{\alpha} \right\rangle - \left\langle \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{w}^{\alpha} \otimes \mathbf{w}^{\alpha} \right\rangle + \left\langle \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{w}^{\alpha} \otimes \frac{d\mathbf{F}}{dt}\mathbf{\Xi}^{\alpha} \right\rangle$$

$$= -\left\langle \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{w}^{\alpha} \otimes \mathbf{w}^{\alpha} \right\rangle + \left\langle \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{w}^{\alpha} \otimes \frac{d\mathbf{F}}{dt}\mathbf{\Xi}^{\alpha} \right\rangle \tag{47}$$

given the definition of $\mathbf{\Xi}^{\alpha}$, and the fact that time averages $\langle \bullet \rangle$ of exact differentials of bounded quantities are zero. The identity (47) is a simply a version of the virial theorem and if we assume a steady state, where $\frac{d\mathbf{F}}{dt}$ must be zero, then we have

$$\left\langle \sum_{\alpha=1}^{N}\mathbf{f}^{\alpha} \otimes \mathbf{z}^{\alpha} \right\rangle + \left\langle \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{w}^{\alpha} \otimes \mathbf{w}^{\alpha} \right\rangle = \mathbf{0}, \tag{48}$$

This does not mean that $\mathbf{F}$ is necessarily fixed at the identity; rather, it means that (48) is satisfied only for truly steady systems. Now we can return to (45) and show that the (time-averaged) expressions for the transformed 1st Piola–Kirchhoff stress and the Cauchy stress are consistent:

$$\left\langle \frac{1}{J}\mathbf{P} \cdot \mathbf{F}^{T} - \boldsymbol{\sigma} \right\rangle = \frac{1}{V}\left\langle \sum_{\alpha=1}^{N}\mathbf{f}^{\alpha} \otimes \mathbf{z}^{\alpha} + m^{\alpha}\mathbf{w}^{\alpha} \otimes \mathbf{w}^{\alpha} \right\rangle = \mathbf{0} \tag{49}$$

by use of (48).

The main difficulty in extending this proof to the general case is that the atoms contributing to the sums in (34) and (37) may be different depending on how atoms are flowing through space. Moreover, mapping the reference frame function $B^{\alpha\beta}(\mathbf{X}) = B_{\mathbf{X}}^{\alpha\beta}$ to the spatial $\widetilde{B}^{\alpha\beta}(\mathbf{x}) = B_{\mathbf{x}}^{\alpha\beta}$ is non-trivial (as alluded to in Section 2.2). Rather than attempting to do this analysis, in Section 3 we will explore how the expression for $\mathbf{P}$ in Eq. (30) performs for cases where the thermal fluctuations are significant, and compare our results with expectations from continuum mechanics and with the usual Hardy definition for Cauchy stress.

2.4.3. Balance of energy

Starting with the Lagrangian expression for the system energy (12),

$$\frac{d(\rho_0 e)}{dt} = \rho_0 \frac{de}{dt} = \frac{d}{dt}\left\{\sum_{\alpha=1}^{N}\left\{\frac{1}{2}m^{\alpha}(v^{\alpha})^2 + \phi^{\alpha}\right\}\psi(\mathbf{X}^{\alpha} - \mathbf{X})\right\} = \sum_{\alpha=1}^{N}\left\{m^{\alpha}\left(\frac{d\mathbf{v}^{\alpha}}{dt}\cdot\mathbf{v}^{\alpha}\right) + \frac{d\phi^{\alpha}}{dt}\right\}\psi(\mathbf{X}^{\alpha} - \mathbf{X})$$

$$= \sum_{\alpha=1}^{N}\left\{(\mathbf{f}^{\alpha} + m^{\alpha}\mathbf{b}^{\alpha})\cdot\mathbf{v}^{\alpha} + \frac{d\phi^{\alpha}}{dt}\right\}\psi(\mathbf{X}^{\alpha} - \mathbf{X}).$$

By imposing the second and third force assumptions, this simplifies to

$$\rho_0\frac{de}{dt} = \nabla_{\mathbf{x}}\cdot\left(\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\sum_{\gamma\neq\alpha}^{N}\left(\frac{\partial\phi^{\gamma}}{\partial x^{\alpha\beta}}\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}\cdot\mathbf{v}^{\alpha}\right)\mathbf{X}^{\alpha\gamma}B^{\alpha\gamma}(\mathbf{X})\right) + \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{b}^{\alpha}\cdot\mathbf{v}^{\alpha}\psi(\mathbf{X}^{\alpha} - \mathbf{X}). \tag{50}$$

Eq. (50) can be further simplified by using the fourth force assumption:

$$\rho_0\frac{de}{dt} = \nabla_{\mathbf{x}}\cdot\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\sum_{\gamma\neq\alpha}^{N}\left(\frac{\partial\phi^{\gamma}}{\partial x^{\alpha\beta}}(\delta_{\alpha\gamma} + \delta_{\beta\gamma})\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}\cdot\mathbf{v}^{\alpha}\right)\mathbf{X}^{\alpha\gamma}B^{\alpha\gamma}(\mathbf{X}) + \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{b}^{\alpha}\cdot\mathbf{v}^{\alpha}\psi(\mathbf{X}^{\alpha} - \mathbf{X}) \tag{51}$$

$$= \nabla_{\mathbf{x}}\cdot\left(\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\left(\frac{\partial\phi^{\beta}}{\partial x^{\alpha\beta}}\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}\cdot\mathbf{v}^{\alpha}\right)\mathbf{X}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X})\right) + \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{b}^{\alpha}\cdot\mathbf{v}^{\alpha}\psi(\mathbf{X}^{\alpha} - \mathbf{X}) \tag{52}$$

To proceed further, we separate atomic motion from continuum motion in two ways. First, we split the atomic velocities $\mathbf{v}^{\alpha}$ into the continuum velocity $\mathbf{v}(\mathbf{X}, t)$ and a relative velocity $\mathbf{w}^{\alpha}(\mathbf{X}, t)$ as in (35). Next we recall that earlier we recognized that the total energy, e, contains contributions from both internal energy and continuum-scale kinetic energy. We separate this using the expression $e = \epsilon + \frac{1}{2}v^2$:

$$\rho_0\frac{de}{dt} = \rho_0\frac{d\epsilon}{dt} + \rho_0\frac{d\mathbf{v}}{dt}\cdot\mathbf{v} \tag{53}$$

Application of (53) to the LHS of (52) and (35) to the RHS of (52) produces:

$$\rho_0\frac{d\epsilon}{dt} + \rho_0\frac{d\mathbf{v}}{dt}\cdot\mathbf{v} = \nabla_{\mathbf{x}}\cdot\left(\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\left(\frac{\partial\phi^{\beta}}{\partial x^{\alpha\beta}}\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}\cdot(\mathbf{v} + \mathbf{w}^{\alpha})\right)\mathbf{X}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X})\right) + \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{b}^{\alpha}\cdot(\mathbf{v} + \mathbf{w}^{\alpha})\psi(\mathbf{X}^{\alpha} - \mathbf{X})$$

$$= \nabla_{\mathbf{x}}\cdot(\mathbf{v}\cdot\mathbf{P}) + \nabla_{\mathbf{x}}\cdot\left(\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\left(\frac{\partial\phi^{\beta}}{\partial x^{\alpha\beta}}\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}\cdot\mathbf{w}^{\alpha}\right)\mathbf{X}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X})\right) + \rho_0\mathbf{b}\cdot\mathbf{v} + \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{b}^{\alpha}\cdot\mathbf{w}^{\alpha}\psi(\mathbf{X}^{\alpha} - \mathbf{X})$$

$$= (\nabla_{\mathbf{x}}\mathbf{v}):\mathbf{P} + \mathbf{v}\cdot(\nabla_{\mathbf{x}}\cdot\mathbf{P} + \rho_0\mathbf{b}) + \nabla_{\mathbf{x}}\cdot\left(\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\left(\frac{\partial\phi^{\beta}}{\partial x^{\alpha\beta}}\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}\cdot\mathbf{w}^{\alpha}\right)\mathbf{X}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X})\right) + \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{b}^{\alpha}\cdot\mathbf{w}^{\alpha}\psi(\mathbf{X}^{\alpha} - \mathbf{X})$$

Using the balance of linear momentum Eq. (8), this simplifies to

$$\rho_0\frac{d\epsilon}{dt} = (\nabla_{\mathbf{x}}\mathbf{v}):\mathbf{P} + \nabla_{\mathbf{x}}\cdot\left(\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\left(\frac{\partial\phi^{\beta}}{\partial x^{\alpha\beta}}\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}\cdot\mathbf{w}^{\alpha}\right)\mathbf{X}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X})\right) + \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{b}^{\alpha}\cdot\mathbf{w}^{\alpha}\psi(\mathbf{X}^{\alpha} - \mathbf{X}). \tag{54}$$

Since the $\nabla_{\mathbf{x}}$ and $\frac{d}{dt}$ operators are commutative, $\nabla_{\mathbf{x}}\mathbf{v} = \frac{d\mathbf{F}}{dt}$. Hence,

$$\rho_0\frac{d\epsilon}{dt} = \mathbf{P}:\frac{d\mathbf{F}}{dt} - \nabla_{\mathbf{x}}\cdot\mathbf{Q} + \rho_0 h, \tag{55}$$

where

$$\mathbf{Q}(\mathbf{X}, t) = -\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\left(\frac{\partial\phi^{\beta}}{\partial x^{\alpha\beta}}\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}\cdot\mathbf{w}^{\alpha}\right)\mathbf{X}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X}) \tag{56}$$

is the heat flux as expressed in the reference configuration. We note that like the expression for stress this expression contains only a potential term and not a kinetic term, unlike the spatial frame heat flux expression derived by Hardy [33]. Nevertheless, thermal motion does enter this expression through the derivatives of the potential energy, the inter-atomic positions $\mathbf{x}^{\alpha\beta}$, and the relative velocities $\mathbf{w}^{\alpha}$.

Comparison of (54) with (55) also produces the relation defining energy generation per unit mass:

$$h(\mathbf{X}, t) = \frac{1}{\rho_0(\mathbf{X})} \sum_{\alpha=1}^{N} m^\alpha \mathbf{b}^\alpha \cdot \mathbf{w}^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X}) = \frac{\sum_{\alpha=1}^{N} m^\alpha \mathbf{b}^\alpha \cdot \mathbf{w}^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X})}{\sum_{\alpha=1}^{N} m^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X})} \tag{57}$$

We note that for a uniform body force field this term simplifies to zero. This term would be also be negligible for a non-uniform body force field for which significant variations in the field are defined at larger length scales that the localization volume size associated with ψ. However, for situations where $\mathbf{b}$ truly varies from atom to atom, it appears that the work done by the field against the relative velocity field generates energy. The term h may also be related to other energy source terms that can be introduced into the atomic energy, although none are present in the above analysis.

Hardy and colleagues also derived [33] an expression for temperature by considering the equipartition theorem and the kinetic energy associated with atomic velocities relative to the velocity of the continuum at a spatial point,

$$T(\mathbf{x}, t) = \frac{1}{3k_B} \frac{\sum_{\alpha=1}^{N} m^\alpha (w^\alpha)^2 \psi(\mathbf{x}^\alpha - \mathbf{x})}{\sum_{\alpha=1}^{N} \psi(\mathbf{x}^\alpha - \mathbf{x})}, \tag{58}$$

which is a simple weighted average as opposed to the volume average in (10) for example. Here k_B is Boltzman's constant. Similarly, we can define a temperature field using our densities expressed in the reference configuration,

$$T(\mathbf{X}, t) = \frac{1}{3k_B} \frac{\sum_{\alpha=1}^{N} m^\alpha (w^\alpha)^2 \psi(\mathbf{X}^\alpha - \mathbf{X})}{\sum_{\alpha=1}^{N} \psi(\mathbf{X}^\alpha - \mathbf{X})}. \tag{59}$$

This definition is consistent with the allocation of $\frac{1}{2} k_B T$ of kinetic energy per degree of freedom for an atomic system. For solids, this allocation is somewhat inexact due to constraints, e.g. periodic boundary conditions, that may be acting on the system, but this difference is minimal for systems where the number of atoms is much larger than the number of constraints.

3. Evaluation of material frame expressions

In this section, we examine the behavior of our P–K stress expression for several molecular dynamics simulations. These simulations will confirm that our expression for P–K stress is consistent with both the virial stress and the Cauchy stress expression defined by Hardy.[6] All of our simulations involve systems of copper modeled using the EAM potential by Foiles et al. [29]. This potential creates an equilibrium, face-centered-cubic crystal of Cu of lattice parameter equal to 3.615 Å at zero temperature. For molecular dynamics simulations, a timestep of 0.001 ps is used.

Calculations are done using specialized routines written for ParaDyn [34] and the large-scale atomic/molecular massively parallel simulator (LAMMPS) [35], molecular simulation codes developed at Sandia National Laboratories. For the analyses presented in this section, the choice of the zero temperature, undeformed system is used as our material configuration. The rationale for this selection will be elaborated upon in the subsequent discussion section.

3.1. Stress for a constrained finite temperature system

In this and the following section, we present simulations of a system containing 4000 atoms ($10 \times 10 \times 10$ unit cells), where periodic boundary conditions are enforced on all sides of the simulation box. Two sets of calculations are performed: one using a single point in the center of system with a spherical localization volume of radius 15 Å and a quartic polynomial localization function, and another using a step function where both ψ and $B^{\alpha\beta}$ equal the quantity V_0^{-1} (where V_0 is the system size at zero temperature and deformation).

We first examine the situation where our system is constrained to remain at the reference volume, but heated to a finite, non-zero temperature. In this instance $\mathbf{F} = \mathbf{1}$ and $J = 1$; hence, the values of 1st P–K and Cauchy stress should coincide. Unless otherwise stated, the results presented here refer to the continuum stress measures evaluated for the single point simulations. The results obtained in the step-based simulations were similar in all cases, with stress values much closer in agreement to the system virial as one would expect since all atoms and bonds contribute uniformly in that analysis.

Fig. 2 shows the variation of instantaneous pressure with time for a system that is heated to 100 K. 'Pressure' in this case refers to the negative of the hydrostatic stress for each stress measure, i.e. the P–K pressure equals $-\frac{1}{3}\text{Trace}(\mathbf{P}) = -\frac{1}{3}P_{kK}$, the Cauchy pressure equals $-\frac{1}{3}\text{Trace}(\boldsymbol{\sigma})$ and the same relation is used for the system virial. The distributions of P–K and Cauchy nearly perfectly overlap with one another, and both distributions are centered around the virial distribution. Also, since the volume of material used for evaluation is a subset of the whole system, the variations from the mean value are larger in magnitude for both P–K and Cauchy pressures as compared with the variation observed in the virial. It is interesting to note that while the mathematical analysis presented in the previous section showed that the P–K and Cauchy stress expressions agree with one another (through the $J\boldsymbol{\sigma} = \mathbf{P} \cdot \mathbf{F}^T$ transformation) only if a long time average is taken, Fig. 2 shows that close

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[6] In this section, all calculations of Cauchy stress ($\boldsymbol{\sigma}$) are determined using Eq. (34), where the fixed spatial point $\mathbf{x}$ coincides with the material point $\mathbf{X}$ used to calculate $\mathbf{P}$ via Eq. (30).
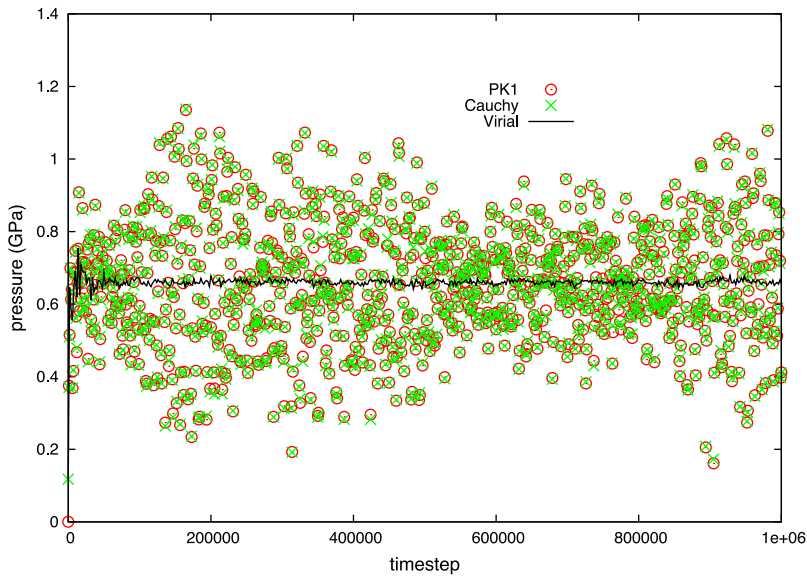
Fig. 2. Variation of instantaneous pressure with time for a constrained system at 100 K.

agreement also exists for stress evaluations at specific instants in time. We suspect that this is due to the ensemble averaging provided by the Hardy method.

The agreement between our stress measures and the virial is easier to see by using the data in Fig. 2 to calculate cumulative time-averaged pressures. Fig. 3 shows the variation of these time-averaged pressures with time for the same duration, 10^6 timesteps. This figure shows that the time-averaged pressures essentially converge within 500,000 timesteps (0.5 ns), and that the converged values of P–K, Cauchy and virial pressures are very close to one another. This agreement is more clearly shown in Table 1, which compares the converged values of P–K pressure (after 10^6 timesteps) with the virial pressure for both the point-based analysis shown in Fig. 3 and the step-based analysis. We note in Table 1 that the percent difference between P–K and virial pressures is much less than 1%, and that this difference is smaller for the step-based analysis (which uses all atoms in the system) than for the point-based analysis.

Table 1 also shows the converged time-averaged pressures for systems heated to 300 K and 675 K, values approximately 22% and 50%, respectively, of the melting temperature of copper. It can be seen that the agreement between P–K pressure and the virial remains excellent even at these high temperatures and stress levels. This close agreement is emphasized in Fig. 4, which graphically shows the variation of pressure with increasing temperature for this constrained system. It was also observed that, at the highest temperature simulated of 675 K, agreement between the P–K pressure and the virial improved if a longer time average is taken.

The above analyses show that our derived expression for P–K stress is consistent with a thermomechanical measure of stress despite the fact that it contains only a potential and not a kinetic term, unlike the Cauchy stress expression derived by Hardy. The small level of error between P–K stress and the system virial noted in Table 1 is much smaller than the amount of stress attributed to the kinetic part of Hardy's Cauchy stress or the virial itself. That kinetic part is approximately equal to 0.1169, 0.3507 and 0.7891 GPa for the temperatures considered (100, 300 and 675 K, respectively). Comparison of these values with the virial pressure listed for each temperature, given in Table 1, shows that they are significant fractions of
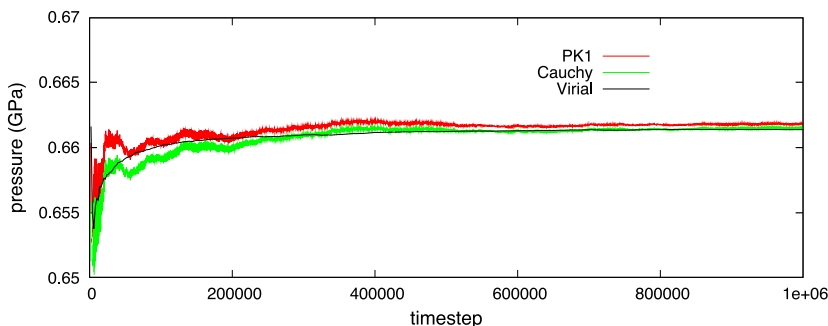

Fig. 3. Variation of time-averaged pressure with time for a constrained system at 100 K.

Table 1
Time-averaged pressures after 10^6 timesteps for constrained volume simulations.

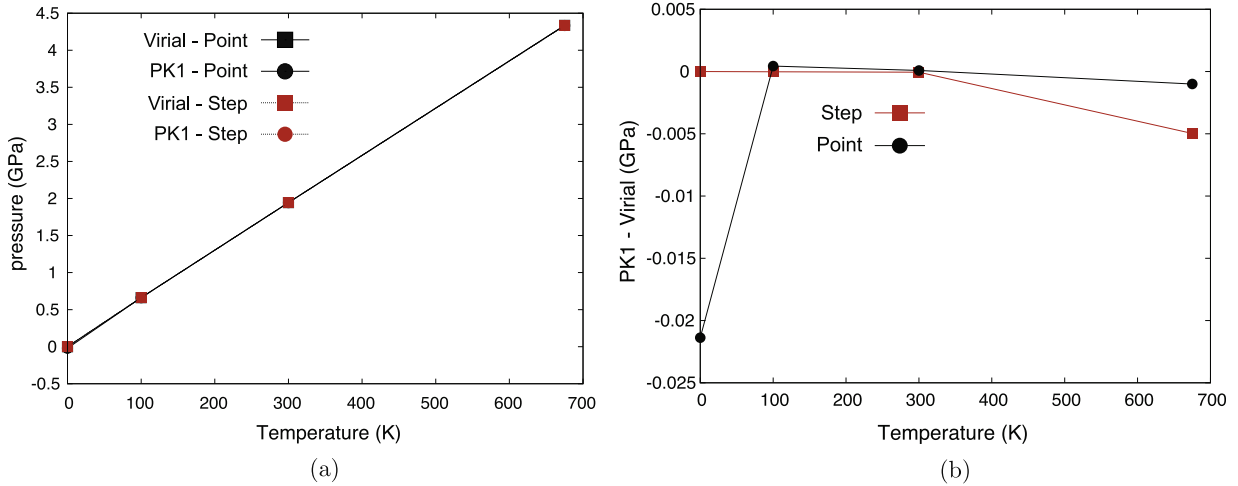| Temperature (K)	Point/step	Virial pressure (GPa)	P–K pressure (GPa)	% Difference
100	Point	0.6613775	0.6618136	0.06653
100	Step	0.6614168	0.6613937	−0.00350
300	Point	1.944335	1.944422	0.00448
300	Step	1.944465	1.944413	−0.00264
675	Point	4.335872	4.334868	−0.02316
675	Step	4.335840	4.336577	0.01699

Fig. 4. (a) Time-averaged pressures after 10^6 timesteps for constrained volume simulations performed at various temperatures. (b) Differences between P–K and virial measures of pressure at various temperatures.

the virial, about 17.7%, 18.0% and 18.2%, respectively. This finding confirms that for cases where the kinetic contribution to the stress tensor is significant, the P–K stress expression yields a full measure of stress in agreement with the expression for the total Cauchy stress, which explicitly includes this kinetic contribution.

3.2. Finite temperature deformation

For the situation of a constrained volume, the values of P–K and Cauchy stress were not anticipated to differ by any significant amount. However, we have yet to consider a case for which deformation occurs and the two values should be related by the Piola transform $\boldsymbol{\sigma} = \frac{1}{J}\mathbf{P} \cdot \mathbf{F}^T$. We now examine the scenario where our system starts out at zero temperature, is heated over the course of 10^6 timesteps (1 ns) to a finite temperature but allowed to expand in order to maintain a condition of zero pressure, is equilibrated for an additional 10^6 timesteps at that non-zero temperature and zero pressure, and is then triaxially stretched an additional 1% or 5% from this expanded state.

Fig. 5 shows the variation of the hydrostatic stresses for $\mathbf{P}$, $\boldsymbol{\sigma}$ (as measured using the original Hardy formulation) and the system virial for a stretch of 1% after equilibration at 100 K. In this section, we plot and discuss only values measured from the simulations performed with the point-based analysis; however, values calculated with step-based analysis were virtually the same. Fig. 5 shows large variations in the instantaneous estimates of $\mathbf{P}$ and $\boldsymbol{\sigma}$ as compared with the system virial. It is observed that this variation stays within a limit of approximately ±15% of the long time average after 400,000 timesteps (0.4 ns) have elapsed. As expected, the values of $\mathbf{P}$ are slightly higher than the values of $\boldsymbol{\sigma}$ and the virial. Fig. 6 compares the transformed stress $\frac{1}{J}\mathbf{P} \cdot \mathbf{F}^T$ to the Cauchy stress and virial, and demonstrates that the transformed P–K stress is in close correspondence with the Cauchy measure. In this figure, we see that the distributions of transformed Piola–Kirchhoff stress and Cauchy stress nearly perfectly overlap with one another, and both distributions are centered around the virial distribution. Again, we note that although the mathematical analysis presented in the previous section showed that the P–K and Cauchy stress expressions agree with one another only if a long time average is taken, Fig. 6 shows that close agreement also exists for stress evaluations at specific instants in time.

Fig. 7 shows the cumulative time averages of the four stress values ($\mathbf{P}$, σ, virial and transformed $\mathbf{P}$). It is observed that the system virial approaches its long time average in a short amount of time, ~20,000 timesteps (0.02 ns), and that both the Cauchy stress and transformed P–K stress approach this same value within approximately 200,000 timesteps (0.2 ns). The P–K stress also approaches its own long time average within this same amount of time, and the value is appropriately higher.
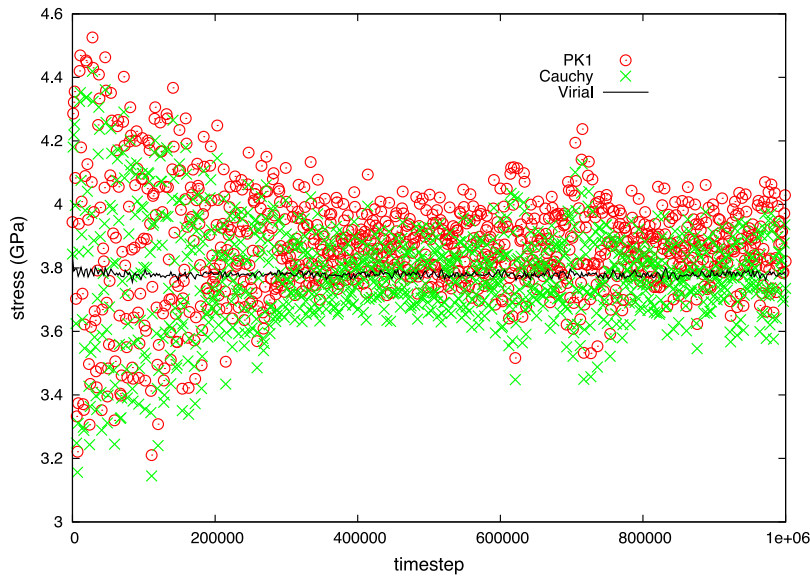
Fig. 5. Variation of the instantaneous hydrostatic stresses for **P** Eq. (30), $\boldsymbol{\sigma}$ Eq. (34) and the system virial for a stretch of 1% after equilibration at 100 K and zero pressure.
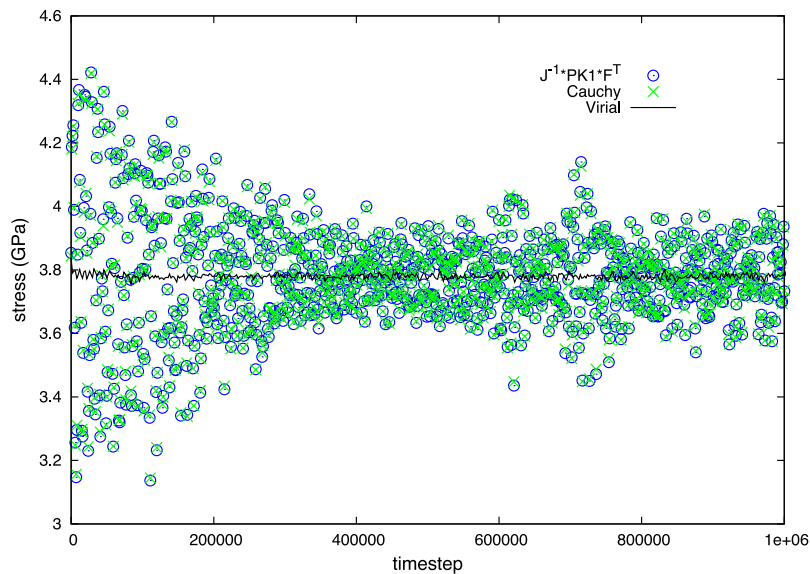

Fig. 6. Variation of the instantaneous hydrostatic stresses for $\frac{1}{J}\mathbf{P}\cdot\mathbf{F}^T, \boldsymbol{\sigma}$ and the system virial for a stretch of 1% after equilibration at 100 K and zero pressure.

Values of these long time averages are listed in Table 2. These results clearly show a negligible difference between the transformed P–K stress value and the virial of the system. Thus, we again conclude that our derived expression is consistent with the continuum relation between Cauchy and P–K stress despite the absence of a kinetic term.

In addition to our simulation results for the case of 1% stretch at 100 K, Table 2 also shows results for systems heated to 300 K and 675 K for stretches of both 1% and 5% following thermal equilibration at zero pressure. We observe that in all cases, the difference between the hydrostatic virial stress and the hydrostatic transformed P–K stress is very small with a difference of, at most, 1%. The results in Figs. 8(a) and (b) show near perfect agreement of the virial and the transformed P–K stress across a range of temperatures.[7]

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[7] These figures reveal that at higher temperatures a lower amount of stress is produced within the system. This result can be attributed to the temperature dependence of the elastic constants that softens (decreases) their value with increasing temperature.
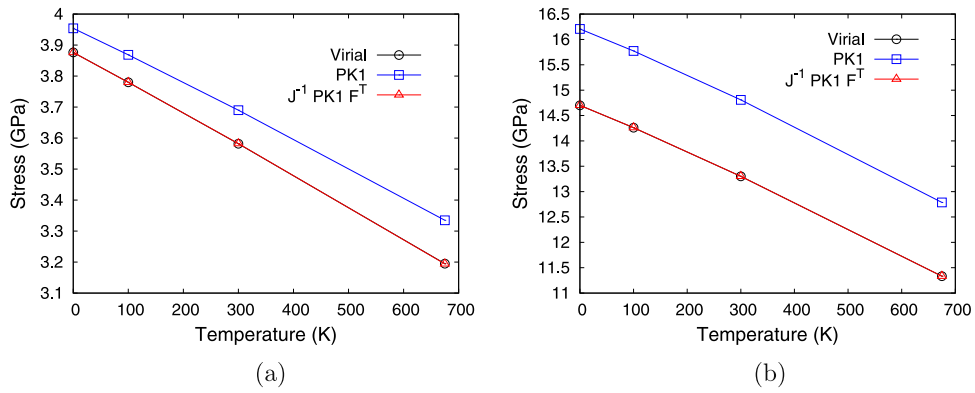
Fig. 8. Variation of time-averaged hydrostatic stress measures after 10^6 timesteps with temperature for a stretch of (a) 1%, and (b) 5% after equilibration at that temperature.
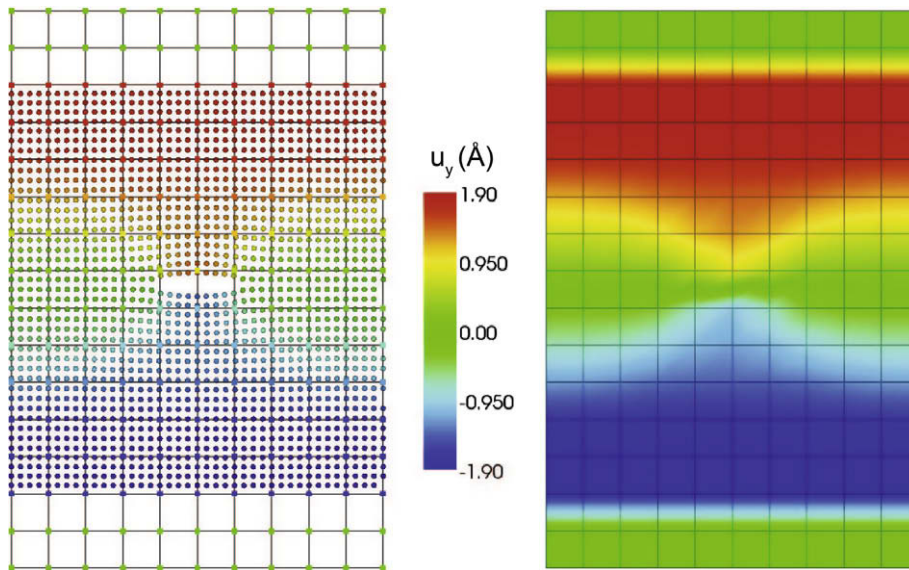

Fig. 9. Displacement field u_y for a center-cracked body vertically stretched 6.9%. (Left) Atoms pictured with overlaying mesh and nodes. (Right) Mesh elements showing contours of continuum displacement field; mesh is shown with gray lines to identify elements.

Table 2
Time-averaged stresses after 10^6 timesteps for simulations of a heated and triaxially strained system. Here, '% difference' refers to the difference between transformed P–K stress (the 6th) column) and the virial.

T (K)	Point/step	Total strain	Virial (GPa)	P–K (GPa)	$\frac{1}{J}(P-K)\mathbf{F}^T$	% Difference
0	Point	0.01	3.876275	3.954033	3.876123	−0.00394
0	Step	0.01	3.876273	3.954190	3.876277	−0.00009
0	Point	0.05	14.70036	16.20713	14.70035	−0.00009
0	Step	0.05	14.70036	16.20710	14.70032	−0.00026
100	Point	0.01168	3.779846	3.868452	3.779658	−0.00499
100	Step	0.01163	3.782552	3.871040	3.782538	−0.00038
100	Point	0.05169	14.26000	15.77334	14.26085	0.00597
300	Point	0.01495	3.581698	3.690054	3.582124	0.01190
300	Step	0.01495	3.579387	3.687273	3.579472	0.002386
300	Point	0.05515	13.30167	14.80901	13.30142	−0.00186
675	Point	0.02174	3.194773	3.334715	3.194304	−0.01469
675	Step	0.02174	3.194821	3.303813	3.164701	−0.94278
675	Point	0.06221	11.33258	12.78735	11.33345	0.00768

method. For this system, our mesh consists of $10 \times 15 \times 1 = 150$ elements where our mesh extends beyond the atomic system in the vertical direction by 2.5 unit cells at both the upper and lower boundaries.

Fig. 9 shows the displaced atoms, colored by the values of the component u_y of their displacement vector, as well as u_y displacement field evaluated at nodes and interpolated through elements, for the center-cracked body vertically stretched by approximately 6.9%. The left portion of Fig. 9 clearly shows that the nodal values of displacement agree with the values of nearby atoms, while the right portion displays a displacement field consistent with expectations from fracture mechanics. It is interesting to note that the normalization present in Eq. (15) enables approximately correct values of u_y to be calculated at nodes bordering the boundaries of the atomic system, even though 1/2 of each node's localization volume is empty. This is because the normalization produces a displacement value corresponding to the center of mass of the localization volume and assigns that value to the node. And, since each element only contains a small number of atoms, the difference between the nodal position and the center of mass position is relatively small. Obviously, special care should be taken to use small elements near the boundary of an enclosed atomistic system, or near any region for which mass is unevenly distributed within the localization volume in the reference configuration. Nodes with localization volumes that are completely empty of atoms are assigned a zero value.

Fig. 10 shows the fields of P_{yy} and σ_{yy} for the same stretch state of 6.9%. These fields are consistent with expectations from fracture mechanics, possessing features such as zero stress in the crack opening region and concentrations of tensile stress near the crack tips. Consistency between our formulation and Hardy's is shown by the qualitative similarity of the fields, with values of σ_{yy} having, in general, a slightly higher magnitude than the corresponding value of P_{yy}. Quantitative consistency can be evaluated by comparing the values at a specific material point. We choose a node near the crack tip, at a position of {21.69 Å, 10.845 Å, 10.845 Å} (six elements down from the top of the system, and two elements from the right edge). At this node, the value of P_{yy} equals 9.40327 GPa, and the value of σ_{yy} is 10.0719 GPa. Using our method to estimate displacement gradient $\nabla_{\mathbf{X}}\mathbf{u}$, and by using the relation $\mathbf{F} = \mathbf{1} + \nabla_{\mathbf{X}}\mathbf{u}$, the value of transformed P–K stress is calculated to be 9.48638 GPa. This value is somewhat lower than the expected value from the Hardy expression (a difference of about -5.81%). However, our earlier simulation examples indicate that this agreement may improve if the system is fixed at a given (inhomogeneous) deformation state and stress values are time-averaged for periods $\sim$1 ns. It may also be the case that displacement gradient values are actually higher in magnitude than estimated here due to the small size of the system and the use of (relatively) large localization volumes near the crack tip, i.e. the estimated displacement gradient also has errors associated with it.

4. Formulation for a micromorphic continuum

In Section 2.3, we noted that Hardy makes four assumptions about the forms of the energies of, and forces on, the atoms in the system. We also noted that arbitrary multi-body potentials do not necessarily satisfy all four assumptions. For example, the Stillinger–Weber potential for silicon [30], contains a 3-body term that violates the fourth assumption. This assump-
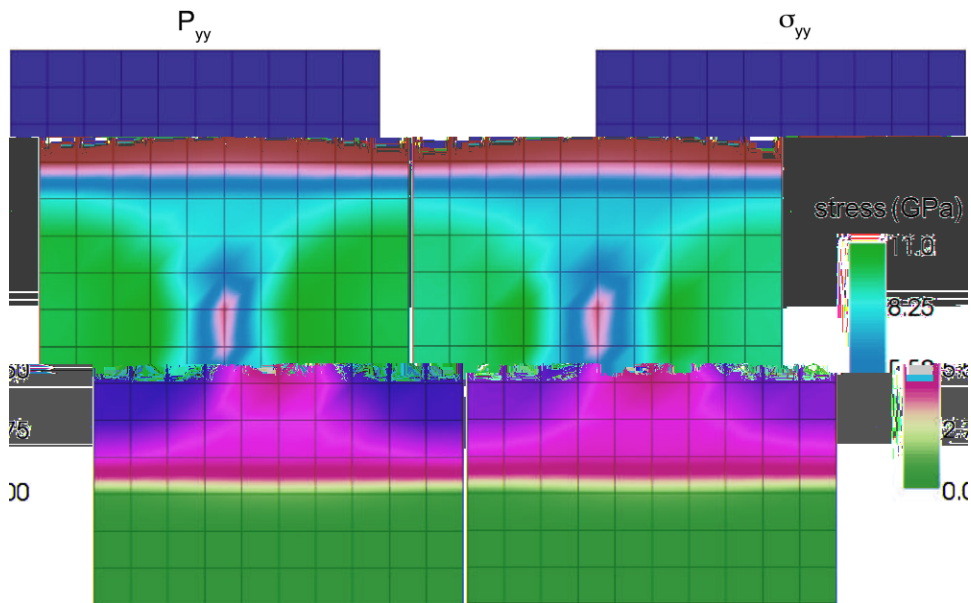

Fig. 10. Stress fields for a center-cracked body vertically stretched 6.9%. (Left) Mesh elements showing contours of continuum field P_{yy}. (Right) Mesh elements showing contours of continuum field σ_{yy} as determined from the original Hardy formulation. In both pictures, the mesh is shown with gray lines to identify elements.

tion is pivotal as it leads to a simplified form of the inter-atomic force between two atoms, which is then used to isolate the expression for stress in the balance of energy. Without this relationship, it is not straightforward to show that the stress expression derived from momentum balance also satisfies energy balance.

This issue has been examined further by both Delph [38] and Chen [39]. In his work, Delph uses the linear momentum balance to derive a generalized expression for stress that includes multi-body terms up to Nth order (where N is the number of atoms in the system). However, this same expression is not present within his analysis of the balance of energy. On the other hand, Chen restricts her analysis to consider only potentials with 2-body and 3-body terms, such as the aforementioned Stillinger–Weber potential and the potential by Tersoff [40,41]. While Chen does manage to show that the stress expression defined by linear momentum appears in the energy balance, her derivation is unclear in its consistency with regard to the expression for the inter-atomic force between two atoms.

We hypothesize that the difficulties experienced by both Delph and Chen are due to the underlying assumption that potential energies that use multi-body terms representative of directional bonding constitute a standard continuum at the microscopic scale. Rather, we conjecture that an enhanced continuum theory is required in order to represent such a material. One such theory is that of a micromorphic continuum as put forth by Eringen [42,43]. This theory is attractive as it is based on the supposition of microscopic deformations and rotations and includes the concepts of asymmetric stress and a couple stress tensor, both of which act to balance angular or rotational momentum in a body. Such concepts would seemingly be vital when defining volumes associated with continuum material points of arbitrary size and shape for a material governed by directional bonding between atoms. (This point is further addressed in Appendix A.)

In this section, we apply our material frame version of the Hardy formulation to the set of balance laws for a micromorphic continuum. The choice of a material frame analysis is not happenstance; indeed, the authors have attempted to perform a spatial frame analysis consistent with the original formulation by Hardy. However, this analysis is not trivial as an inconsistency exists between the notion of a fixed spatial point $\mathbf{x}$ from the Hardy formulation with the material point $\bar{\mathbf{x}}$ of Eringen's theory. In micromorphic theory, $\bar{\mathbf{x}}$ represents the center of mass of a "microvolume" or "microelement" at the current state of deformation. However, Hardy's analysis requires that $\mathbf{x}$ represent a fixed spatial point. Combining the two formulations requires the introduction of additional terms to account for the offset of the center of mass from the spatial point $\mathbf{x}$. We have thus far been unable to define a unambiguous set of balance laws that includes such additional variables. Eringen's original derivation for balance laws in the material frame, as shown in [42], does include such variables. For a material frame analysis (as presented in Section 2), this inclusion is unnecessary: a set of material points $\mathbf{X}$ can be selected that satisfy the center of mass requirement and these points remain fixed over time in the reference configuration. This statement is not true for spatial points that coincide with the material points when the system occupies the reference configuration as, at a later time, they will no longer represent mass centers.

Before proceeding, we note that Chen and Lee previously performed an analysis to connect atomistic quantities to micromorphic theory [44,45]. In their work, they consider both instantaneous and time-averaged forms of thermomechanical variables and the consistency of these variables with the balance laws for a micromorphic continuum. However, their analysis was performed using a mixture of material and spatial frames as they use the spatial forms of the balance laws and consider current positions of microelements but define quantities relative to fixed sets of atoms associated with each microelement. In addition, they use the original form of Eringen's theory without consideration of the mass center issue discussed above. Our work will involve manipulation of the material frame versions of the balance laws, thereby avoiding this inconsistency. It is worth noting that Zhou and McDowell considered a similar "equivalent continuum" analysis for a micropolar continuum [13] (a continuum with microelements that undergo rigid rotations only), but proceeded in an entirely different manner than we do or that Chen and Lee have. Also, Murdoch has performed an analysis in which he defined a couple stress tensor that satisfies a moment of momentum balance [15]. It will be seen that our expression for couple stress contains significant differences as compared to Murdoch's expression, and that, unlike Murdoch, we consider the full set of micromorphic balance laws as established by Eringen.

4.1. Balance laws

The material frame balance laws for a micromorphic continuum, as derived by Eringen in [42], are as follows:

$$\frac{d\rho_0}{dt} = 0 \tag{61}$$

$$\rho_0 \frac{d\mathbf{I}}{dt} = 0 \tag{62}$$

$$\rho_0 \frac{d\mathbf{v}}{dt} = \nabla_{\mathbf{x}} \cdot \mathbf{P} + \rho_0 \mathbf{b} \tag{63}$$

$$\rho_0 \frac{d^2 \boldsymbol{\chi}}{dt^2} \cdot \mathbf{I} = \nabla_{\mathbf{x}} \cdot \mathbf{M} + \mathbf{P} - \bar{\mathbf{P}} + \rho_0 \mathbf{c} \tag{64}$$

$$\rho_0 \frac{d\epsilon}{dt} = \mathbf{P} : \frac{d\mathbf{F}}{dt} + \mathbf{M} : \left(\nabla_{\mathbf{x}} \frac{d\boldsymbol{\chi}}{dt} \right) + (\bar{\mathbf{P}} - \mathbf{P}) : \frac{d\boldsymbol{\chi}}{dt} - \nabla_{\mathbf{x}} \cdot \mathbf{Q} + \rho_0 h \tag{65}$$

where $\mathbf{I}$ is the micro-inertia tensor, $\boldsymbol{\chi}$ is the micro-deformation gradient, and $\mathbf{M}$ is the couple stress tensor.[8] The stress $\overline{\mathbf{P}}$ is a quantity related to $\mathbf{P}$ in the sense that the latter is considered by Eringen to be a surface averaged limit of a traction while the former is a volume averaged limit of that same traction (for a more precise explanation, the reader is referred to Ref. [42]). We note that the total energy contains contributions from internal energy, continuum translational kinetic energy and continuum micro-rotational kinetic energy: $e = \epsilon + \frac{1}{2}v^2 + \frac{1}{2}\mathbf{I} : \left(\frac{d\boldsymbol{\chi}}{dt}^T \cdot \frac{d\boldsymbol{\chi}}{dt}\right)$.[9] These equations appear in a more generalized form in [42]; however, to simplify our analysis we have made the assumption of Cartesian coordinates (instead of curvilinear coordinates) and do not separate out intrinsic surface energy density. We also assume that the material points $\mathbf{X}$ coincide with the centers of mass of the localization volumes they are associated with, as in (39). Hence,

$$\mathbf{X} = \frac{1}{\rho_0(\mathbf{X})}\sum_{\alpha=1}^{N}m^\alpha\mathbf{X}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X}) = \frac{\sum_{\alpha=1}^{N}m^\alpha\mathbf{X}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X})}{\sum_{\alpha=1}^{N}m^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X})}. \tag{66}$$

The consequences of this assumption were mentioned earlier in this paper.

4.2. Densities

The expressions for $\rho_0, \mathbf{p}_0$ and $\rho_0 e$ defined in Eqs. (10)–(12), respectively, are reused for the micromorphic formulation. In addition, we define the following expression for micro-inertia tensor $\mathbf{I}$:

$$\rho_0\mathbf{I}(\mathbf{X}) = \sum_{\alpha=1}^{N}m^\alpha\boldsymbol{\Xi}^\alpha \otimes \boldsymbol{\Xi}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X}) \tag{67}$$

In this expression, $\boldsymbol{\Xi}^\alpha \equiv \mathbf{X}^\alpha - \mathbf{X}$ using Eringen's notation.[10] We also note that micro-inertia is the second moment of mass for the localization volume centered at $\mathbf{X}$ (using relative position vectors $\boldsymbol{\Xi}^\alpha$), while mass density is the zeroth moment. Eq. (66) can be used to show that the first moment of mass is, in-fact, zero:

$$\sum_{\alpha=1}^{N}m^\alpha\boldsymbol{\Xi}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X}) = \sum_{\alpha=1}^{N}m^\alpha(\mathbf{X}^\alpha - \mathbf{X})\psi(\mathbf{X}^\alpha - \mathbf{X}) = \sum_{\alpha=1}^{N}m^\alpha\mathbf{X}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X}) - \sum_{\alpha=1}^{N}m^\alpha\mathbf{X}\psi(\mathbf{X}^\alpha - \mathbf{X})$$

$$= \rho_0\mathbf{X} - \mathbf{X}\left(\sum_{\alpha=1}^{N}m^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X})\right) = \rho_0\mathbf{X} - \rho_0\mathbf{X} = 0$$

We also define a micro-rotational momentum tensor $\boldsymbol{\Upsilon}$,

$$\rho_0\boldsymbol{\Upsilon}(\mathbf{X}, t) = \sum_{\alpha=1}^{N}m^\alpha\mathbf{v}^\alpha \otimes \boldsymbol{\Xi}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X}). \tag{68}$$

As for standard continuum theory, there are several interesting aspects of this expression. Consistency between equations (64) and (68) requires that $\boldsymbol{\Upsilon} = \frac{d\boldsymbol{\chi}}{dt} \cdot \mathbf{I}$. This makes sense; just as we earlier defined a continuum velocity field as the product of linear momentum density and the inverse of the mass density, now we define a "micro-deformational velocity tensor" $(\frac{d\boldsymbol{\chi}}{dt})$ as the product of micro-rotational momentum tensor and the inverse of the micro-inertia tensor:

$$\frac{d\boldsymbol{\chi}}{dt}(\mathbf{X}, t) = (\rho_0\boldsymbol{\Upsilon}) \cdot (\rho_0\mathbf{I})^{-1} = \left(\sum_{\alpha=1}^{N}m^\alpha\mathbf{v}^\alpha \otimes \boldsymbol{\Xi}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X})\right) \cdot \left(\sum_{\alpha=1}^{N}m^\alpha\boldsymbol{\Xi}^\alpha \otimes \boldsymbol{\Xi}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X})\right)^{-1}. \tag{69}$$

We also note that since the only time-dependent quantities in the above expression are the individual atomic velocities, we can integrate the expression to obtain the micro-deformation gradient,

$$\boldsymbol{\chi}(\mathbf{X}, t) = \left(\sum_{\alpha=1}^{N}m^\alpha\mathbf{x}^\alpha \otimes \boldsymbol{\Xi}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X})\right) \cdot \left(\sum_{\alpha=1}^{N}m^\alpha\boldsymbol{\Xi}^\alpha \otimes \boldsymbol{\Xi}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X})\right)^{-1}. \tag{70}$$

Using the expression $\mathbf{X}^\alpha = \mathbf{X} + \boldsymbol{\Xi}^\alpha$ with Eq. (66), we notice that $\boldsymbol{\chi} \to \mathbf{1}$ in the limit of zero deformation. We can use (69) and (70) to estimate the micro-gyration tensor defined by Eringen,

$$\nu \equiv \frac{d\boldsymbol{\chi}}{dt} \cdot \boldsymbol{\chi}^{-1} = \left(\sum_{\alpha=1}^{N}m^\alpha\mathbf{v}^\alpha \otimes \boldsymbol{\Xi}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X})\right) \cdot \left(\sum_{\alpha=1}^{N}m^\alpha\mathbf{x}^\alpha \otimes \boldsymbol{\Xi}^\alpha\psi(\mathbf{X}^\alpha - \mathbf{X})\right)^{-1}. \tag{71}$$

Comparison of this expression with the expression by Chen and Lee [44] shows that our formulation, while similar, does display significant differences.

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[8] As the couple stress is a third order tensor, the divergence operator is taken to act on the outermost index of $\mathbf{M}$, i.e. $\nabla_\mathbf{X} \cdot \mathbf{M} = M_{ijK,K}$.

[9] Note that in Eq. (65), the notation $\mathbf{A} : \mathbf{B}$ represents the quantity $\sum_{i=1}^{3}\sum_{j=1}^{3}A_{ij}B_{ij}$ when $\mathbf{A}$ and $\mathbf{B}$ are second order tensors and the quantity $\sum_{i=1}^{3}\sum_{j=1}^{3}\sum_{K=1}^{3}A_{ijK}B_{ijK}$ when $\mathbf{A}$ and $\mathbf{B}$ are third order tensors.

[10] Recall that this same definition was used in (39).

4.3. Derivation of continuum expressions

4.3.1. Balance of mass and micro-inertia
As before, inspection of Eq. (10) reveals that $\frac{d\rho_0}{dt} = 0$. Similarly, we notice that the expression for micro-inertia given in Eq. (67) contains no atomic variables that are time-dependent. Hence,

$$\rho_0 \frac{d\mathbf{I}}{dt} = \frac{d(\rho_0 \mathbf{I})}{dt} = 0.$$

4.3.2. Balance of linear momentum
We choose not to repeat the derivation shown in Section 2.4.2, but merely refer to our derived expressions for the 1st Piola–Kirchhoff stress tensor in Eq. (30),

$$\mathbf{P}(\mathbf{X}, t) = -\frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \mathbf{X}^{\alpha\beta} B^{\alpha\beta}(\mathbf{X}),$$

and the body force vector in Eq. (31),

$$\mathbf{b}(\mathbf{X}, t) = \frac{\sum_{\alpha=1}^{N} m^{\alpha} \mathbf{b}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X})}{\sum_{\alpha=1}^{N} m^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X})}.$$

We note that in this derivation it was not necessary to define the quantity $\mathbf{f}^{\alpha\beta}$, but merely acknowledge the relations $\mathbf{f}^{\alpha} = \sum_{\beta \neq \alpha}^{N} \mathbf{f}^{\alpha\beta}$ and $\mathbf{f}^{\beta\alpha} = -\mathbf{f}^{\alpha\beta}$. We will address the specific form of $\mathbf{f}^{\alpha\beta}$ in a later section.

4.3.3. Balance of rotational momentum
We start with the expression for micro-rotational momentum given in (68) and take its time derivative:

$$\rho_0 \frac{d^2\boldsymbol{\chi}}{dt^2} \cdot \mathbf{I} = \frac{d}{dt}\left(\rho \frac{d\boldsymbol{\chi}}{dt} \cdot \mathbf{I}\right) = \frac{d}{dt}(\rho_0 \Upsilon) = \frac{d}{dt}\left(\sum_{\alpha=1}^{N} m^{\alpha} \mathbf{v}^{\alpha} \otimes \boldsymbol{\Xi}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X})\right) = \sum_{\alpha=1}^{N} m^{\alpha} \frac{d\mathbf{v}^{\alpha}}{dt} \otimes \boldsymbol{\Xi}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X})$$

$$= \sum_{\alpha=1}^{N} (\mathbf{f}^{\alpha} + m^{\alpha} \mathbf{b}^{\alpha}) \otimes \boldsymbol{\Xi}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X})$$

By using the relation $\mathbf{f}^{\alpha} = \sum_{\beta \neq \alpha}^{N} \mathbf{f}^{\alpha\beta}$ and acknowledging that α and β are dummy indices, one obtains:

$$\rho_0 \frac{d^2\boldsymbol{\chi}}{dt^2} \cdot \mathbf{I} = \frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes (\boldsymbol{\Xi}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X}) - \boldsymbol{\Xi}^{\beta} \psi(\mathbf{X}^{\beta} - \mathbf{X})) + \sum_{\alpha=1}^{N} m^{\alpha} \mathbf{b}^{\alpha} \otimes \boldsymbol{\Xi}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X}) \tag{72}$$

In order to use the relationship shown in Eq. (23), we rearrange the first term on the RHS of (72) (labeled RHS$_1$ for convenience) into the following expression:

$$\text{RHS}_1 = \frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes (\mathbf{X}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X}) - \mathbf{X}^{\beta} \psi(\mathbf{X}^{\beta} - \mathbf{X}) - \mathbf{X}[\psi(\mathbf{X}^{\alpha} - \mathbf{X}) - \psi(\mathbf{X}^{\beta} - \mathbf{X})])$$

This can now be simplified to

$$\text{RHS}_1 = \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \mathbf{X}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X}) + \frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \mathbf{X} \otimes \mathbf{X}^{\alpha\beta} \cdot \nabla_{\mathbf{X}} B^{\alpha\beta}(\mathbf{X}).$$

We then use the chain rule to bring the divergence operator to the outside of the second term. Hence,

$$\rho_0 \frac{d^2\boldsymbol{\chi}}{dt^2} \cdot \mathbf{I} = \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \mathbf{X}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X}) + \nabla_{\mathbf{X}} \cdot \left(\frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \mathbf{X} \otimes \mathbf{X}^{\alpha\beta} B^{\alpha\beta}(\mathbf{X})\right) - \frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \mathbf{X}^{\alpha\beta} B^{\alpha\beta}(\mathbf{X})$$

$$+ \sum_{\alpha=1}^{N} m^{\alpha} \mathbf{b}^{\alpha} \otimes \boldsymbol{\Xi}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X}). \tag{73}$$

At this point, we note that the third term on the RHS is none other than $\mathbf{P}$. Also, the first two terms on the RHS of Eq. (73) appear to lack frame invariance, i.e. the value of these terms will depend on the material frame coordinate origin. In order to correct this, we add (to the first term) and subtract (from the second term) the quantity

$$\nabla_{\mathbf{X}} \cdot \left(\frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \mathbf{X}^{\alpha} \otimes \mathbf{X}^{\alpha\beta} B^{\alpha\beta}(\mathbf{X})\right),$$

and again use the relation in Eq. (23). This simplifies Eq. (73) to

$$\rho_0 \frac{d^2\boldsymbol{\chi}}{dt^2} \cdot \mathbf{I} = \frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta\neq\alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \mathbf{X}^\alpha (\psi(\mathbf{X}^\alpha - \mathbf{X}) + \psi(\mathbf{X}^\beta - \mathbf{X})) + \nabla_\mathbf{X} \cdot \left(-\frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta\neq\alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \boldsymbol{\Xi}^\alpha \otimes \mathbf{X}^{\alpha\beta} B^{\alpha\beta}(\mathbf{X}) \right) + \mathbf{P}$$
$$+ \sum_{\alpha=1}^{N} m^\alpha \mathbf{b}^\alpha \otimes \boldsymbol{\Xi}^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X}).$$

Finally, by separating the first term on the RHS into two separate terms, switching dummy indices α and β and using the relation $\mathbf{f}^{\beta\alpha} = -\mathbf{f}^{\alpha\beta}$, we arrive at

$$\rho_0 \frac{d^2\boldsymbol{\chi}}{dt^2} \cdot \mathbf{I} = \frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta\neq\alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \mathbf{X}^{\alpha\beta} \psi(\mathbf{X}^\alpha - \mathbf{X}) + \nabla_\mathbf{X} \cdot \left(-\frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta\neq\alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \boldsymbol{\Xi}^\alpha \otimes \mathbf{X}^{\alpha\beta} B^{\alpha\beta}(\mathbf{X}) \right) + \mathbf{P} + \sum_{\alpha=1}^{N} m^\alpha \mathbf{b}^\alpha \otimes \boldsymbol{\Xi}^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X}).$$
(74)

Comparing Eq. (74) with (64), we identify the expressions for couple stress,

$$\mathbf{M}(\mathbf{X}, t) = -\frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta\neq\alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \boldsymbol{\Xi}^\alpha \otimes \mathbf{X}^{\alpha\beta} B^{\alpha\beta}(\mathbf{X}),$$
(75)

for $\overline{\mathbf{P}}$,

$$\overline{\mathbf{P}}(\mathbf{X}, t) = -\frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta\neq\alpha}^{N} \mathbf{f}^{\alpha\beta} \otimes \mathbf{X}^{\alpha\beta} \psi(\mathbf{X}^\alpha - \mathbf{X}),$$
(76)

and for the body couple,

$$\mathbf{c}(\mathbf{X}, t) = \frac{1}{\rho_0(\mathbf{X})} \sum_{\alpha=1}^{N} m^\alpha \mathbf{b}^\alpha \otimes \boldsymbol{\Xi}^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X}) = \frac{\sum_{\alpha=1}^{N} m^\alpha \mathbf{b}^\alpha \otimes \boldsymbol{\Xi}^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X})}{\sum_{\alpha=1}^{N} m^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X})}$$
(77)

Before proceeding to the next section, we again point out that, with regard to the inter-atomic forces, we have only used the relations $\mathbf{f}^\alpha = \sum_{\beta\neq\alpha}^{N} \mathbf{f}^{\alpha\beta}$ and $\mathbf{f}^{\beta\alpha} = -\mathbf{f}^{\alpha\beta}$. We have not yet specified a form for the quantity $\mathbf{f}^{\alpha\beta}$.

4.3.4. Balance of energy
As before, we begin with Hardy's expression for the system energy (12),

$$\rho_0 \frac{de}{dt} = \frac{d(\rho_0 e)}{dt} = \frac{d}{dt} \left\{ \sum_{\alpha=1}^{N} \left\{ \frac{1}{2} m^\alpha (v^\alpha)^2 + \phi^\alpha \right\} \psi(\mathbf{X}^\alpha - \mathbf{X}) \right\} = \sum_{\alpha=1}^{N} \left\{ m^\alpha \left(\frac{d\mathbf{v}^\alpha}{dt} \cdot \mathbf{v}^\alpha \right) + \frac{d\phi^\alpha}{dt} \right\} \psi(\mathbf{X}^\alpha - \mathbf{X})$$
$$= \sum_{\alpha=1}^{N} \left\{ (\mathbf{f}^\alpha + m^\alpha \mathbf{b}^\alpha) \cdot \mathbf{v}^\alpha + \frac{d\phi^\alpha}{dt} \right\} \psi(\mathbf{X}^\alpha - \mathbf{X}) = \sum_{\alpha=1}^{N} \left\{ \mathbf{f}^\alpha \cdot \mathbf{v}^\alpha + \frac{d\phi^\alpha}{dt} \right\} \psi(\mathbf{X}^\alpha - \mathbf{X}) + \sum_{\alpha=1}^{N} m^\alpha \mathbf{b}^\alpha \cdot \mathbf{v}^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X}).$$

Using Hardy's second assumption, $\mathbf{f}^\alpha = \sum_{\eta=1}^{N} \mathbf{f}^{\alpha\eta}$, this can be also written as

$$\rho_0 \frac{de}{dt} = \sum_{\alpha=1}^{N} \left\{ \sum_{\eta\neq\alpha}^{N} \mathbf{f}^{\alpha\eta} \cdot \mathbf{v}^\alpha + \frac{d\phi^\alpha}{dt} \right\} \psi(\mathbf{X}^\alpha - \mathbf{X}) + \sum_{\alpha=1}^{N} m^\alpha \mathbf{b}^\alpha \cdot \mathbf{v}^\alpha \psi(\mathbf{X}^\alpha - \mathbf{X}).$$
(78)

In order to simplify the expression above, we must (as did Hardy) provide a relationship between the inter-atomic force $\mathbf{f}^{\alpha\eta}$ and the atomic potential energies ϕ^α and ϕ^η. Earlier, we noted that Hardy's third and fourth assumptions combined are only valid for pair and central force (e.g. EAM) potentials and not for potentials representative of directional bonding such as the Stillinger–Weber potential. Here, we substitute a new third assumption: each atom's potential energy depends only on the vectors that connect the atom under consideration to all other atoms. Hence, $\phi^\alpha = \phi^\alpha(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\gamma}, \ldots, \mathbf{x}^{\alpha N})$. We acknowledge that this form of ϕ^α is not invariant with respect to orientation of the coordinate system origin. (It is invariant with respect to translation.)[11] The actual form of ϕ^α is based on invariant arguments such as the angle between three neighboring atoms $\theta_\alpha^{\beta\gamma}$ which we express here in terms of relative position vectors, i.e. $\theta_\alpha^{\beta\gamma} = \frac{\mathbf{x}^{\beta\alpha} \cdot \mathbf{x}^{\gamma\alpha}}{\|\mathbf{x}^{\beta\alpha}\| \|\mathbf{x}^{\gamma\alpha}\|}$, for convenience in the subsequent mathematical developments. Using this new relation, the force between atoms α and η can be defined as

$$\mathbf{f}^{\alpha\eta} = -\left\{ \frac{\partial\phi^\alpha}{\partial\mathbf{x}^{\alpha\eta}} + \frac{\partial\phi^\eta}{\partial\mathbf{x}^{\alpha\eta}} \right\},$$
(79)

our new fourth assumption.

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[11] Appendix A of Ref. [16], discusses the fact that the system potential energy Φ must depend on its configuration through invariant quantities such as bond lengths, angles between bonds involving common atoms, areas and volumes.

Inserting Eq. (79) into the first term on the RHS of (78), this term (RHS_1) becomes the following:

$$\text{RHS}_1 = \sum_{\alpha=1}^{N} \left\{ -\sum_{\eta\neq\alpha}^{N} \left\{ \frac{\partial\phi^{\alpha}}{\partial\mathbf{x}^{\alpha\eta}} + \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \right\} \cdot \mathbf{v}^{\alpha} + \frac{d\phi^{\alpha}}{dt} \right\} \psi(\mathbf{X}^{\alpha} - \mathbf{X}) = \sum_{\alpha=1}^{N} \left\{ -\sum_{\eta\neq\alpha}^{N} \left\{ \frac{\partial\phi^{\alpha}}{\partial\mathbf{x}^{\alpha\eta}} + \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \right\} \cdot \mathbf{v}^{\alpha} + \sum_{\eta\neq\alpha}^{N} \frac{\partial\phi^{\alpha}}{\partial\mathbf{x}^{\alpha\eta}} \cdot \mathbf{v}^{\alpha\eta} \right\} \psi(\mathbf{X}^{\alpha} - \mathbf{X})$$

$$= \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \left\{ -\frac{\partial\phi^{\alpha}}{\partial\mathbf{x}^{\alpha\eta}} \cdot \mathbf{v}^{\alpha} - \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \cdot \mathbf{v}^{\alpha} + \frac{\partial\phi^{\alpha}}{\partial\mathbf{x}^{\alpha\eta}} \cdot \mathbf{v}^{\alpha} - \frac{\partial\phi^{\alpha}}{\partial\mathbf{x}^{\alpha\eta}} \cdot \mathbf{v}^{\eta} \right\} \psi(\mathbf{X}^{\alpha} - \mathbf{X})$$

$$= \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \left\{ -\frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \cdot \mathbf{v}^{\alpha} - \frac{\partial\phi^{\alpha}}{\partial\mathbf{x}^{\alpha\eta}} \cdot \mathbf{v}^{\eta} \right\} \psi(\mathbf{X}^{\alpha} - \mathbf{X}) = -\sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \cdot \mathbf{v}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X}) - \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \frac{\partial\phi^{\alpha}}{\partial\mathbf{x}^{\alpha\eta}} \cdot \mathbf{v}^{\eta} \psi(\mathbf{X}^{\alpha} - \mathbf{X})$$

We now switch dummy indices on the right term of the above expression (i.e. $\alpha \leftrightarrow \eta$) and use the relation $\mathbf{x}^{\eta\alpha} = -\mathbf{x}^{\alpha\eta}$ to obtain

$$\text{RHS}_1 = -\sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \cdot \mathbf{v}^{\alpha}(\psi(\mathbf{X}^{\alpha} - \mathbf{X}) - \psi(\mathbf{X}^{\eta} - \mathbf{X})). \tag{80}$$

Combining this result with Eqs. (23) and (78), we arrive at

$$\rho_0 \frac{de}{dt} = \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \left(\frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \cdot \mathbf{v}^{\alpha} \right) (\mathbf{X}^{\alpha\eta} \cdot \nabla_{\mathbf{X}} B^{\alpha\eta}(\mathbf{X})) + \sum_{\alpha=1}^{N} m^{\alpha} \mathbf{b}^{\alpha} \cdot \mathbf{v}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X}). \tag{81}$$

As before, this can be modified to

$$\rho_0 \frac{de}{dt} = \nabla_{\mathbf{X}} \cdot \left(\sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \left(\frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \cdot \mathbf{v}^{\alpha} \right) \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}) \right) + \sum_{\alpha=1}^{N} m^{\alpha} \mathbf{b}^{\alpha} \cdot \mathbf{v}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X}). \tag{82}$$

Similar to our material frame analysis of the balance of energy for standard continuum theory, we separate atomic motion from continuum motion by splitting the atomic velocities $\mathbf{v}^{\alpha}$. However, for a micromorphic continuum, this velocity becomes the sum of three terms,

$$\mathbf{v}^{\alpha} = \mathbf{v}(\mathbf{X}, t) + \frac{d\boldsymbol{\chi}}{dt}(\mathbf{X}, t) \cdot \boldsymbol{\Xi}^{\alpha} + \mathbf{w}^{\alpha}(\mathbf{X}, t), \tag{83}$$

where $\frac{d\boldsymbol{\chi}}{dt}(\mathbf{X}, t) \cdot \boldsymbol{\Xi}^{\alpha}$ now represents a continuum velocity associated with the microscale rotation and deformation of the microelement containing atom α. Substitution of this expression into (82), along with the aforementioned relation $e = \epsilon + \frac{1}{2}v^2 + \frac{1}{2}\mathbf{I} : \left(\frac{d\boldsymbol{\chi}^T}{dt} \cdot \frac{d\boldsymbol{\chi}}{dt} \right)$, results in the following upon simplification:

$$\rho_0 \frac{d\epsilon}{dt} + \rho_0 \frac{d\mathbf{v}}{dt} \cdot \mathbf{v} + \left(\rho_0 \frac{d^2\boldsymbol{\chi}}{dt^2} \cdot \mathbf{I} \right) : \frac{d\boldsymbol{\chi}}{dt}$$

$$= \nabla_{\mathbf{X}} \cdot \left(\mathbf{v} \cdot \left\{ \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}) \right\} \right) + \nabla_{\mathbf{X}} \cdot \left(\frac{d\boldsymbol{\chi}}{dt} : \left\{ \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \otimes \boldsymbol{\Xi}^{\alpha} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}) \right\} \right)$$

$$+ \nabla_{\mathbf{X}} \cdot \left(\sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \left(\frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \cdot \mathbf{w}^{\alpha} \right) \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}) \right) + \rho_0 \mathbf{b} \cdot \mathbf{v} + \frac{d\boldsymbol{\chi}}{dt} : \left(\sum_{\alpha=1}^{N} m^{\alpha} \mathbf{b}^{\alpha} \otimes \boldsymbol{\Xi}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X}) \right)$$

$$+ \sum_{\alpha=1}^{N} m^{\alpha} \mathbf{b}^{\alpha} \cdot \mathbf{w}^{\alpha} \psi(\mathbf{X}^{\alpha} - \mathbf{X}) \tag{84}$$

Eq. (84) can be further simplified in two ways. On the LHS, the expressions $\rho_0 \frac{d\mathbf{v}}{dt}$ and $\rho_0 \frac{d^2\boldsymbol{\chi}}{dt^2} \cdot \mathbf{I}$ are replaced using the balance of linear and rotational momentum equations shown in Eqs. (63) and (64), respectively. On the RHS, we can relate each divergence term to a corresponding continuum quantity. By using our new expression for inter-atomic forces defined in Eq. (79), we notice that the 1st Piola–Kirchhoff stress $\mathbf{P}$ is

$$\mathbf{P} = -\frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \mathbf{f}^{\alpha\eta} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}) = \frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \left\{ \frac{\partial\phi^{\alpha}}{\partial\mathbf{x}^{\alpha\eta}} + \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \right\} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X})$$

$$= \frac{1}{2} \left\{ \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \frac{\partial\phi^{\alpha}}{\partial\mathbf{x}^{\alpha\eta}} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}) + \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}) \right\}$$

$$= \frac{1}{2} \left\{ \sum_{\eta=1}^{N} \sum_{\alpha\neq\eta}^{N} \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\eta\alpha}} \otimes \mathbf{X}^{\eta\alpha} B^{\eta\alpha}(\mathbf{X}) + \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}) \right\}$$

$$= \frac{1}{2} \left\{ \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}) + \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}) \right\} = \sum_{\alpha=1}^{N} \sum_{\eta\neq\alpha}^{N} \frac{\partial\phi^{\eta}}{\partial\mathbf{x}^{\alpha\eta}} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}).$$

Hence,

$$\nabla_{\mathbf{x}} \cdot \left(\mathbf{v} \cdot \left\{ \sum_{\alpha=1}^{N} \sum_{\eta \neq \alpha}^{N} \frac{\partial \phi^{\eta}}{\partial \mathbf{x}^{\alpha\eta}} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}) \right\} \right) \rightarrow \nabla_{\mathbf{x}} \cdot (\mathbf{v} \cdot \mathbf{P}) = \mathbf{P} : \frac{d\mathbf{F}}{dt} + \mathbf{v} \cdot (\nabla_{\mathbf{x}} \cdot \mathbf{P}). \tag{85}$$

Regarding the second divergence term in (84), we notice that the couple stress tensor (Eq. (75)) now has the form

$$\mathbf{M} = \frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\eta \neq \alpha}^{N} \left\{ \frac{\partial \phi^{\alpha}}{\partial \mathbf{x}^{\alpha\eta}} + \frac{\partial \phi^{\eta}}{\partial \mathbf{x}^{\alpha\eta}} \right\} \otimes \boldsymbol{\Xi}^{\alpha} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}).$$

Admittedly, it is not as easy to simplify this expression as it was to simplify the expression for $\mathbf{P}$. However, we note here that Delph asserted that any potential energy expression dependent on M atoms within the N-atom system is equally divided among the M atoms [38]. For example, the contribution for a 3-body energy term between atoms α, β and γ is divided equally into thirds for $\phi^{\alpha}, \phi^{\beta}$ and ϕ^{γ} respectively. Hence, this assertion results in the conclusion that while, in general, $\phi^{\alpha} \neq \phi^{\eta}$, it is the case that $\frac{\partial \phi^{\alpha}}{\partial \mathbf{x}^{\alpha\eta}} = \frac{\partial \phi^{\eta}}{\partial \mathbf{x}^{\alpha\eta}}$ since the portion of potential energy that provides non-zero values of this derivative is the same for both atoms α and η. Hence,

$$\mathbf{M} = \sum_{\alpha=1}^{N} \sum_{\eta \neq \alpha}^{N} \frac{\partial \phi^{\eta}}{\partial \mathbf{x}^{\alpha\eta}} \otimes \boldsymbol{\Xi}^{\alpha} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}),$$

and,

$$\nabla_{\mathbf{x}} \cdot \left(\frac{d\boldsymbol{\chi}}{dt} : \left\{ \sum_{\alpha=1}^{N} \sum_{\eta \neq \alpha}^{N} \frac{\partial \phi^{\eta}}{\partial \mathbf{x}^{\alpha\eta}} \otimes \boldsymbol{\Xi}^{\alpha} \otimes \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}) \right\} \right) \rightarrow \nabla_{\mathbf{x}} \cdot \left(\frac{d\boldsymbol{\chi}}{dt} : \mathbf{M} \right) = \mathbf{M} : \left(\nabla_{\mathbf{x}} \frac{d\boldsymbol{\chi}}{dt} \right) + \frac{d\boldsymbol{\chi}}{dt} : (\nabla_{\mathbf{x}} \cdot \mathbf{M}) \tag{86}$$

The third divergence term provides us with the definition for heat flux vector for a micromorphic system:

$$\mathbf{Q}(\mathbf{X}, t) = -\sum_{\alpha=1}^{N} \sum_{\eta \neq \alpha}^{N} \left(\frac{\partial \phi^{\eta}}{\partial \mathbf{x}^{\alpha\eta}} \cdot \mathbf{w}^{\alpha} \right) \mathbf{X}^{\alpha\eta} B^{\alpha\eta}(\mathbf{X}) \tag{87}$$

Combining (85)–(87) into Eq. (84), along with the earlier definitions for energy generation per unit mass (57) and body couple (77), we obtain:

$$\rho_0 \frac{d\epsilon}{dt} + (\nabla_{\mathbf{x}} \cdot \mathbf{P} + \rho_0 \mathbf{b}) \cdot \mathbf{v} + (\nabla_{\mathbf{x}} \cdot \mathbf{M} + \mathbf{P} - \overline{\mathbf{P}} + \rho_0 \mathbf{c}) : \frac{d\boldsymbol{\chi}}{dt} = \mathbf{P} : \frac{d\mathbf{F}}{dt} + \mathbf{v} \cdot (\nabla_{\mathbf{x}} \cdot \mathbf{P}) + \mathbf{M} : \left(\nabla_{\mathbf{x}} \frac{d\boldsymbol{\chi}}{dt} \right)$$
$$+ \frac{d\boldsymbol{\chi}}{dt} : (\nabla_{\mathbf{x}} \cdot \mathbf{M}) - \nabla_{\mathbf{x}} \cdot \mathbf{Q} + \rho_0 \mathbf{b} \cdot \mathbf{v} + \frac{d\boldsymbol{\chi}}{dt} : \rho_0 \mathbf{c} + \rho_0 h \tag{88}$$

Upon simplifying this equation, we obtain

$$\rho_0 \frac{d\epsilon}{dt} = \mathbf{P} : \frac{d\mathbf{F}}{dt} + \mathbf{M} : \left(\nabla_{\mathbf{x}} \frac{d\boldsymbol{\chi}}{dt} \right) + (\overline{\mathbf{P}} - \mathbf{P}) : \frac{d\boldsymbol{\chi}}{dt} - \nabla_{\mathbf{x}} \cdot \mathbf{Q} + \rho_0 h, \tag{89}$$

which exactly matches the balance of energy equation derived by Eringen [42] and given earlier in Eq. (65).

5. Discussion

By constructing a material frame-based formalism similar to the spatial frame-based formalism developed by Hardy, we have derived expressions for continuum theory variables based on atomic-scale quantities. For an atomistic system governed by central force potentials, these expressions are based on conventional continuum theory and include the 1st Piola–Kirchhoff stress tensor, a body force field, a heat flux vector field, and an energy generation rate. For an atomistic system where the inter-atomic potential is multi-body and directional in nature, these expressions are based on micromorphic continuum theory and also include a couple stress tensor and a body couple tensor field.

Our formulations are suitable for the analysis of solid mechanics problems for which rearrangement of the configuration due to large relative motions of neighboring atoms is minimal. For simulations involving fluid and gaseous states of matter the concepts of a reference configuration and deformation gradient are not well-defined. Hence, our formulations would have limited usefulness for these types of simulations. This would also be true for situations of dramatic molecular rearrangement, such as mixing (as happens in granular materials). For all of these cases, the original spatial frame formulation developed by Hardy would be appropriate. The difficulty inherent to developing a spatial frame formulation for a micromor-

[46, Chapter 4 and Appendix I in Chapter 6] and the articles by Andia and colleagues [22–25]. As mentioned earlier, Andia et al. define an expression for P–K stress as a cell averaged quantity. Our expression is defined at a single material point and depends only on the size of the volume associated with that point in the sense that a minimum volume must be used to show consistency with expected continuum behavior. Additionally, both Andia et al. and Weiner make the distinction between internal and external forces, separating the interactions between atoms within the cell and the interactions between atoms with "ghost" atoms located across the periodic boundaries. This distinction is not needed for our approach.

The analyses presented in the Evaluation section clearly show that our derived expression for P–K stress is a full thermo-mechanical measure of stress despite the fact that it contains only a potential and not a kinetic term, unlike the Cauchy stress expression derived by Hardy. Our analysis also shows that our expression for **P** is consistent with Cauchy stress via the Piola transformation $\boldsymbol{\sigma} = \frac{1}{J}\mathbf{P} \cdot \mathbf{F}^T$. While, in the special case of a system average, Weiner's expression [46, Eq. A44] is equivalent to our expression for **P** (30), we have gone one step further and made a strong connection between (30) and the expressions for Cauchy stress (34) and the virial.

In order to show the consistency of our expression with continuum thermodynamics, we chose our material configuration to be the zero temperature, undeformed state of the system simulated. Unlike conventional continuum mechanics where the choice of reference configuration and temperature is arbitrary, the selection of a zero temperature state as the reference configuration is mandatory for our formulation. This requirement was discussed by Weiner [46, Chapter 4], who noted that for the case of anharmonic pair potentials, a zero value of P–K stress is achieved only at zero temperature. This can be more easily understood by examining our expression for P–K stress,

$$\mathbf{P} = -\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta}\otimes\mathbf{X}^{\alpha\beta}B^{\alpha\beta}(\mathbf{X}),$$

and comparing it with the expression derived by Hardy for Cauchy stress,

$$\boldsymbol{\sigma} = -\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta}\otimes\mathbf{x}^{\alpha\beta}\widetilde{B}^{\alpha\beta}(\mathbf{x}) - \sum_{\alpha=1}^{N}m^{\alpha}\mathbf{w}^{\alpha}\otimes\mathbf{w}^{\alpha}\tilde{\psi}(\mathbf{x}^{\alpha}-\mathbf{x}).$$

Here, we see that if we select the given current configuration to represent our material frame, the first term on the right-hand side of the Cauchy expression will exactly equal the full value of the P–K expression. However, this term will not equal zero for any system that has been equilibrated to a non-zero temperature. For that case, it is apparent that the second term on the right-hand side will be equal to a non-zero value. Ergo, the P–K and Cauchy stresses will differ by exactly this amount and the expected relationship between P–K and Cauchy stresses will not hold.

Although our continuum formulations are distinctly different from the works by Delph [38] and Chen [39] due to our use of a material frame basis, it is interesting to notice that our formulations offers two advantages. First, unlike in Delph's derivation, our stress expression appears in both the linear momentum and energy balance laws without modification. Second, unlike the work by Chen, the balance laws our expressions satisfy are the same as from micromorphic continuum theory; no specialized "microscale balance laws" need to be postulated.

Our formulation, as applied to micromorphic theory, yields an expression for the couple stress tensor **M**, Eq. (75). As couple stress has dimensions of stress times length, it is reasonable to ask if there is a characteristic length. The terms present in this expression include $\mathbf{f}^{\alpha\beta}$, $B^{\alpha\beta}(\mathbf{X})$, $\boldsymbol{\Xi}^{\alpha}$, and $\mathbf{X}^{\alpha\beta}$. The first of these, $\mathbf{f}^{\alpha\beta}$, is non-zero only for distances less than or equal to the cut-off distance of the inter-atomic potential used in the simulation. By comparison, $B^{\alpha\beta}(\mathbf{X})$ is non-zero over a region corresponding to the localization volume. The two remaining terms, $\boldsymbol{\Xi}^{\alpha}$ and $\mathbf{X}^{\alpha\beta}$, have no intrinsic length scale connected with them, as they span distances ranging from zero to the system size. Given the fact that both $\mathbf{f}^{\alpha\beta}$ and $B^{\alpha\beta}(\mathbf{X})$ go to zero outside their respective ranges, it is clear that the shorter of the two distances, i.e. the potential's cut-off distance or localization volume's size, constitutes an appropriate characteristic length. In most instances, the volume size is larger than the cut-off distance (a recommendation made in [16] for producing smooth continuum fields), and hence the latter defines the length scale for this microcontinuum.

Finally, in order to relate the material frame variables defined here to their spatial frame counterparts, it is necessary to define kinematic deformation variables such as the deformation gradient. It is interesting to note that few of the aforementioned articles establish such field variables. However, in Eq. (15) we define a displacement field **u** consistent with the same localization function and volumes used to define the thermodynamic variables. This field could easily be used to construct a locally-varying deformation gradient expression. Also, in Eqs. (70) and (71) we derived expressions for the micro-deformation gradient $\boldsymbol{\chi}$ and micro-gyration tensor ν, respectively, the kinematic variables inherent to micromorphic continuum theory. It is interesting to note that if the relationship $\mathbf{x}^{\alpha} = \mathbf{x} + \xi^{\alpha}$ is applied to Eq. (70), where ξ^{α} is the spatial frame counterpart to $\boldsymbol{\Xi}^{\alpha}$, then it can also be shown that

$$\boldsymbol{\chi}(\mathbf{X},t) = \left(\sum_{\alpha=1}^{N}m^{\alpha}\xi^{\alpha}\otimes\boldsymbol{\Xi}^{\alpha}\psi(\mathbf{X}^{\alpha}-\mathbf{X})\right) \cdot \left(\sum_{\alpha=1}^{N}m^{\alpha}\boldsymbol{\Xi}^{\alpha}\otimes\boldsymbol{\Xi}^{\alpha}\psi(\mathbf{X}^{\alpha}-\mathbf{X})\right)^{-1}. \tag{90}$$

This expression for micro-deformation gradient bears a strong resemblance to the expressions developed by both Horstemeyer et al. [47–49] and Zimmerman et al. [50,51] to define an atomic-scale deformation gradient. Detailed comparisons between our micro-deformation gradient and the atomic-scale equivalent defined in these works is deferred for future work.

Acknowledgments

Appendix A

It can be shown that inter-atomic potentials representative of directional bonding will result in a non-symmetric Cauchy stress. To accomplish this, we use the "potential" portion of the Hardy expression, $\boldsymbol{\sigma} = -\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{f}^{\alpha\beta}\otimes\mathbf{x}^{\alpha\beta}\widetilde{B}^{\alpha\beta}(\mathbf{x})$, combined with our new expression for $\mathbf{f}^{\alpha\beta} = -\{\frac{\partial\phi^{\alpha}}{\partial\mathbf{x}^{\alpha\beta}}+\frac{\partial\phi^{\beta}}{\partial\mathbf{x}^{\alpha\beta}}\}$. As a simple case, we consider the interaction of only 3 atoms (α, β and δ) through a single 3-body potential energy term Φ,

$$\Phi = \Phi(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\delta}). \tag{A.1}$$

This form fits the case of the 3-body term in the Stillinger–Weber potential [30] where α is the center atom of the $\beta - \alpha - \delta$ triplet and

$$\Phi(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\delta}) = \varepsilon\lambda\exp\left(\frac{\gamma}{\frac{x^{\alpha\beta}}{\sigma}-a}\right)\exp\left(\frac{\gamma}{\frac{x^{\alpha\gamma}}{\sigma}-a}\right)\left\{\cos(\theta)+\frac{1}{3}\right\}^2, \tag{A.2}$$

where $\varepsilon, \lambda, \gamma, \sigma$ and a are fitted material parameters and

$$\theta \equiv \arccos\left(\frac{\mathbf{x}^{\alpha\beta}\cdot\mathbf{x}^{\alpha\delta}}{x^{\alpha\beta}x^{\alpha\delta}}\right). \tag{A.3}$$

Using the relation $\phi^{\alpha} = \phi^{\alpha}(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\gamma}, \ldots, \mathbf{x}^{\alpha N})$, the full energy Φ is partitioned equally among the 3 atoms, $\phi^{\alpha} = \phi^{\beta} = \phi^{\delta} = \frac{1}{3}\Phi$. However, in order to correctly take partial derivatives of these individual energies, we must express the functional dependency for each energy correctly. For atom α, the expression is trivial,

$$\phi^{\alpha} = \frac{1}{3}\Phi(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\delta}), \tag{A.4}$$

but for atoms β and δ, the expressions are

$$\phi^{\beta} = \phi^{\beta}(\mathbf{x}^{\beta\alpha}, \mathbf{x}^{\beta\delta}) = \frac{1}{3}\Phi(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\beta}+\mathbf{x}^{\beta\delta}) \tag{A.5}$$

$$\phi^{\delta} = \phi^{\delta}(\mathbf{x}^{\delta\alpha}, \mathbf{x}^{\delta\beta}) = \frac{1}{3}\Phi(\mathbf{x}^{\alpha\delta}+\mathbf{x}^{\delta\beta}, \mathbf{x}^{\alpha\delta}) \tag{A.6}$$

In these relations, we have substituted $\mathbf{x}^{\alpha\beta}+\mathbf{x}^{\beta\delta}$ for $\mathbf{x}^{\alpha\delta}$ in the expression for ϕ^{β} since it cannot depend directly on $\mathbf{x}^{\alpha\delta}$. Likewise for the ϕ^{δ} term, we have substituted $\mathbf{x}^{\alpha\delta}+\mathbf{x}^{\delta\beta}$ for $\mathbf{x}^{\alpha\beta}$. Obviously, clarity requires that any expression that uses Φ in a simple way must refer to its original form shown in (A.1). So, when partial derivatives are taken, they must include terms that may indirectly depend on certain variables. For example,

$$\frac{\partial\phi^{\beta}}{\partial\mathbf{x}^{\alpha\beta}} = \frac{1}{3}\left(\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}+\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\frac{\partial\mathbf{x}^{\alpha\delta}}{\partial\mathbf{x}^{\alpha\beta}}\right) = \frac{1}{3}\left(\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}+\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\right). \tag{A.7}$$

Eq. (A.7) is easily understood. The first term inside the parentheses results from the derivative of Φ with respect to $\mathbf{x}^{\alpha\beta}$ as it appears explicitly within the normal functional form of Φ, but the second term is present because Φ also depends on $\mathbf{x}^{\alpha\delta}$, which itself depends on $\mathbf{x}^{\alpha\beta}$ through the relation $\mathbf{x}^{\alpha\delta} = \mathbf{x}^{\alpha\beta}+\mathbf{x}^{\beta\delta}$. Since

$$\frac{\partial\phi^{\alpha}}{\partial\mathbf{x}^{\alpha\beta}} = \frac{1}{3}\left(\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}\right), \tag{A.8}$$

we can now calculate $\mathbf{f}^{\alpha\beta}$ to be

$$\mathbf{f}^{\alpha\beta} = -\left\{\frac{\partial\phi^{\alpha}}{\partial\mathbf{x}^{\alpha\beta}}+\frac{\partial\phi^{\beta}}{\partial\mathbf{x}^{\alpha\beta}}\right\} = -\left\{\frac{1}{3}\left(\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}\right)+\frac{1}{3}\left(\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}+\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\right)\right\} = -\left\{\frac{2}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}+\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\right\}. \tag{A.9}$$

Similarly, for this example

$$\mathbf{f}^{\alpha\delta} = -\left\{\frac{2}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}+\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}\right\}, \tag{A.10}$$

It is interesting to note that the expression for $\mathbf{f}^{\alpha\beta}$ in (A.9) involves derivatives with respect to inter-atomic vectors other than just $\mathbf{x}^{\alpha\beta}$, and that it is not necessarily collinear with $\mathbf{x}^{\alpha\beta}$.

Combining the expressions in Eqs. (A.9) and (A.10) with a similarly derived expression for $\mathbf{f}^{\beta\delta}$, the expression for Cauchy stress becomes:

$$\boldsymbol{\sigma}(\mathbf{x},t) = -\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\mathbf{x}^{\alpha\beta}\otimes\mathbf{f}^{\alpha\beta}\widetilde{B}^{\alpha\beta}(\mathbf{x}) = -\mathbf{x}^{\alpha\beta}\otimes\mathbf{f}^{\alpha\beta}\widetilde{B}^{\alpha\beta}(\mathbf{x}) - \mathbf{x}^{\alpha\delta}\otimes\mathbf{f}^{\alpha\delta}\widetilde{B}^{\alpha\delta}(\mathbf{x}) - \mathbf{x}^{\beta\delta}\otimes\mathbf{f}^{\beta\delta}\widetilde{B}^{\beta\delta}(\mathbf{x})$$

$$= \mathbf{x}^{\alpha\beta}\otimes\left\{\frac{2}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}+\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\right\}\widetilde{B}^{\alpha\beta}(\mathbf{x}) + \mathbf{x}^{\alpha\delta}\otimes\left\{\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}+\frac{2}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\right\}\widetilde{B}^{\alpha\delta}(\mathbf{x}) + \mathbf{x}^{\beta\delta}\otimes\left\{-\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}+\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\right\}\widetilde{B}^{\beta\delta}(\mathbf{x}), \quad \text{(A.11)}$$

which can be simplified to

$$\boldsymbol{\sigma}(\mathbf{x},t) = \mathbf{x}^{\alpha\beta}\otimes\left\{\frac{2}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}+\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\right\}\widetilde{B}^{\alpha\beta}(\mathbf{x}) + \mathbf{x}^{\alpha\delta}\otimes\left\{\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}+\frac{2}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\right\}\widetilde{B}^{\alpha\delta}(\mathbf{x}) + \left\{\mathbf{x}^{\alpha\delta}-\mathbf{x}^{\alpha\beta}\right\}$$

$$\otimes\left\{-\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}+\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\right\}\widetilde{B}^{\beta\delta}(\mathbf{x}). \quad \text{(A.12)}$$

To proceed further, we assume that the potential function Φ can be expressed an an alternative function $\tilde{\Phi}$ that depends only on the invariants $x^{\alpha\beta}, x^{\alpha\delta}$ and θ (as defined in Eq. (A.3)):

$$\Phi = \Phi(\mathbf{x}^{\alpha\beta},\mathbf{x}^{\alpha\delta}) = \tilde{\Phi}(x^{\alpha\beta},x^{\alpha\delta},\cos\theta). \quad \text{(A.13)}$$

This assumption is certainly true for the Stillinger–Weber 3-body term (A.2) and can be generalized for other potentials representative of directional bonding. Using (A.13), we obtain the relations

$$\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}} = \frac{\partial\tilde{\Phi}}{\partial x^{\alpha\beta}}\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} + \frac{\partial\tilde{\Phi}}{\partial c_\theta}\left[\frac{\mathbf{x}^{\alpha\delta}}{x^{\alpha\beta}x^{\alpha\delta}} - \frac{c_\theta}{x^{\alpha\beta}}\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}\right]$$

$$\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}} = \frac{\partial\tilde{\Phi}}{\partial x^{\alpha\delta}}\frac{\mathbf{x}^{\alpha\delta}}{x^{\alpha\delta}} + \frac{\partial\tilde{\Phi}}{\partial c_\theta}\left[\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}x^{\alpha\delta}} - \frac{c_\theta}{x^{\alpha\delta}}\frac{\mathbf{x}^{\alpha\delta}}{x^{\alpha\delta}}\right], \quad \text{(A.14)}$$

where c_θ represents $\cos\theta$. Substituting the above relations into Eq. (A.12), we clearly see that the expression for $\boldsymbol{\sigma}(\mathbf{x},t)$ will contain many terms that are non-symmetric. Specifically, the quantities $\mathbf{x}^{\alpha\beta}\otimes\mathbf{x}^{\alpha\delta}$ and $\mathbf{x}^{\alpha\delta}\otimes\mathbf{x}^{\alpha\beta}$ will both be present but will not have the same scalar coefficient, a requirement for a symmetric tensor.

One result we can obtain is the expression for the average stress, $\bar{\boldsymbol{\sigma}}(t)$, for the entire volume V of the system. Integrating both sides of Eq. (A.12), we obtain

$$\bar{\boldsymbol{\sigma}}(t) = \frac{1}{V}\left(\mathbf{x}^{\alpha\beta}\otimes\left\{\frac{2}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}+\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\right\} + \mathbf{x}^{\alpha\delta}\otimes\left\{\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}+\frac{2}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\right\} + \left\{\mathbf{x}^{\alpha\delta}-\mathbf{x}^{\alpha\beta}\right\}\otimes\left\{-\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}}+\frac{1}{3}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\right\}\right)$$

$$= \frac{1}{V}\left(\mathbf{x}^{\alpha\beta}\otimes\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}} + \mathbf{x}^{\alpha\delta}\otimes\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}}\right) \quad \text{(A.15)}$$

Substitution of (A.14) into (A.15), along with simplification of terms, results in the expression

$$\bar{\boldsymbol{\sigma}}(t) = \frac{1}{V}\left(\left[\frac{\partial\tilde{\Phi}}{\partial x^{\alpha\beta}} - \frac{\partial\tilde{\Phi}}{\partial c_\theta}\frac{c_\theta}{x^{\alpha\beta}}\right]\frac{\mathbf{x}^{\alpha\beta}\otimes\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} + \left[\frac{\partial\tilde{\Phi}}{\partial x^{\alpha\delta}} - \frac{\partial\tilde{\Phi}}{\partial c_\theta}\frac{c_\theta}{x^{\alpha\delta}}\right]\frac{\mathbf{x}^{\alpha\delta}\otimes\mathbf{x}^{\alpha\delta}}{x^{\alpha\delta}} + \frac{\partial\tilde{\Phi}}{\partial c_\theta}\frac{\left\{\mathbf{x}^{\alpha\beta}\otimes\mathbf{x}^{\alpha\delta}+\mathbf{x}^{\alpha\delta}\otimes\mathbf{x}^{\alpha\beta}\right\}}{x^{\alpha\beta}x^{\alpha\delta}}\right). \quad \text{(A.16)}$$

Clearly, the average stress for the system is a symmetric quantity. This explains why standard continuum theory adequately describes the deformation of directional bonded materials such as silicon. At the macroscopic scale, asymmetries in stress are probably minor and unnoticeable. However, at the microscopic scale, these asymmetries may be significant and indicative of the need for a microcontinuum theory.

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