Atomistic counterpart of micromorphic theory

Y. Chen, J. D. Lee and A. Eskandarian, Washington, D.C.

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Summary. This paper aims to connect atomistic model to continuum theories. The fundamentals of micromorphic continuum theory are introduced. The instantaneous mechanical variables in an atomic system and the averaged quantities in a continuum field are derived and related to atomic variables. The balance laws of micromorphic continuum theory are formulated and verified from the viewpoint of molecular motion. Some conclusions and discussions are presented.

1 Introduction

The entire physical science is based on two fundamental physical models: (1) discrete atomic models, (2) continuum field theories. In the range of lengths of $10^{-7}$ cm and below, one would only see collections of discrete particles, moving under the influence of their mutual interaction forces. Hence, the natural description of microscopic physics is in terms of many-body dynamics. On the other hand, continuum physics describes a system in terms of a few macroscopic variables, like mass, temperature, stress et al., that are directly to the sense and measurements, dramatically enlarges the applicability region, and has been proved very successful in describing and predicting macroscopic physical phenomena.

With the present-day computers one can study systems of millions, and soon to be billions, particles. Such studies already simulate some features of real macroscopic physics. Nevertheless, it is important to note that even if an ideal computer existed, which could solve the initial-value problem of a system of $10^{23}$ particles, the solution alone as such would not help us to answer the questions asked in macroscopic physics. Although the underlying physical concept may be the same, the descriptions by two models are thoroughly different. Science necessarily deals with quite complex systems with different ways. What we need, therefore, is a correspondence rule by which we associate a continuum field quantity to a discrete atomic function, and so that seeks the correspondence between the two models.

Micromorphic Theory, developed by Eringen [1], [2], constitutes extensions of the classical field theories concerned with the deformations, motions, and electromagnetic interactions of material media, as continua, in microscopic space and short time scales. It treats a material body as a continuous collection of a large number of deformable particles, each particle possesses finite size and inner structure. Upon some assumptions such as infinitesimal deformation, slow motion and spin isotropy, microcontinuum theory can be reduced to Mindlin’s Microstructure Theory [3]. When the microstructure of the material is considered as rigid, it becomes the Micropolar Theory [4]. Assuming a constant microinertia, micropolar theory is identical to
the Cosserat Theory [5]. Eliminating the distinction of macromotion of the particle and the micromotion of its inner structure, it results Toupin’s Couple Stress theory [6]. When the particle reduces to the mass point, all the theories reduce to the classical or ordinary continuum mechanics.

This paper aims at relating an atomistic model to the micromorphic theory. The fundamentals of micromorphic theory are introduced in Sect. 2; instantaneous mechanical variables are derived and related to atomic coordinates and velocities in Sect. 3; averaged continuum field quantities are obtained from the atomic model in Sect. 4; time evolution laws for dynamical variables and statistical consideration are presented in Sect. 5; balance laws of micromorphic theory are derived and verified in Sect. 6; the results are discussed in Sect. 7. In this work, standard dyadic notation is adopted.

2 Fundamentals of the micromorphic theory

From atomistic viewpoint, a material is treated as a collection of discrete mass points, representing atoms, which interact with each other and with its environment. From the viewpoint of micromorphic theory, a material body is considered as a continuous collection of a large number of deformable particles, called material particles, which at any given instant can be placed in a one-to-one correspondence with the points of closed region of three-dimensional Euclidean space. The particle differs from that of both classic continuum mechanics and general atomic models by possessing finite size and direction representing its inner structure. The deformable particle may be considered as a polyatomic molecule, a unit cell of a crystalline, or a chopped fiber in a composite, et al.

Geometrically, a deformable particle is characterized by its centroid \( C \) (located at \( X \)) and vector \( \Xi \) attached to \( C \). As shown in Fig.1, a generic point \( P \) is represented by the vector sum of \( X \) and \( \Xi \) in the reference state at time \( t = 0 \). The motions that carry \( P(X, \Xi) \) to \( P(x, \xi, t) \) in deformed state at time \( t \) can be expressed as

\[
\begin{align*}
\chi_k &= x_k(X, t), & (2.1) \\
\omega_k &= \omega_k(X, t)\Xi_k. & (2.2)
\end{align*}
\]

It is seen that the macromotion, Eq. (2.1), accounts for the motion of the centroid of the material particle while the micromotion, Eq. (2.2), specifies the changing of orientation and deformation of the inner structure of the material particle. Thus the particle has 9 independent degrees of freedom for both stretches and rotations in addition to the 3 classical translation degrees of freedom of the center. There are three strain tensors:

Fig. 1. Macro- and micro-motions of a material particle
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\[ E_{KL} \equiv \chi_{KL} \hat{x}_{KL} - \delta_{KL}, \quad (2.3) \]
\[ F_{KL} \equiv \chi_{KL} \hat{x}_{KL} - \delta_{KL} = F_{L,K}, \quad (2.4) \]
\[ \Gamma_{KLM} \equiv \hat{x}_{KL} \hat{x}_{KL,M}, \quad (2.5) \]

where \( \hat{x} \) is the inverse of \( X \), i.e., \( \chi_{KL} \hat{x}_{KL} = \delta_{KL} \). In case of small macro- and micro-motions, the strains can be approximated as

\[ E_{KL} \equiv u_{L,K} - \phi_{L,K}, \quad (2.6) \]
\[ F_{KL} \equiv \phi_{KL} + \phi_{L,K}, \quad (2.7) \]
\[ \Gamma_{KLM} \equiv \phi_{KL,M}, \quad (2.8) \]

where \( u_{K} \) is the displacement at the mass center of the particle, \( \phi_{KL} \) is the generalized deformation of the inner structure of the particle. Correspondingly there are three thermodynamics conjugates, \( t, s, m \), named as Cauchy stress, microstress average, and moment stress, respectively.

The continuous description makes use of the mass density \( \rho \), microinertia \( \rho \dot{t} \), velocity \( \dot{r} \), gyration tensor \( \omega \), body force \( f \), body couple \( l \), internal energy \( \epsilon \), three stresses \( (t, s, m) \) and heat flux \( q \) as fundamental variables. The fundamental equations for classical continuum mechanics are the balance laws for mass, linear momentum, angular momentum, and energy and the principle of entropy. For micromorphic theory, a balance law for microinertia is added, the balance law for angular momentum is generalized to the balance law for moment of momentum, may also be named as generalized spin, and the balance law of energy is upgraded. They can be written in terms of the fundamental variables as follows [1], [2]:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \dot{r}) = 0. \quad (2.9) \]
\[ \frac{\partial (\rho \dot{r})}{\partial t} + \nabla \times (v \otimes \rho \dot{r}) = \rho \phi + \rho \phi^\parallel. \quad (2.10) \]
\[ \frac{\partial (\rho \dot{v})}{\partial t} + \nabla \cdot (\rho \dot{v} \otimes v - \dot{t}) = f. \quad (2.11) \]
\[ \frac{\partial (\rho \phi)}{\partial t} + \nabla \times (v \otimes \rho \phi - m) = \omega \cdot \dot{r} \cdot \omega^\parallel + \dot{t}^\parallel - s + l, \quad (2.12) \]
\[ \frac{\partial (\rho \omega)}{\partial t} + \nabla \cdot (v \rho \omega - q) = t : \nabla \otimes v + m : \nabla \otimes \omega + \omega : (s - t)^\parallel + h, \quad (2.13) \]

where \( \rho \phi = \omega \cdot \rho \dot{r} \) is called generalized spin.

3 Instantaneous mechanical variables in an atomic system

3.1 The geometric model of an atomic system

A geometric model of a crystal is taken as an example. An ideal crystal is constructed by the infinite regular repetition in space of identical structural units. A unit cube of diamond structure crystal is shown in Fig. 2. A schematic representation of the lattice of a molecular crystal is shown in Fig. 3. A unit cell or a molecule can be viewed as a material particle in the micromorphic theory.
In a general case, consider a unit cell \( k \) in a crystal \((k = 1, 2, 3, \ldots n)\), each unit cell is composed of \( v \) atoms with the mass \( m^x \) \((x = 1, 2, \ldots v)\). The state of a unit cell \( k \) is given by the position \( R^{ka} \) and the velocity \( V^{ka} \) of the atoms, with the center coordinate \( R^k \) and the velocity \( V^k \).

\[
m = \sum_{x=1}^{v} m^x, \tag{3.1}
\]

\[
R^k = \frac{1}{m} \sum_{x=1}^{v} m^x R^{ka}, \tag{3.2}
\]

\[
V^k = \frac{1}{m} \sum_{x=1}^{v} m^x V^{ka}. \tag{3.3}
\]

The relative positions and velocities between atoms and the center of the unit cell are

\[
\Delta r^{ka} = R^{ka} - R^k, \quad \Delta v^{ka} = V^{ka} - V^k. \tag{3.4}
\]

The crystal is then represented by the phase-space coordinates \((r, p)\), i.e., the positions and momenta of atoms with

\[
\begin{align*}
  r &= \{ R^{ka} | k = 1, 2, 3, \ldots n, x = 1, 2, 3, \ldots v \} \\
  p &= \{ m^x V^{ka} | k = 1, 2, 3, \ldots n, x = 1, 2, 3, \ldots v \}. \tag{3.5}
\end{align*}
\]

3.2 Instantaneous mechanical variables corresponding to one-particle contributions

The instantaneous mechanical variables, mass, momentum, microinertia, generalized spin, body force, body couple, temperature, and internal energy, are independent of interatomic interactions. The microscopic expressions are straightforward. According to the atomic model, the mass densities can be expressed as

\[
\eta = \frac{m}{\Delta V} = \frac{m^x}{\Delta V^x}, \tag{3.6}
\]

the microinertia density as

\[
\rho^b = \sum_{x=1}^{v} m^x \frac{\Delta r^{ka} \otimes \Delta v^{ka}}{\Delta V}, \tag{3.7}
\]

![Fig. 2. A unit cube of a covalent crystal](image1.png)

![Fig. 3. The lattice of a molecular crystal](image2.png)
and the density of the moment of momentum, or the generalized spin, as
\[
\rho_\phi = \sum_{k=1}^{n} \sum_{x=1}^{m} \frac{(m^x \Delta \mathbf{r}^k \times \Delta \mathbf{r}^x)}{\Delta V},
\]
where $\Delta V$ is the volume of a unit cell, $\Delta V^x$ is the volume associated with $x$-th atom. Assume that
the material is micromorphic of grade 1, then
\[
\Delta \mathbf{r}^k = \mathbf{o}^k \cdot \Delta \mathbf{r}^x,
\]
where $\mathbf{o}^k$ is the called gyration tensor of the unit cell $k$.

The interatomic forces can be derived from the potential functions such as the hard sphere or
Lennard-Jones pair potential [7] or the many body embedded-atom potential [8]. Three kinds of
forces are assumed to act on an atom:

(1) $f_1^{k_a^{\beta}}$: interatomic force between the $(k, \alpha)$ and $(l, \beta)$ atoms, which is corresponding to the
potential $u_1^{k_a^{l_b}},$ with

\[
u_1^{k_a^{l_b}} = u_1^{k_a^{l_b}},
\]
\[
f_1^{k_a^{l_b}} = \frac{\partial}{\partial \mathbf{R}^{k_a^{l_b}}} u_1^{k_a^{l_b}} = \frac{\partial}{\partial \mathbf{R}^{k_a^{l_b}}} u_1^{k_a^{l_b}} = -f_1^{l_b^{k_a}}.
\]

(2) $f_2^{k_a^{\beta}}$: interatomic force between the atoms $\alpha$ and $\beta$ in the same unit cell $k$, which is corre-
sponding to potential $u_2^{k_a^{l_b}},$ with

\[
u_2^{k_a^{l_b}} = u_2^{k_a^{l_b}},
\]
\[
f_2^{k_a^{l_b}} = \frac{\partial}{\partial \mathbf{R}^{k_a^{l_b}}} u_2^{k_a^{l_b}} = \frac{\partial}{\partial \mathbf{R}^{k_a^{l_b}}} u_2^{k_a^{l_b}} = -f_2^{l_b^{k_a}}.
\]

(3) $f_3^{k_a^{\beta}}$: body force on atom $(k, \alpha)$ due to external fields, which gives body force density

\[
f \equiv \sum_{a=1}^{n} \mathbf{f}_3^{k_a^{\alpha}} / \Delta V,
\]
and the body couples density

\[
l = \sum_{a=1}^{n} \mathbf{f}_3^{k_a^{\alpha}} \otimes \Delta \mathbf{r}^{k_a^{\alpha}} / \Delta V.
\]

Hence, the total force acting on an atom $(k, \alpha)$ can be written as

\[
\mathbf{F}^{k_a^{\alpha}} = \sum_{i=1}^{n} \sum_{\beta=1}^{n} \mathbf{f}_1^{k_a^{l_b}} + \sum_{i=1}^{n} \mathbf{f}_2^{k_a^{l_b}} + \mathbf{f}_3^{k_a^{\alpha}},
\]
and simplest form of the total potential energy of an atom is

\[
U^{k_a^{\alpha}} = \frac{1}{2} \left( \sum_{i=1}^{n} \sum_{\beta=1}^{n} u_1^{k_a^{l_b}} + \sum_{i=1}^{n} u_2^{k_a^{l_b}} \right).
\]

The potential $u_1$ or $u_2$ may include more than one type of potentials if the material has more than
type of atoms, and the above additive expression still holds. In this work, it is understood that
the summation over $k$ and $l$, when $f_1^{k_a^{l_b}}$ and/or $u_1^{k_a^{l_b}}$ are involved, does not include the case $k = l$, and
when $f_2^{k_a^{l_b}}$ and/or $u_2^{k_a^{l_b}}$ are involved, the summation over $x$ and $\beta$ does not include $x = \beta$. 
Instantaneous temperature $T$ for $N$-body system can be most simply defined in terms of kinetic energy by the mean-squared velocity, relative to the local stream velocity, as

$$T = \frac{1}{3nk_b} \sum_{i=1}^{n} m (V_i - \bar{v})^2,$$

where $k_b$ is the Boltzmann constant, $\bar{v}$ is the stream velocity or averaged velocity. This equilibrium temperature definition, giving the fluctuation of the microscopic velocity about the mean at equilibrium, also serves as a convenient and consistent non-equilibrium generalization of temperature to far-from-equilibrium state.

In microscopic $N$-body dynamics system, the internal energy can be divided into a thermal kinetic part and a potential part [9]. Hence the internal energy density has the form:

$$\rho e = \frac{1}{2} \sum_{i=1}^{n} \left[ \frac{1}{2m}(V_i - \bar{v})^2 + \sum_{x=1}^{x} \left( \frac{1}{2m}(\alpha^x - \bar{\omega}) \cdot \Delta r_{ij} \right)^2 + U_{ij} \right],$$

where $\bar{v}$ and $\bar{\omega}$ are the ensemble averages of $v$ and $\omega$, respectively.

### 3.2 Instantaneous mechanical variables that involve two atom contributions

Stresses (Cauchy stress, microstress average, moment stress) and heat flux involve not only one-particle kinetic parts, but also two-or-more-particle potential contributions. The microscopic expressions are thus more complicated than those that do not involve atomic interactions. The work in this paper is restricted to pair potential in order to simplify the derivation.

Virial theorem (cf. [10]) relates the microscopic pressure tensor $P$ to particle coordinate and momentum. Its derivation begins with a canonical partition function. Its expression has been used for over 30 years in obtaining pressure from many-body simulations. But, for nonequilibrium systems, where no analytical expressions for a partition function can be conveniently used, the Virial theorem is not applicable. An alternative and more useful derivation has been provided by Hoover [10], [11] by returning to the fundamental definition of pressure as a momentum flux. From the more detailed atomistic viewpoint, on a microscopic basis there are two kinds of contributions to the pressure tensor, “kinetic” and “potential”. The “kinetic” contribution to the momentum flux, summed over all particles within a volume $dV$, is

$$P_{\text{kin}} = \sum_{i} \frac{p_i \otimes p_i}{mdV}.$$  

The additional “potential” flow of momentum, between all pairs of particles within $dV$ occurs through the mechanism of the interparticle forces. For a pair of particles $i$ and $j$, the rate at which momentum is transported from particle $i$ to particle $j$, i.e., the force on particle $j$ due to particle $i$, is given by the pair force $f_{ij} = -f_{ji}$. For each such pair the direction of this transport is along the direction of the line of centers, parallel to $R_{ij} = R_i - R_j$. Then the “potential” contribution of all pairs of particles to the pressure tensor is

$$P_{\text{pot}} = \frac{1}{2} \sum_{ij} \frac{R_{ij} \otimes f_{ij}}{dV}.$$  

In continuum mechanics it is usually to discuss the stress tensor rather than the pressure tensor. The stress tensor $\sigma$ is just the negative of the pressure tensor $P$. The microscopic stress tensor has the form:
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\[ \mathbf{\sigma} = \mathbf{\sigma}^{\text{kin}} + \mathbf{\sigma}^{\text{pot}} = -\sum_i \mathbf{p}_i \otimes \frac{\mathbf{p}_i}{mdV} - \frac{1}{2} \sum_{ij} \left( \mathbf{R}_i - \mathbf{R}_j \right) \otimes \frac{\mathbf{f}_{ij}}{dV}. \]  

(3.22)

The best feature of this most useful, direct derivation of the stress or pressure tensor from the momentum flux by Hoover is that the unpleasant and impractical time-averaging as well as the fluctuation in the body forces is not required, and the instantaneous form applies equally well for systems far from equilibrium.

Following this approach the three kinds of stresses, as well as the heat flux, in micromorphic theory can be derived. In this paper, we use the particle coordinates and velocities instead of coordinates and mementa for the sake of the later derivation of the conservation laws and constitutive relations. By virtue of the possible macroscopic motion of the whole body of molecules, the velocity that makes contribution to stresses and heat flux is \( \mathbf{V}^k - \mathbf{\bar{v}} \), the difference between the instantaneous velocity and the stream velocity.

The Cauchy stress \( \mathbf{t} \) is the stress evaluated at the center of a material particle, the center of a unit cell in an atomic system. Replacing the momentum \( \mathbf{p}_i \) by \( m(\mathbf{V}^k - \mathbf{\bar{v}}) \) for the kinetic part in Eq. (3.22), the kinetic part, i.e., the flow of momentum due to the particle motion, is

\[ \mathbf{t}^{\text{kin}} = -m(\mathbf{V}^k - \mathbf{\bar{v}}) \otimes \frac{(\mathbf{V}^k - \mathbf{\bar{v}})}{\Delta V}. \]  

(3.23)

and the “potential” flow due to the interparticle force is

\[ \mathbf{t}^{\text{pot}} = -\frac{1}{2} \sum_i \left( \mathbf{R}_i^k - \mathbf{R}_i^l \right) \otimes \frac{\mathbf{f}_i^{kl}}{dV}. \]  

(3.24)

On the other hand, for an atom \( (k, z) \), the momentum is \( m^z(\mathbf{V}^{kz} - (\mathbf{\bar{v}} + \mathbf{\omega} \cdot \Delta \mathbf{r}^{kz})) \), hence if the stress evaluated at the atomic position, the microscopic stress can be then written as

\[ \mathbf{s} = \mathbf{s}^{\text{kin}} + \mathbf{s}^{\text{pot}} = -m^z(\mathbf{V}^{kz} - (\mathbf{\bar{v}} + \mathbf{\omega} \cdot \Delta \mathbf{r}^{kz})) \otimes \frac{(\mathbf{V}^{kz} - (\mathbf{\bar{v}} + \mathbf{\omega} \cdot \Delta \mathbf{r}^{kz}))}{dV^z} \]

\[ -\frac{1}{2} \left( \sum_{l=1}^n \left( \mathbf{R}^{kz} - \mathbf{R}^{lz} \right) \otimes \frac{\mathbf{f}_l^{kz}}{dV^z} + \sum_{l=1}^n \left( \mathbf{R}^{kz} - \mathbf{R}^{lz} \right) \otimes \frac{\mathbf{f}_l^{kz}}{dV^z} \right) \right), \]

(3.25)

where \( dV^z \) is the volume associated with the \( z \)-th atom in a unit cell \( k \). So, the stresses averaging over all atoms in the unit cell, called the microstress average in the continuum field, can be obtained as

\[ \mathbf{s}^{\text{kin}} = -\sum_{z=1}^n m^z(\mathbf{V}^{kz} - (\mathbf{\bar{v}} + \mathbf{\omega} \cdot \Delta \mathbf{r}^{kz})) \otimes \frac{(\mathbf{V}^{kz} - (\mathbf{\bar{v}} + \mathbf{\omega} \cdot \Delta \mathbf{r}^{kz}))}{\Delta V^z}, \]

(3.26)

\[ \mathbf{s}^{\text{pot}} = -\frac{1}{2} \sum_{l=1}^n \sum_{z=1}^n \left( \mathbf{R}^{kz} - \mathbf{R}^{lz} \right) \otimes \frac{\mathbf{f}_l^{kz}}{\Delta V^z} - \frac{1}{2} \sum_{z=1}^n \left( \mathbf{R}^{kz} - \mathbf{R}^{lz} \right) \otimes \frac{\mathbf{f}_l^{kz}}{\Delta V^z}. \]

(3.27)

It can be seen that \( s \) is symmetric tensor, because \( \mathbf{R}^{kz} - \mathbf{R}^{lz} \) and \( \mathbf{R}^{kz} - \mathbf{R}^{lz} \) are parallel to \( \mathbf{f}_l^{kz} \) and \( \mathbf{f}_l^{kz} \), respectively. The symmetry of the microstress average, an important character in the micromorphic theory, is now confirmed by the use of pair potential. On the other hand, the Cauchy stress \( \mathbf{t} \), from Eqs. (3.24), is not symmetric.

**Moment stress**, \( \mathbf{m} \), measures the flux of the spin. Following Hoover’s approach it can be divided into the flow of spin caused by the atomic motion and by the moment of interatomic force. Following the same derivation for the momentum flux, the kinetic part of microscopic moment stress can be obtained as
and the potential part

\[
m_{\text{pot}} = -\frac{1}{2} \sum_{l=1}^{n} \mathbf{R}^k - \mathbf{R}_l^l \otimes \left\{ \sum_{k \beta=1}^{\nu} f^k_{\beta} \otimes \Delta r^{k \beta} \right\} \frac{1}{\Delta V}.
\]  

(3.29)

Heats flux vector measures the conductive flow of energy per unit time and area. Heat theorem relates the heat flux vector to a time-averaged sum of atomistic quantities (cf. Hoover [11]). An alternative approach is from the flow of energy ([10], [11]). The flow of energy, for all particles in the volume \( dV \), gives the kinetic contributions to the heat flux. It comes from the rate at which each particle carries energy with single-particle contribution:

\[
q_{\text{kin}} = \sum_{i} \frac{p_i}{m} E \frac{1}{dV},
\]  

(3.30)

where \( E \) is the energy associated with the particle. While the potential contributions to heat flux occur whenever two moving particles interact in such a way that one particle transfers a part of their joint energy to the other particle. It comes from the rate at which energy is transported through the action of interparticle forces:

\[
q_{\text{pot}} = \frac{1}{2} \sum_{i,j} R_i(p_i + p_j) - \frac{1}{2m} \frac{\mathbf{f}_i}{dV}. \]  

(3.31)

In the notation of this paper and also following the convention used in micromorphic theory, the kinetic part of heat flux can be expressed as

\[
q_{\text{kin}} = -\left( V_k - \bar{v} \right) \frac{[\frac{1}{2m} (V_k - \bar{v})^2 + \sum_{x=1}^{\nu} (\mathbf{0} - \bar{x} \cdot \Delta r^{k x}) \cdot \Delta r^{k x}]^{1/2}_x} {\Delta V},
\]  

(3.32)

and the potential part as

\[
q_{\text{pot}} = -\frac{1}{2} \sum_{l=1}^{n} (\mathbf{R}^k - \mathbf{R}_l^l) \sum_{x \beta=1}^{\nu} (V_k - \bar{v} \cdot \Delta r^k \cdot \Delta r^{k \beta}) \frac{f^k_{\beta}} {\Delta V} = -\frac{1}{2} \sum_{l=1}^{n} (\mathbf{R}^k - \mathbf{R}_l^l) \sum_{x \beta=1}^{\nu} (V_k - \bar{v} \cdot \Delta r^k \cdot (V^\beta - \bar{v} \cdot \Delta r^\beta) \frac{f^k_{\beta}} {2\Delta V}. \]  

(3.33)

4 Averaged field quantities

4.1 General relation between instantaneous variables and continuum field quantities

The continuum quantities are described by continuous functions of the physical space coordinates \( x \) and time \( t \). They are fields in physical space-time. The discrete atomic quantities, on the other hand, are functions of the phase-space coordinates \( (r, p) \). The link of the quantities between the two models can be established through the ensemble averages. This was called the mapping of the phase space into the physical space (Balescu [12], [13]). The \( \delta \) function with its
integration is employed as an important tool to link the discrete expressions to the properties in a field. So, a continuum field quantity is defined as the average of a dynamical function with the following characteristic form:

$$\bar{A} = \langle A \rangle = \int \int A(\mathbf{r}, \mathbf{p}, t) f(\mathbf{r}, \mathbf{p}, t) \, d\mathbf{r} \, d\mathbf{p},$$

(4.1)

where $f$ is the normalized distribution function, i.e.,

$$\int \int f(\mathbf{r}, \mathbf{p}, t) \, d\mathbf{r} \, d\mathbf{p} = 1,$$

(4.2)

and

$$A(\mathbf{r}, \mathbf{p}, x) = \sum_k \alpha(\mathbf{R}^k, \mathbf{V}^k) \delta(\mathbf{R}^k - \mathbf{x})$$

(4.3)

or

$$A(\mathbf{r}, \mathbf{p}, x) = \sum_{k=1}^{n} \left( \sum_{s=1}^{v} a^{s}(\mathbf{R}^{ks}, \mathbf{V}^{ks}) \right) \delta(\mathbf{R}^k - \mathbf{x})$$

(4.4)

is called the corresponding local density of the phase-space dynamic function $a(\mathbf{R}^k, \mathbf{V}^k)$ at point $x$. In a discrete atomic description, there can be a contribution to the density function only if the center of a unit cell $k$ happens to be located at $x$. In the following sections, we use $\bar{A} = \langle A \rangle$ to distinguish from the corresponding instantaneous quantity $A$.

### 4.2 Averaged field quantities corresponding to one-particle contributions

Substituting the expressions of instantaneous mechanical variables in Sect. 3.1 into Eq. (4.1), the corresponding averaged field quantities can be immediately obtained as

1. **Mass density:**

$$\bar{\rho} = \left( \sum_{k=1}^{n} m \delta(\mathbf{R}^k - \mathbf{x}) / \Delta V \right) = \left( \sum_{k=1}^{n} \eta \delta(\mathbf{R}^k - \mathbf{x}) \right).$$

(4.5)

2. **Linear momentum density:**

$$\bar{\rho} \mathbf{v} = \left( \sum_{k=1}^{n} \eta \mathbf{V}^k \delta(\mathbf{R}^k - \mathbf{x}) \right).$$

(4.6)

3. **Microinertia density:**

$$\bar{\rho} \mathbf{I} = \left( \sum_{k=1}^{n} \left( \sum_{s=1}^{v} (m^s \mathbf{A}^{ks} \otimes \mathbf{A}^{ks}) \delta(\mathbf{R}^k - \mathbf{x}) / \Delta V \right) \right).$$

(4.7)

4. **Generalized spin density:**

$$\bar{\rho} \mathbf{\Omega} = \left( \sum_{k=1}^{n} \sum_{s=1}^{v} (m^s \mathbf{A}^{ks} \otimes \mathbf{A}^{ks}) \delta(\mathbf{R}^k - \mathbf{x}) / \Delta V \right).$$

(4.8)
(4) Internal energy density:
\[ \overline{\rho e} = \sum_{k=1}^{n} \left[ \frac{2}{3} m (V^k - \bar{v})^2 + \sum_{x=1}^{y} \left( \frac{1}{2} m^x \left( \sigma^k - \bar{\sigma} \right) \cdot \Delta r^{kx} \right)^2 + U^{kx} \right] \delta (R^k - x) / \Delta V \].

(5) Body force density:
\[ \bar{f} = \sum_{k=1}^{n} \left( \sum_{x=1}^{y} f_{kx}^{b} \right) \delta (R^k - x) / \Delta V \].

(6) Body couple density:
\[ \bar{i} = \left( \sum_{k=1}^{n} \left( \sum_{x=1}^{y} f_{kx}^{b} \otimes \Delta r^{kx} \right) \delta (R^k - x) / \Delta V \right). \]

4.3 Averaged field quantities that involve two-atom contributions

Stresses and heat flux involve both one-atom kinetic contribution and two-atom potential contributions. Therefore the kinetic parts are nonvanishing only when the center of a unit cell is at \( x \), and the corresponding averaged field quantities can be obtained through Eq. (4.1). While the "potential" flows have contributions from every pair of particles when the line of centers passing through \( x \), and may vary with position \( x \). Hence, the corresponding averaged potential parts have to be modified by linear interpolations. It then follows

(1) Cauchy stress:
\[ \bar{t}^{\text{kin}} = -\left( \sum_{k=1}^{n} m(V^k - \bar{v}) \otimes (V^k - \bar{v}) \delta (R^k - x) / \Delta V \right). \]

(2) Microstress average:
\[ \bar{s}^{\text{kin}} = \sum_{k=1}^{n} \sum_{x=1}^{y} m^x (V^{kx} - (\bar{v} + \bar{\sigma} \cdot \Delta r^{kx})) \otimes (V^{kx} - (\bar{v} + \bar{\sigma} \cdot \Delta r^{kx})) \delta (R^k - x) / \Delta V \].

(3) Moment stress:
\[ \bar{m}^{\text{kin}} = -\left( \sum_{k=1}^{n} (V^k - \bar{v}) \otimes (\sigma^k - \bar{\sigma}) \cdot \left( \sum_{x=1}^{y} m^x \Delta r^{kx} \otimes \Delta r^{kx} \right) \delta (R^k - x) / \Delta V \right). \]
Atomistic counterpart of micromorphic theory

\[ \mathbf{m}^{pol} = -\left\langle \frac{1}{2} \int \sum_{k=1}^{n} (\mathbf{R}^k - \mathbf{R}') \otimes \left\{ \sum_{\beta, \beta'=1}^{v} f_{\beta}^{k} \otimes [\Delta r^{k}\xi(1-\zeta) + \Delta r^{\beta}\xi] \right\} \right\rangle \times \delta(\mathbf{R}^k(1-\zeta) + \mathbf{R}^\xi - \mathbf{x}) \frac{d\xi}{\Delta V}. \]  

(4.17)

Heat flux:

\[ \mathbf{q}^{kin} = -\left\langle \sum_{k=1}^{n} \left( \mathbf{v}^k - \mathbf{v} \right) \left[ \frac{1}{2} m (\mathbf{v}^k - \mathbf{v})^2 + \sum_{\beta=1}^{v} \left[ \frac{1}{2} m^\beta (\mathbf{\omega}^k - \mathbf{\omega}) \cdot \Delta r^{k}\xi \right]^2 + U^{k}\right] \right\rangle \delta(\mathbf{R}^k - \mathbf{x}) / \Delta V, \]  

(4.18)

\[ \mathbf{q}^{pol} = -\left\langle \sum_{k=1}^{n} \left( \mathbf{v}^k - \mathbf{v} \right) \sum_{\beta, \beta'=1}^{v} V^{k} f_{\beta}^{k} \delta(\mathbf{R}^k(1-\zeta) + \mathbf{R}^\xi - \mathbf{x}) d\xi \right\rangle \times \frac{\delta(\mathbf{R}^k - \mathbf{x})}{\Delta V} \]  

(4.19)

With the identities of \( \delta \) function (McLennan [14])

\[ \delta(\mathbf{R}^k - \mathbf{x}) - \delta(\mathbf{R}^l - \mathbf{x}) = -\nabla_x \cdot \int_0^1 (\mathbf{R}^k - \mathbf{R}^l) \delta|\mathbf{R}^k - \mathbf{x} - \zeta(\mathbf{R}^k - \mathbf{R}^l)| d\zeta, \]  

(4.20)

\[ \delta(\mathbf{R}^l - \mathbf{x}) = \nabla_x \cdot \int_0^1 \zeta(\mathbf{R}^k - \mathbf{R}^l) \delta|\mathbf{R}^k - \mathbf{x} - \zeta(\mathbf{R}^k - \mathbf{R}^l)| d\zeta \]  

(4.21)

it can be proved that the divergence of the fluxes have following features:

\[ \nabla_x \cdot \mathbf{f}^{pol} = \left\langle \sum_{k=1}^{n} \sum_{\beta, \beta'=1}^{v} f_{\beta}^{k} \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle. \]  

(4.22)

\[ \nabla_x \cdot \mathbf{m}^{pol} + (\mathbf{f}^{pol} - \mathbf{q}^{pol})^{T} = \left\langle \sum_{k=1}^{n} \sum_{\beta, \beta'=1}^{v} \left( \sum_{\beta, \beta'=1}^{v} f_{\beta}^{k} \otimes \Delta r^{k}\xi + f_{\beta}^{\beta'} \otimes \Delta r^{\xi} \right) \delta(\mathbf{R}^k - \mathbf{x}) / \Delta V \right\rangle, \]  

(4.23)

\[ \nabla_x \cdot (\mathbf{q}^{pol} + \mathbf{m}^{pol} \cdot \mathbf{\omega} + \mathbf{f}^{pol} \cdot \mathbf{v}) = \frac{1}{2} \left\langle \sum_{k, \beta, \beta'=1}^{n} \sum_{\beta, \beta'=1}^{v} (V^{k\beta} + V^{\beta\xi}) \cdot f_{\beta}^{k} \delta(\mathbf{R}^k - \mathbf{x}) / \Delta V \right\rangle. \]  

(4.24)

The above expressions for averaged potential parts of stresses and heat flux can be reduced to the corresponding expressions of instantaneous variables. Also, for the cases \( \mathbf{x} = \mathbf{R}^k \), they still follow Eq. (4.1). While if \( \mathbf{x} \neq \mathbf{R}^k \), but \( \mathbf{x} = \mathbf{R}^k (1 - \zeta) + \mathbf{R}^\xi, 0 < \zeta < 1 \), the linear interpolations come to play. The discrete microscropic expression have thus modified so that they can be evaluated at any position \( \mathbf{x} \) in physical space. The stresses and heat flux defined this way possess a periodic character, which resembles the characteristic of a crystal due to the periodic arrangement of the atoms.
5 Time evolution of conserved dynamical quantities

Among the mechanical variables, the mass density $\rho$, microinertia density $\rho \dot{\mathbf{r}}$, momentum density $\rho \mathbf{v}$, generalized spin density $\rho \mathbf{\omega}$, and the internal energy density $\rho e$, are conserved properties. The continuum field quantity is defined as the average of a dynamical function through the ensemble average, Eq. (4.1). With the identity
\[
\nabla \mathbf{R}_k \cdot \delta(\mathbf{R}_k - \mathbf{x}) = -\nabla \mathbf{x} \cdot \delta(\mathbf{R}_k - \mathbf{x}).
\]  
(5.1)

The time evolution of the averaged field quantity $\langle A \rangle$ takes the form:
\[
\frac{\partial \langle A \rangle}{\partial t} \bigg|_x = \left( \sum_{k=1}^{n} (\mathbf{V}_k \cdot \nabla \mathbf{R}_k + \dot{\mathbf{V}}_k \cdot \nabla \mathbf{v}_k) \right) \langle a(\mathbf{R}_k, \mathbf{V}_k) \delta(\mathbf{R}_k - \mathbf{x}) \rangle + \int \int A f d\mathbf{r} d\mathbf{p}.
\]  
(5.2)

It can be seen that the information about the rate of change of the distribution function $f$ is then critical for the time evolution of $\langle A \rangle$.

The logical foundation for Gibbs equilibrium statistical mechanics is Liouville theorem, which describes the flow of phase-space probability density function $f(\mathbf{r}, \mathbf{p}, t)$. Liouville theorem guarantees $\dot{f} = 0$. Therefore, equilibrium statistical mechanics yields the time evolution law in the following form:
\[
\frac{\partial \langle A \rangle}{\partial t} = \left( \sum_{k=1}^{n} (\mathbf{V}_k \cdot \nabla \mathbf{R}_k + \dot{\mathbf{V}}_k \cdot \nabla \mathbf{v}_k) \right) \langle a(\mathbf{R}_k, \mathbf{V}_k) \delta(\mathbf{R}_k - \mathbf{x}) \rangle.
\]  
(5.3)

For conserved properties, this is the form of local conservation law or balance law.

While for non-equilibrium system, the main analytical tool available is the Boltzmann transport equation. The goal of Boltzmann transport equation is to calculate the evolution of the one-particle probability density function $f(\mathbf{r}, \mathbf{p}, t)$ by analyzing the effect of gas collisions statistically. The collision term has been obtained as the difference between a “gain” term and a “loss” term as
\[
\dot{f}_i = \left( \frac{\partial f}{\partial t} \right)_{\text{coll}} - \left( \frac{\partial f}{\partial t} \right)_{\text{gain}} - \left( \frac{\partial f}{\partial t} \right)_{\text{loss}} = \int d\Omega \int d\mathbf{p}_1 \sigma(\Omega) |\mathbf{p}_1 - \mathbf{p}_2| (f^0_{j_3, j_4} - f_{j_3} f_{j_4}),
\]  
(5.4)

where
\[
f_i = f(\mathbf{r}, \mathbf{p}_i, t), \quad f^0_i = f(\mathbf{r}, \mathbf{p}'_i, t), \quad (i = 1, 2).
\]

Multiplying the Boltzmann transport equation on both side by the conserved property $A(\mathbf{r}, \mathbf{p})$, and then integrating over $\mathbf{p}$, interchanging the integration variables $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}'_1, \mathbf{p}'_2$ each to other, yields the following conservation theorem [15]:
\[
\int \int A(\mathbf{r}, \mathbf{p}) \left( \frac{\partial f_i}{\partial t} \right)_{\text{coll}} d\mathbf{p} d\mathbf{r} = 0.
\]  
(5.5)

This means that for conserved properties, the net change due to molecular collision is zero. Grad [16] has argued that Boltzmann equation should be an exact statement in a gas of N particles interacting via a potential, in other words, the total net change of the conserved property due to particle interactions will be balanced. Boltzmann equation thus provides an approach to derive conservation laws. Based on Boltzmann equation conservation laws for hydrodynamics, fluid dynamics and continuum mechanics have been derived and the results have exactly matched those of phenomenological field theories [15], [17–21]. One of the consequences of Boltzmann equation, therefore, is the local conservation law
\[ \frac{\partial (A)}{\partial t} = \left( \sum_{k=1}^{n} (V^k \cdot \nabla \rho^k + V^k \cdot \nabla \rho^k) [\alpha(R^k, V^k) \delta([R^k-x])] \right). \quad (5.6) \]

It has the same form as (5.3), but with a distribution function \( f(r, p, t) \) of a non-equilibrium system (\( f \neq 0 \)).

Despite the approximate nature of the theorem’s derivation, Boltzmann equation has provided an exact description for low-density gases. It satisfies the required property of implying the conservation equations, correctly identifies collisions as the mechanism leading to chaos and irreversible behavior in nonequilibrium gas systems, and is able to explain irreversible behavior for isolated systems obeying reversible Newtonian mechanics. From the viewpoint of continua, the kinetic gas is in all respects a special kind of continuum. All the requirements of continuum mechanics are satisfied by the solutions of Boltzmann equation. Thus the solutions represent the kinetic gas as a material in the sense of the thermodynamics of continua [19]. From the viewpoint of physics, the conservation equations express the basic conservation principles of physics: mass, momentum, and energy. Thus a necessary requirement for a kinetic equation to be a valid relation is that it implies these conservation laws [21]. Since the conservation laws of a continuum theory are independent of materials, phases, and equilibrium or nonequilibrium processes, the conservation laws that satisfy the gas dynamics would apply to the dynamics of fluid and solid as well. The consequence of Boltzmann equation,

\[ \int \int f(r, p, t) A \, dr \, dp = 0, \]

for conserved properties is therefore employed in this paper to verify the balance laws in micromorphic theory.

### 6 Balance laws of micromorphic continuum

#### 6.1 Conservation of mass

With \( \bar{\rho} = \left( \sum_{k=1}^{n} \eta \delta(R^k-x) \right) \), Eq. (5.6) immediately results

\[ \frac{\partial \bar{\rho}}{\partial t} = -\nabla \cdot \left( \sum_{k=1}^{n} \eta V^k \delta([R^k-x]) \right). \quad (6.1) \]

With the expression of density of linear momentum, the well-known conservation law of mass is obtained

\[ \frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{v}}) = 0. \quad (6.2) \]

#### 6.2 Conservation of microinertia

With

\[ \overline{\mathbf{a}} = \left( \sum_{k=1}^{n} \left( \sum_{j=1}^{n} (m_j \Delta r^{kj} \otimes \Delta r^{kj})(R^k-x)/\Delta V \right) \right), \]
and
\[ \sum_{z=1}^{v} m^z \Delta r^z = 0, \]
it follows
\[ \frac{\partial}{\partial t} \left( \left( \sum_{z=1}^{v} \sum_{x=1}^{n} (V^z \cdot \nabla_{R^z}) \left[ (m^z \Delta r^z \otimes \Delta r^z) \delta(R^z - x)/\Delta V \right] \right) \right) \]
\[ = \left( \sum_{z=1}^{v} \left( \sum_{x=1}^{n} m^z V^z \otimes \Delta r^z \right) \delta(R^z - x)/\Delta V \right) + \left( \sum_{z=1}^{v} \left( \sum_{x=1}^{n} m^z \Delta r^z \otimes V^z \right) \delta(R^z - x)/\Delta V \right) \]
\[ - \nabla_x \cdot \left( \left[ \sum_{z=1}^{v} V^z \otimes \sum_{x=1}^{n} m^z \Delta r^z \otimes \Delta r^z \delta(R^z - x)/\Delta V \right] \right). \]

Denoting
\[ \gamma \equiv \sum_{z=1}^{v} \left( V^z - \bar{v} \right) \otimes \sum_{x=1}^{n} m^z \Delta r^z \otimes \Delta r^z \delta(R^z - x)/\Delta V \]
\[ = \sum_{z=1}^{v} \left( V^z - \bar{v} \right) \otimes (\rho \dot{r}^z) \delta(R^z - x), \]
its averaged value can be obtained as
\[ \langle \gamma \rangle \equiv \left( \sum_{z=1}^{v} \left( V^z - \bar{v} \right) \otimes (\rho \dot{r}^z) \delta(R^z - x) \right) \]
\[ = \int \int \sum_{z=1}^{v} \left( V^z - \bar{v} \right) \otimes (\rho \dot{r}^z) \delta(r^z - x) \int \int \int \left( V^z - \bar{v} \right) \otimes (\rho \dot{r}^z) \delta(x - p) \right) \]
\[ = \left[ \int \int \int \left( V^z - \bar{v} \right) \otimes (\rho \dot{r}^z) \delta(x - p) \right] \otimes (\rho \dot{r}^z) \delta(R^z - x) \]
\[ = 0. \]

With
\[ \sum_{z=1}^{v} m^z \Delta r^z = 0 \]
and the definition of \( \bar{p} \bar{v} \), the balance law of microinertia is then obtained as
\[ \frac{\partial}{\partial t} (\bar{p} \bar{v}) + \nabla_x \cdot (\dot{v} \otimes \bar{p} \bar{v}) = \bar{p} \bar{\phi} + \bar{p} \bar{v} \bar{v}. \]

It is seen that, \( \langle \gamma \rangle = 0 \), whereas \( \gamma \neq 0 \), the balance law of microinertia for microscopic atomic system would have different form from a continuum system.

### 6.3 Balance of linear momentum

With
\[ \bar{p} \bar{v} = \left( \sum_{z=1}^{v} \eta V^z \delta(R^z - x) \right), \]
and
\[
\left\langle \sum_{k=1}^{n} V^{k} \otimes V^{k} \delta(R^{k} - x) \right\rangle = \left\langle \sum_{k=1}^{n} [(V^{k} - \bar{v}) \otimes (V^{k} - \bar{v}) + \bar{v} \otimes \bar{v}] \delta(R^{k} - x) \right\rangle,
\]
Eq. (6.7)

Eq. (5.6) leads to
\[
\frac{\partial}{\partial t} (\bar{p} \bar{v}) = \left\langle \sum_{k=1}^{n} \left( \frac{1}{m} \sum_{s=1}^{r} F^{k,s} \right) \nabla_{x} (\eta V^{k}) \delta(R^{k} - x) \right\rangle - \nabla_{x} \left\langle \sum_{k=1}^{n} \eta V^{k} \otimes V^{k} \delta(R^{k} - x) \right\rangle
\]
\[
= \left\langle \sum_{k=1}^{n} \left( \sum_{s=1}^{r} F^{k,s} \right) \delta(R^{k} - x)/\Delta V \right\rangle - \nabla_{x} \left\langle \sum_{k=1}^{n} \eta [(V^{k} - \bar{v}) \otimes (V^{k} - \bar{v}) + \bar{v} \otimes \bar{v}] \delta(R^{k} - x) \right\rangle.
\]
Eq. (6.8)

Because within a unit cell \( k \),
\[
\sum_{x=1}^{r} f^{k} = 0,
\]
Eq. (6.8) becomes
\[
\frac{\partial}{\partial t} (\bar{p} \bar{v}) + \nabla_{x} \cdot \left\langle \bar{p} \bar{v} \otimes \bar{v} + \sum_{k=1}^{n} \eta [(V^{k} - \bar{v}) \otimes (V^{k} - \bar{v})] \delta(R^{k} - x) \right\rangle
\]
\[
= \left\langle \sum_{k=1}^{n} \sum_{s=1}^{r} f^{k,s} \delta(R^{k} - x)/\Delta V \right\rangle + \left\langle \sum_{k=1}^{n} \sum_{s=1}^{r} f^{k,s} \delta(R^{k} - x)/\Delta V \right\rangle.
\]
Eq. (6.9)

Combining Eq. (4.22) with the definitions of the body force \( \bar{f} \) and the Cauchy stresses \( \bar{t}^{(u)} \), it results the balance law of momentum
\[
\frac{\partial}{\partial t} (\bar{p} \bar{v}) + \nabla_{x} \cdot (\bar{p} \bar{v} \otimes \bar{v} - \bar{t}) = \bar{f}.
\]
Eq. (6.10)

6.4 Balance of generalized spin

With
\[
\bar{p} \bar{v} = \left\langle \sum_{k=1}^{n} \sum_{s=1}^{r} (m^{s} \Delta r^{k,s} \otimes \Delta r^{k,s}) \delta(R^{k} - x)/\Delta V \right\rangle.
\]
we have
\[
\frac{\partial}{\partial t} (\bar{p} \bar{v}) = \left\langle \sum_{k=1}^{n} \sum_{s=1}^{r} \left( \frac{m^{s} \Delta r^{k,s} \otimes \Delta r^{k,s}}{m} \right) \delta(R^{k} - x)/\Delta V \right\rangle
\]
\[
- \nabla_{x} \left\langle \sum_{k=1}^{n} \frac{m^{s} \Delta r^{k,s} \otimes \Delta r^{k,s}}{m} \delta(R^{k} - x)/\Delta V \right\rangle
\]
\[
= - \nabla_{x} \left\langle \sum_{k=1}^{n} \frac{m^{s} \Delta r^{k,s} \otimes \Delta r^{k,s}}{m} \delta(R^{k} - x)/\Delta V \right\rangle
\]
\[
+ \left\langle \sum_{k=1}^{n} \sum_{s=1}^{r} \frac{m^{s} \Delta r^{k,s} \otimes \Delta r^{k,s}}{m} \delta(R^{k} - x)/\Delta V \right\rangle + \left\langle \sum_{k=1}^{n} \sum_{s=1}^{r} \frac{m^{s} \Delta r^{k,s} \otimes \Delta r^{k,s}}{m} \delta(R^{k} - x)/\Delta V \right\rangle
\]
\[
\equiv B + C + D.
\]
Eq. (6.11)
According to the definitions of the kinetic part of moment stress and the generalized spin, and the vanishing \( \ddot{\gamma} \), we have

\[
B = -\nabla_x \cdot \left[ \bar{\nu} \otimes \bar{\rho} \bar{\gamma} + \sum_{k=1}^n \left( (V^k - \bar{\nu}) \otimes (\omega^k - \bar{\omega}) \right) \cdot \left( \sum_{s=1}^v m_s \Delta r^{ks} \otimes \Delta r^{ks} \right) \delta(R^k - x)/\Delta V \right]
\]

\[
= -\nabla_x \cdot \left( \bar{\nu} \otimes \bar{\rho} \bar{\gamma} - \bar{m}^{km} \right).
\]

(6.12)

Using the definitions of the microinertia, kinetic part of Cauchy stress, kinetic part of microstress average, and the definition of the generalized spin \( \bar{\rho} \bar{\gamma} = \bar{\omega} \otimes \bar{m} \), it results

\[
C = \bar{\omega} \cdot \bar{m} \bar{\omega}^T + \sum_{k=1}^n \left( (\omega^k - \bar{\omega}) \cdot \left( \sum_{s=1}^v m_s \Delta r^{ks} \otimes \Delta r^{ks} \right) \delta(R^k - x)/\Delta V \right)
\]

\[
= \bar{\omega} \cdot \bar{m} \bar{\omega}^T + \bar{t}^{km} - \bar{s}^{km}.
\]

(6.13)

With Eq. (4.23)

\[
D = \left( \sum_{k=1}^n \left( \sum_{s=1}^v F^{ks} \otimes \Delta r^{ks} \right) \right) \delta(R^k - x)/\Delta V
\]

\[
= \sum_{k=1}^n \left( \sum_{s=1}^v \sum_{s'=1}^v F^{ks} \Delta r^{ks} + \sum_{s=1}^v \sum_{s'=1}^v F^{s's} \Delta r^{k's} + \sum_{s=1}^v \sum_{s'=1}^v F^{sk's} \Delta r^{sk'} \right) \delta(R^k - x)/\Delta V
\]

\[
= \nabla_x \cdot \left( \bar{m}^{km} + (\bar{t}^{km} - \bar{s}^{km}) \right) + \bar{l}.
\]

(6.14)

Combining \( B, C, D \), and the definition of \( t, s, m \), it yields

\[
\frac{\partial}{\partial t}(\bar{\rho} \bar{\gamma}) + \nabla_x \cdot \left( \bar{\nu} \otimes \bar{\rho} \bar{\gamma} - \bar{m} \right) = \bar{\omega} \cdot \bar{m} \bar{\omega}^T + \bar{t}^{km} - \bar{s}^{km} + \bar{l}.
\]

(6.15)

6.5 Conservation of energy

With

\[
(\rho v) = \sum_{k=1}^n \left[ \frac{1}{2} m(V^k - \bar{\nu})^2 + \frac{1}{2} \sum_{s=1}^v m^s ((\omega^k - \bar{\omega}) \cdot \Delta r^{ks})^2 + \sum_{s=1}^v U^{ks} \right] \delta(R^k - x)/\Delta V
\]

we have

\[
\frac{\partial}{\partial t} [\rho v] = \sum_{k=1}^n \left[ \frac{1}{2} m(V^k - \bar{\nu})^2 + \frac{1}{2} \sum_{s=1}^v m^s ((\omega^k - \bar{\omega}) \cdot \Delta r^{ks})^2 + \sum_{s=1}^v U^{ks} \right] \delta(R^k - x)/\Delta V
\]

\[
+ \left( \sum_{k=1}^n \nabla_{R^k}^2 \left[ \frac{1}{2} m(V^k - \bar{\nu})^2 + \frac{1}{2} \sum_{s=1}^v m^s ((\omega^k - \bar{\omega}) \cdot \Delta r^{ks})^2 + \sum_{s=1}^v U^{ks} \right] \delta(R^k - x)/\Delta V \right)
\]

\[
= \left( \sum_{k=1}^n \sum_{s=1}^v \left( \frac{1}{m^s} F^{sk's} \cdot \nabla u^{ks} \right) \delta(R^k - x)/\Delta V \right)
\]

\[
= P + Q + R
\]

(6.16)
Atomistic counterpart of micromorphic theory

where \( P, Q, \) and \( R \) can be further derived as follows:

\[
P = -\nabla_x \left( \sum_{k=1}^n (V^k - \bar{v}) + \bar{v} \left[ \frac{1}{2} m(V^k - \bar{v})^2 + \sum_{a=1}^y m_a^2 ((\sigma^k - \bar{\sigma}) : \Delta r^{k\alpha})^2 + \sum_{a=1}^y U_{k\alpha}^a \right] \delta(R^k - \bar{x}) / \Delta V \right) \\
+ \sum_{k=1}^n (V^k - \bar{v} + \bar{v}) \cdot \nabla_x \left( \frac{1}{2} m(V^k - \bar{v})^2 + \sum_{a=1}^y m_a^2 ((\sigma^k - \bar{\sigma}) : \Delta r^{k\alpha})^2 \right) \delta(R^k - \bar{x}) / \Delta V \right) \\
- \nabla_x \cdot (\bar{v} \bar{\sigma} - \bar{q}^{k\text{lin}}) - \sum_{k=1}^n (V^k - \bar{v} + \bar{v}) \\
\otimes \left( m(V^k - \bar{v}) : \nabla_x \otimes \bar{v} + \sum_{a=1}^y m_a^2 ((\sigma^k - \bar{\sigma}) : \Delta r^{k\alpha}) : \nabla_x \otimes (\bar{\sigma} : \Delta r^{k\alpha}) \right) \delta(R^k - \bar{x}) / \Delta V \right) \\
- \nabla_x \cdot (\bar{v} \bar{\sigma} - \bar{q}^{k\text{lin}}) + t^{k\text{lin}} : \nabla_x \otimes v + \bar{m}^{k\text{lin}} : \nabla_x \otimes \sigma \\
- \left( \sum_{k=1}^n (V^k - \bar{v}) : \nabla_x \otimes \bar{v} + \sum_{a=1}^y m_a^2 ((\sigma^k - \bar{\sigma}) : \Delta r^{k\alpha}) : \nabla_x \otimes (\bar{\sigma} : \Delta r^{k\alpha}) \right) \delta(R^k - \bar{x}) / \Delta V \right).
\]

(6.17)

According to the definitions of linear momentum, Eq. (4.2), and generalized spin, Eq. (4.4), the last term on the right-hand side of above equation vanishes. This leaves

\[
P = -\nabla_x \cdot (\bar{v} \bar{\sigma} - \bar{q}^{k\text{lin}}) + t^{k\text{lin}} : \nabla_x \otimes v + \bar{m}^{k\text{lin}} : \nabla_x \otimes \sigma.
\]

Taking into account the relations
\[
\nabla_{\kappa^\mu} u_{1\gamma} = -f_{1\gamma}^\mu \delta_{\beta \sigma} - f_{1\beta}^\mu \delta_{\kappa \nu} \\
\nabla_{\kappa^\mu} u_{2\beta} = -f_{2\beta}^\mu \delta_{\sigma \alpha} - f_{2\sigma}^\mu \delta_{\kappa \nu},
\]

(6.19)

recalling the definition of \( s^{k\text{lin}}, t^{k\text{lin}}, \) and \( (\rho \phi) = (\rho \cdot \phi) = (\rho \phi) \), \( Q \) becomes

\[
Q = \left( \sum_{k=1}^n \sum_{s=1}^y (V^{ks} : \nabla_{\kappa^s} \bar{\sigma}) \left[ \sum_{l=1}^n \sum_{\beta=1}^y f_{1\gamma}^\beta \delta(R^k - \bar{x}) / \Delta V \right] + \sum_{s=1}^y \sum_{\beta=1}^y f_{2\beta}^\gamma \delta(R^k - \bar{x}) / \Delta V \right) \\
= -\frac{1}{2} \sum_{k=1}^n \sum_{s=1}^y (V^{ks} - V^{k\phi}) f_{1\gamma}^\beta \delta(R^k - \bar{x}) / \Delta V \right) - \frac{1}{2} \sum_{k=1}^n \sum_{s=1}^y (V^{ks} - V^{k\phi}) f_{2\beta}^\gamma \delta(R^k - \bar{x}) / \Delta V \right) \\
- \left( \sum_{k=1}^n \sum_{s=1}^y m_a^2 ((\sigma^k - \bar{\sigma} + \sigma^s - \bar{\sigma}) : \Delta r^{k\alpha} : \nabla_x \otimes \sigma) \delta(R^k - \bar{x}) / \Delta V \right) \\
= -\frac{1}{2} \sum_{k=1}^n \sum_{s=1}^y (V^{ks} - V^{k\phi}) f_{1\gamma}^\beta \delta(R^k - \bar{x}) / \Delta V \right) - \left( \sum_{k=1}^n \sum_{s=1}^y \Delta r^{k\alpha} \cdot f_{1\gamma}^\beta \delta(R^k - \bar{x}) / \Delta V \right) \\
+ \bar{\sigma} : (\bar{s}^{k\text{lin}} - t^{k\text{lin}}).
\]

(6.20)
If we hold to the usual viewpoint that the potential energy $U^{ks}$ is not a function of atomic velocity $V^{ks}$, then

$$R = \left\langle \sum_{k=1}^{n} \sum_{\beta=1}^{v} \frac{1}{m^{\beta}} \cdot \nabla^{\beta} \left( \frac{1}{2} m V^{k} - \bar{v} \right)^{2} + \sum_{x=1}^{v} m^{x} \left( (a^{k} - \bar{a}) \cdot \Delta r^{x/k} \right)^{2} \delta(R^{k} - x)/\Delta V \right\rangle$$

$$= \left\langle \sum_{k=1}^{n} \left( V^{k} - \bar{v} + (a^{k} - \bar{a}) \cdot \Delta r^{x/k} \cdot F^{x} \delta(R^{k} - x)/\Delta V \right) \left( V^{k} - \bar{v} + (a^{k} - \bar{a}) \cdot \Delta r^{x/k} \cdot F^{x} \delta(R^{k} - x)/\Delta V \right) \right\rangle$$

$$= \left\langle \sum_{k=1}^{n} \left( \left( V^{k} - \bar{v} + (a^{k} - \bar{a}) \cdot \Delta r^{x/k} \cdot F^{x} \delta(R^{k} - x)/\Delta V \right) \cdot \left( \frac{1}{2} m V^{k} - \bar{v} \right)^{2} + \sum_{x=1}^{v} m^{x} \left( (a^{k} - \bar{a}) \cdot \Delta r^{x/k} \right)^{2} \delta(R^{k} - x)/\Delta V \right) \right\rangle$$

$$+ \left\langle \sum_{k=1}^{n} \Delta t^{x/k} \cdot \left( \frac{1}{2} m V^{k} - \bar{v} \right)^{2} \delta(R^{k} - x)/\Delta V \right\rangle$$

$$+ \left\langle \sum_{k=1}^{n} \left( V^{k} - \bar{v} + (a^{k} - \bar{a}) \cdot \Delta r^{x/k} \cdot F^{x} \delta(R^{k} - x)/\Delta V \right) \right\rangle.$$  

(6.21)

Denoting

$$\lambda \equiv \sum_{k=1}^{n} \sum_{x=1}^{v} \left( V^{k} - \bar{v} + (a^{k} - \bar{a}) \cdot \Delta r^{x/k} \cdot F^{x} \delta(R^{k} - x)/\Delta V \right),$$

(6.22)

$$Q + R = -\frac{1}{2} \left\langle \sum_{k=1}^{n} \sum_{x=1}^{v} \left( V^{k} - \bar{v} + (a^{k} - \bar{a}) \cdot \Delta r^{x/k} \cdot F^{x} \delta(R^{k} - x)/\Delta V \right) \right\rangle$$

$$- \left\langle \sum_{k=1}^{n} \left( \sum_{x=1}^{v} \Delta r^{x/k} \cdot F^{x} \delta(R^{k} - x)/\Delta V \right) \right\rangle$$

$$+ \left\langle \sum_{k=1}^{n} \sum_{x=1}^{v} \left( V^{k} - \bar{v} + (a^{k} - \bar{a}) \cdot \Delta r^{x/k} \cdot \left( \frac{1}{2} m V^{k} - \bar{v} \right)^{2} \delta(R^{k} - x)/\Delta V \right) \right\rangle + \lambda$$

$$= \left\langle \sum_{k=1}^{n} \sum_{x=1}^{v} \left( \frac{1}{2} \left( V^{k} + V^{\bar{v}} \cdot F^{x} \delta(R^{k} - x)/\Delta V \right) \right) - \bar{v} \cdot \left( \nabla_{x} \cdot \bar{t}^{\text{pot}} \right) \right\rangle$$

$$- \bar{v} \cdot \left( \nabla_{x} \cdot \bar{m}^{\text{pot}} + \left( \bar{t}^{\text{pot}} - \bar{m}^{\text{kin}} \right) \right) + \lambda.$$

(6.23)

With Eq. (4.28), finally

$$P + Q + R = -\nabla_{x} \cdot \left( \bar{v} \bar{e} - \bar{q}^{\text{kin}} \right) + \left( \bar{t}^{\text{kin}} + \bar{t}^{\text{pot}} \right) \cdot \left( \nabla_{x} \otimes \bar{v} \right) + \left( \bar{m}^{\text{pot}} + \bar{m}^{\text{kin}} \right) \cdot \left( \nabla_{x} \otimes \bar{a} \right) + \lambda.$$  

(6.24)

The balance law of energy is then obtained as
Atomistic counterpart of micromorphic theory

\[
\frac{\partial(\rho \mathbf{e})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{e} - \mathbf{q}) = \mathbf{f} : \mathbf{e} + \mathbf{m} : \nabla \otimes \mathbf{e} + \rho \mathbf{e} : (\mathbf{s} - \mathbf{t}) + \mathbf{\lambda}.
\]  
(6.25)

If the energy source of non-mechanical origin, denoted by \( h \), is included, then the balance law of energy would have the form:

\[
\frac{\partial(\rho \mathbf{e})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{e} - \mathbf{q}) = \mathbf{f} : \mathbf{e} + \mathbf{m} : \nabla \otimes \mathbf{e} + \rho \mathbf{e} : (\mathbf{s} - \mathbf{t}) + \mathbf{\lambda} + \rho h.
\]  
(6.26)

7 Discussions

7.1 Summary and discussions of the results

All the instantaneous mechanical variables, corresponding to the variables describing the micromorphic continuum, have been derived and related to atomic coordinates and velocities. The expressions for the instantaneous mechanical variables presented in this paper apply equally well to gas, fluid, and solid, and to both equilibrium and nonequilibrium systems. With the definition of those fundamental variables in both atomic model and continuum theory, we have the necessary tools to relate the discrete atomic description and the continuous field description of matter to each other.

Atomistic flow mechanisms make it possible to define the fluxes as sums of one- and two-atom contributions. The internal energy \( e \), heat flux \( q \), and the generalized stress tensors, namely, Cauchy stress \( t \), microstress average \( s \), and moment stress \( m \), are composed of the kinetic parts and the potential parts. With the definition of temperature, it is seen that the kinetic parts of \( t, s, m, q \), and \( e \) are caused by the thermal motion of atoms, and can be linked to temperature. The potential parts are caused by interatomic forces, and can be decided if the potential functions are known. Therefore, the corresponding constitutive relations and the material constants can also be obtained by an atomic model.

Also, for each atom \((k, x)\), the interatomic force is taken from all other atoms in the body considered. The action-at-a-distance interactions described by the interparticle forces give the related quantities a nonlocal character. The derivation in this paper is therefore in the nonlocal arena.

Comparing the balance laws introduced in Sect. 2 and those derived in Sect. 6, it is seen that the first four equations are identical, while the energy equation has an additional term \( \mathbf{\lambda} \). If the external field is the gravitational field, i.e., \( \mathbf{f}_{\text{3}} = m^2 \mathbf{g} \), then

\[
\mathbf{\lambda} = \sum_{k=1}^{n} \sum_{x=1}^{y} \left( \mathbf{V}^k - \mathbf{v} + (\omega^k - \bar{\omega}) \cdot \Delta \mathbf{r}^{k3} \right) \cdot \mathbf{f}_{\text{3}}^{k3} \delta(\mathbf{R}^k - \mathbf{x})
\]

\[
= \sum_{k=1}^{n} \sum_{x=1}^{y} m^2 (\mathbf{V}^k - \mathbf{\bar{v}} + (\omega^k - \bar{\omega}) \cdot \Delta \mathbf{r}^{k3}) \delta(\mathbf{R}^k - \mathbf{x}) \cdot \mathbf{g} = 0,
\]

and also the body couple \( \mathbf{\tilde{l}} \) (cf. Eq. (4.7)) will vanish. If this external field is not the gravitational field, e.g., electromagnetic attractions, then both \( \mathbf{l} \) and \( \mathbf{\lambda} \) would not vanish, and other terms would be included in the balance laws [2]. Therefore, the balance laws derived in this paper have agreed exactly with those derived by Eringen in a top-down approach. On the other hand, it is noticed that \( \mathbf{\gamma} \) and \( \mathbf{\lambda} \) vanish, whereas \( \mathbf{\gamma} \) and \( \mathbf{\lambda} \) are nonvanishing. This implies that the balance laws for instantaneous mechanical variables and for continuum field quantities are different.
Hence the balance laws introduced in Sect. 2 only hold in the statistical sense when the ensemble average is meaningful.

It is also worthwhile to note that if the material particle is reduced to a mass point, i.e., the unit cell contains only one atom, \( \nu = 1 \), then it is straightforward to obtain \( m = m^a \), \( R = R^a \), \( V = V^a \), \( \rho = \rho^a = 0 \), \( \Delta v^a = 0 \), \( f^a = 0 \), \( \rho \phi = 0 \), \( \rho \phi = 0 \). These lead to \( s = t \) and \( m = 0 \). Hence the micromorphic theory will be reduced to the classical continuum theory in the limiting case \( \nu = 1 \), and all the derivations and expressions can then be applied to classical continuum theory.

### 7.2 Applicability analysis of continua theories

(1) Micromorphic theory \([1], [2]\)

From the results obtained in this paper it is seen that micromorphic theory can be obtained based on the kinematics and interactions of atoms. Analytical correspondence can be achieved between the atomic model and the continuum micromorphic model whenever an ensemble average is meaningful so that the continuum treatment is valid. The applicability of the micromorphic theory in microscopic time and length scales is confirmed from the viewpoint of atomic motion and interaction.

(2) Microstructure theory \([3]\)

Compared with Eringen’s micromorphic theory, Mindlin’s microstructure theory is an elastic theory without thermal effect. This is corresponding to the low temperature case in the atomic level. The magnitude of the atomic motion is very small so that the kinetic parts of the stresses, \( t \), \( s \), \( m \), heat flux, \( q \), and the internal energy, \( \varepsilon \), can be ignored. The microscopic expressions of the \( t \), \( s \), \( m \), and \( \varepsilon \), with the potential part only, can then be linked to the mechanical variables in Mindlin’s microstructure theory of elasticity, but the balance laws still take the same form. Therefore, from the viewpoint of atomic motion, Mindlin’s microstructure theory is also a special case of micromorphic theory, valid for low temperature and, as a consequence, small deformation problems.

(3) Micropolar theory \([4]\)

If there is a very large difference between the atomic forces \( f_{1}^{k} \) and \( f_{2}^{k} \), and \( f_{2}^{k} \) is much larger, then the microstructure of the deformable particle can be approximated as rigid. Therefore, the gyration tensor reduces to an angular velocity, and \( \Delta v^{k} = \omega^{k} \times \Delta r^{k} \), this then results in the micropolar theory.

One typical example is the molecular crystals. In molecular crystal the intramolecular bonds are essentially the first order bonds while the intermolecular bonds are generally second order, or in any case considerably weaker than the former. Consequently the intramolecular binding energies are much higher and the intermolecular binding does not change significantly the structure of the molecule. As a consequence, the oscillation frequencies of the atoms within the molecules with respect to each other are much higher than the relative oscillation frequencies of the molecular groups. Hence the molecular groups can, to a reasonable approximation, be taken as rigid.

Apparently, this is not the case for metallic, covalent and ionic crystals. Micropolar theory, therefore, can be applied to molecular crystal, or materials that have rigid or near rigid microstructure.
(4) Cosserat theory [5]
Without the balance law of microinertia, micropolar theory is identical to Cosserat theory. The absence of the time evolution law of microinertia tensor implies that the microinertia tensor is assumed to be constant. This is the case when the deformation and motion within the microstructure of the particle is very small, and the change of the microstructure and its orientation can be ignored. Hence, compared with micropolar theory, Cosserat theory is not suited for problems involve significant change of the orientation of the microstructure.

The couple stress theory, by including higher order stress, provides a model that can yield results depending on the size of specimen. However, there is no distinction between micromotion and macromotion, and hence it is only suited for material without microstructure (Mindlin [3]). The material that does not have microstructure, is usually referred as microscopically homogeneous, and is corresponding to crystal with only one atom in the primitive unit cell. From the results of this paper, this will give \( s = t \) and \( m = 0 \). The couple stress theory is thus closer to nonlocal theory than to micromorphic or microstructure theory, and for the purpose of nonlocal effect, there is no need to have a higher-order stress \( m \).

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Authors' address: Y. Chen, J. D. Lee, and A. Eskandarian, School of Engineering and Applied Science, The George Washington University, 801 22nd Street, NW, Academic Center, Washington, DC 20052, USA (E-mail: lee@seas.gwu.edu)