Chapter 12
Extending Micromorphic Theory to Atomic Scale

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Abstract Micromorphic theory envisions a material body as a continuous collection of deformable particles; each possesses finite size and inner structure. It may be considered as the most successful top-down formulation of a two-level continuum model, in which the deformation is expressed as a sum of macroscopic continuous deformation and microscopic deformation of the inner structure. To enlarge the domain of applicability of the micromorphic theory, starting from many-body dynamics, we took a bottom-up approach to formulate a generalized continuum field theory in which a crystalline material is viewed as a continuous collection of lattice points while embedded within each lattice point is a group of discrete atoms. In this work, atomistic definitions and the corresponding field representations of fundamental physical quantities are introduced. The balance laws and the constitutive relations are obtained through the atomistic formulation, which naturally leads to a generalized continuum field theory. It is identical to molecular dynamics at atomic scale and can be reduced to classical continuum field theory at macroscopic scale.

12.1 Introduction to Micromorphic Theory

Microcontinuum field theories constitute extensions of the classical field theories concerned with deformations, motions, and electromagnetic interactions of material media, as continua, in microscopic space and short time scales. In terms of a

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physical picture, a microcontinuum may be envisioned as a continuous collection of deformable point particles, each with finite size and inner structure. It is worthwhile to note that in the classical continuum theory a point particle is represented by a geometrical point, which is infinitesimal in size. Then the question arises: *How can one represent the intrinsic deformation of a point particle in microcontinuum*? Eringen settled this question by replacing the deformable particle with a geometric point P and some vectors attached to P, which denote the orientations and intrinsic deformations of all the material points in the deformable point particle. This is compatible with the classical picture where a material point in a continuum is endowed with physical properties such as mass density, displacement vector, electric field, stress tensor, etc. Therefore, the vectors assigned to P represent the additional degrees of freedom arising from the motions, relative to P, of all the material points in the particle. Geometrically, a particle P is identified by its position vector $\mathbf{X}$, in the reference (Lagrangian or material) state B, and vectors attached to P, representing the inner structure of P by Ξ^α $(\alpha = 1, 2, 3, \ldots, N)$ while N is the number of material points in the particle. The motions may be expressed as

$$\mathbf{x} = \mathbf{x}(\mathbf{X}, t), \tag{12.1}$$

$$\boldsymbol{\xi}^\alpha = \xi^\alpha\big(\mathbf{X}, \Xi^\alpha, t\big) \quad \alpha \in [1, 2, 3, \ldots, N], \tag{12.2}$$

where t is the time; $\mathbf{x}$ and ξ^α, corresponding to $\mathbf{X}$ and Ξ^α, respectively, are the position vectors in the deformed (Eulerian or spatial) state b. A medium with such general motions is named microcontinuum of grade N by Eringen. In the two-level continuum model, let the position vector of a material point be decomposed as the sum of the position vector of the centroid (mass center) of the particle and the position vector of the material point relative to the centroid (cf. Fig. 1.1.2 of Eringen [6]), i.e.,

$$\mathbf{x}' = \mathbf{x} + \xi, \qquad \mathbf{X}' = \mathbf{X} + \Xi, \tag{12.3}$$

and let the motions be expressed as

$$\mathbf{x} = \mathbf{x}(\mathbf{X}, t), \qquad \xi = \xi(\mathbf{X}, \Xi, t). \tag{12.4}$$

If the micromotion $\xi = \xi(\mathbf{X}, \Xi, t)$ is further reduced to an affine motion, i.e.,

$$\boldsymbol{\xi} = \boldsymbol{\chi}_K(\mathbf{X}, t)\Xi_K \quad \text{or} \quad \xi_k = \chi_{kK}(\mathbf{X}, t)\Xi_K, \tag{12.5}$$

we arrive at the doorstep of the *micromorphic theory*. It is seen that the macromotion $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$ accounts for the motion of the centroid of the particle; the micromotion $\xi_k = \chi_{kK}(\mathbf{X}, t)\Xi_K$ accounts for the intrinsic motions of the particle; and χ_{kK} is called the microdeformation tensor. Because χ_{kK} is a second order tensor, the particle has 9 independent degrees of freedom in addition to the 3 classical translational degrees of freedom of the centroid. A unit cell or a polyatomic molecule may be viewed as a point particle in micromorphic theory [6, 7].

12.2 Balance Laws of Micromorphic Theory

The balance laws of micromorphic theory, namely conservation of mass, microinertia, energy and balance of linear momentum and momentum moments, were first derived by Eringen and Suhubi [8, 11] and Eringen [5] by means of a "microscopic space-averaging" process. Later Eringen [6] derived the balance laws in a more elegant way: balance of linear momentum and momentum moments are the consequences of the objectivity of conservation of energy:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho\nabla_{\mathbf{x}}\cdot\mathbf{v} = 0, \tag{12.6}$$

$$\rho\frac{\mathrm{d}\mathbf{i}}{\mathrm{d}t} = \rho\boldsymbol{\varphi} + \rho\boldsymbol{\varphi}^{T}, \tag{12.7}$$

$$\rho\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \nabla_{\mathbf{x}}\cdot\mathbf{t} + \mathbf{f}, \tag{12.8}$$

$$\rho\frac{\mathrm{d}\boldsymbol{\varphi}}{\mathrm{d}t} = \nabla_{\mathbf{x}}\cdot\mathbf{m} + \mathbf{t}^{T} - \mathbf{s} + \boldsymbol{\upsilon}\cdot\rho\mathbf{i}\cdot\boldsymbol{\upsilon}^{T} + \mathbf{l}, \tag{12.9}$$

$$\rho\frac{De}{Dt} = \mathbf{m}\dddot{\nabla}_{\mathbf{x}}\otimes\boldsymbol{\upsilon} + \mathbf{t}:\nabla_{\mathbf{x}}\otimes\mathbf{v} + (\mathbf{s}-\mathbf{t})^{T}:\boldsymbol{\upsilon} + \nabla_{\mathbf{x}}\cdot\mathbf{q} + h, \tag{12.10}$$

where ρ is the mass density; $\rho\mathbf{i}$ is the microinertia tensor; $\rho\boldsymbol{\varphi} = \boldsymbol{\upsilon}\cdot\rho\mathbf{i}$ is the generalized spin tensor; $\mathbf{t}$ is the Cauchy stress; $\mathbf{s} = \mathbf{s}^{T}$ is the microstress; $\mathbf{m}$ is a third order tensor, called the moment stress; $\mathbf{v}$ is the velocity; $\boldsymbol{\upsilon}$ is a second order tensor, called the gyration tensor; $\mathbf{l}$ is a second order tensor, called the body couple density; e is the internal energy density; $\mathbf{q}$ is the heat flux; and h is the heat source.

To demonstrate that the micromorphic theory can be built on a more profound physical foundation, in this work, we follow the approach of Hardy [9] to link variables between the phase space and the physical space of a many-body system and to derive the balance laws for microcontinuum. Microscopic dynamic quantities in many-body dynamics are functions of phase-space coordinates $(\mathbf{r}, \mathbf{p})$, i.e., the positions and momenta of atoms. For a single crystal of a multi-element system

$$\mathbf{r} = \left\{\mathbf{R}^{k\alpha} = \mathbf{R}^{k} + \Delta\mathbf{r}^{k\alpha} \mid k = 1,2,3,\ldots,N_l; \alpha = 1,2,3,\ldots,N_a\right\}, \tag{12.11}$$

$$\mathbf{p} = \left\{m^{\alpha}\mathbf{V}^{k\alpha} = m^{\alpha}\left(\mathbf{V}^{k} + \Delta\mathbf{v}^{k\alpha}\right) \mid k = 1,2,3,\ldots,N_l; \quad \alpha = 1,2,3,\ldots,N_a\right\}, \tag{12.12}$$

where N_l is the total number of unit cells in the system; N_a is the number of atoms in a unit cell; the superscript $k\alpha$ refers to the αth atom in the kth unit cell; m^{α} is the mass of the αth atom; $\mathbf{R}^{k\alpha}$ and $\mathbf{V}^{k\alpha}$ are the position and velocity of the $k\alpha$th atom, respectively; $\mathbf{R}^{k}$ and $\mathbf{V}^{k}$ are the position and velocity of the centroid of the kth unit cell, respectively; $\Delta\mathbf{r}^{k\alpha}$ and $\Delta\mathbf{v}^{k\alpha}$ are the position and velocity of the $k\alpha$th atom relative to the centroid of the kth unit cell, respectively.

A dynamic function $\mathbf{A}(\mathbf{r}, \mathbf{p})$ in phase space can be linked to its corresponding local density function $\mathbf{a}(\mathbf{x}, t)$ in physical space as

$$\mathbf{a}(\mathbf{x},t)=\sum_{k=1}^{N_l}\sum_{\alpha=1}^{N_a}\mathbf{A}(\mathbf{r},\mathbf{p})\delta\big(\mathbf{R}^k-\mathbf{x}\big), \tag{12.13}$$

where the δ-function can be any localization function with $\int_{\Omega(\mathbf{x})}\delta(\mathbf{R}^k-\mathbf{x})\,\mathrm{d}\mathbf{x}=1$ [9]. With the properties of the δ-function [10], the time evolution of physical quantities can be obtained as

$$\begin{aligned}\left.\frac{\partial\mathbf{a}(\mathbf{x},t)}{\partial t}\right|_{\mathbf{x}}&=\sum_{k=1}^{N_l}\sum_{\alpha=1}^{N_a}\dot{\mathbf{A}}(\mathbf{r},\mathbf{p})\delta\big(\mathbf{R}^k-\mathbf{x}\big)\\&\quad-\nabla_{\mathbf{x}}\cdot\sum_{k=1}^{N_l}\sum_{\alpha=1}^{N_a}\mathbf{V}^k\otimes\mathbf{A}(\mathbf{r},\mathbf{p})\delta\big(\mathbf{R}^k-\mathbf{x}\big).\end{aligned} \tag{12.14}$$

When $\mathbf{a}(\mathbf{x},t)$ is the local density of a conserved quantity, (12.14) is the corresponding microscopic balance law. The conserved quantities in micromorphic theory are

$$\rho=\sum_{k=1}^{N_l}\sum_{\alpha=1}^{N_a}m^\alpha\delta\big(\mathbf{R}^k-\mathbf{x}\big)=\sum_{k=1}^{N_l}m\delta\big(\mathbf{R}^k-\mathbf{x}\big), \tag{12.15}$$

$$\rho\mathbf{i}=\sum_{k=1}^{N_l}\sum_{\alpha=1}^{N_a}m^\alpha\Delta\mathbf{r}^{k\alpha}\times\Delta\mathbf{r}^{k\alpha}\delta\big(\mathbf{R}^k-\mathbf{x}\big), \tag{12.16}$$

$$\rho\mathbf{v}=\sum_{k=1}^{N_l}\sum_{\alpha=1}^{N_a}m^\alpha\mathbf{V}^{k\alpha}\delta\big(\mathbf{R}^k-\mathbf{x}\big)=\sum_{k=1}^{N_l}m\mathbf{V}^k\delta\big(\mathbf{R}^k-\mathbf{x}\big), \tag{12.17}$$

$$\rho\boldsymbol{\varphi}=\sum_{k=1}^{N_l}\sum_{\alpha=1}^{N_a}m^\alpha\Delta\mathbf{v}^{k\alpha}\times\Delta\mathbf{r}^{k\alpha}\delta\big(\mathbf{R}^k-\mathbf{x}\big), \tag{12.18}$$

$$\rho E=\sum_{k=1}^{N_l}\left\{\frac{1}{2}m\big(\mathbf{V}^k\big)^2+\sum_{\alpha=1}^{N_a}\left[\frac{1}{2}m^\alpha\big(\boldsymbol{v}^k\cdot\Delta\mathbf{r}^{k\alpha}\big)^2+U^{k\alpha}\right]\right\}\delta\big(\mathbf{R}^k-\mathbf{x}\big). \tag{12.19}$$

Notice that the micromotion of micromorphic material is affine, i.e., $\Delta\mathbf{v}^{k\alpha}=\boldsymbol{v}^k\cdot\Delta\mathbf{r}^{k\alpha}$, we obtained almost the same set of balance laws except

$$\rho\frac{\mathrm{d}\mathbf{i}}{\mathrm{d}t}=\rho\boldsymbol{\varphi}+\rho\boldsymbol{\varphi}^T-\nabla_{\mathbf{x}}\cdot\boldsymbol{\gamma}, \tag{12.20}$$

$$\rho\frac{\mathrm{d}\boldsymbol{\varphi}}{\mathrm{d}t}=\nabla_{\mathbf{x}}\cdot\mathbf{m}+\mathbf{t}^T-\mathbf{s}+\boldsymbol{v}\cdot\rho\mathbf{i}\cdot\boldsymbol{v}^T+\mathbf{l}-\nabla_{\mathbf{x}}\cdot(\boldsymbol{v}\cdot\boldsymbol{\gamma}), \tag{12.21}$$

where

$$\boldsymbol{\gamma}=\sum_{k=1}^{N_l}\big(\mathbf{V}^k-\mathbf{v}\big)\otimes\sum_{\alpha=1}^{N_a}m^\alpha\Delta\mathbf{r}^{k\alpha}\otimes\Delta\mathbf{r}^{k\alpha}\delta\big(\mathbf{R}^k-\mathbf{x}\big). \tag{12.22}$$

It is seen that $\mathbf{V}^k - \mathbf{v}$ is the difference between phase space velocity and physical space velocity and it is easy to understand why γ does not appear in the "microscopic space-averaging" process. The detailed expressions of $\mathbf{m}$, $\mathbf{t}$, $\mathbf{s}$, $\mathbf{q}$, $\mathbf{l}$ and h are referred to Chen and Lee [2, 3].

12.3 Extension of Micromorphic Theory to Atomic Scale

In the process of constructing a multiscale concurrent atomistic/continuum theory, to keep the knowledge and information at the atomistic level as much as possible, we now relax the assumption of affine motion and let the motions be back to the generality as indicated in (12.1), (12.2). Now the link between a dynamic function in phase space and its corresponding local density function in physical space can be established through a localization function and the Kronecker δ-function as [1]

$$\mathbf{a}\big(\mathbf{x}, \mathbf{y}^\alpha, t\big) = \sum_{k=1}^{N_l} \sum_{\xi=1}^{N_a} \mathbf{A}(\mathbf{r}, \mathbf{p}) \delta\big(\mathbf{R}^k - \mathbf{x}\big) \tilde{\delta}\big(\Delta \mathbf{r}^{k\xi} - \mathbf{y}^\alpha\big), \tag{12.23}$$

with

$$\tilde{\delta}\big(\Delta \mathbf{r}^{k\xi} - \mathbf{y}^\alpha\big) \equiv \begin{cases} 1, & \text{if } \xi = \alpha \text{ and } \Delta \mathbf{r}^{k\alpha} = \mathbf{y}^\alpha, \\ 0, & \text{otherwise.} \end{cases} \tag{12.24}$$

Similarly, the time evolution of a physical quantity can be obtained as:

$$\begin{aligned} \left.\frac{\partial \mathbf{a}(\mathbf{x}, \mathbf{y}^\alpha, t)}{\partial t}\right|_{\mathbf{x}, \mathbf{y}^\alpha} &= \sum_{k=1}^{N_l} \sum_{\xi=1}^{N_a} \dot{\mathbf{A}}(\mathbf{r}, \mathbf{p}) \delta\big(\mathbf{R}^k - \mathbf{x}\big) \tilde{\delta}\big(\Delta \mathbf{r}^{k\xi} - \mathbf{y}^\alpha\big) \\ &\quad - \nabla_{\mathbf{x}} \cdot \sum_{k=1}^{N_l} \sum_{\xi=1}^{N_a} \mathbf{V}^k \otimes \mathbf{A}(\mathbf{r}, \mathbf{p}) \delta\big(\mathbf{R}^k - \mathbf{x}\big) \tilde{\delta}\big(\Delta \mathbf{r}^{k\xi} - \mathbf{y}^\alpha\big) \\ &\quad - \nabla_{\mathbf{y}^\alpha} \cdot \sum_{k=1}^{N_l} \sum_{\xi=1}^{N_a} \Delta \mathbf{v}^{k\xi} \otimes \mathbf{A}(\mathbf{r}, \mathbf{p}) \delta\big(\mathbf{R}^k - \mathbf{x}\big) \tilde{\delta}\big(\Delta \mathbf{r}^{k\xi} - \mathbf{y}^\alpha\big). \end{aligned} \tag{12.25}$$

Following the pattern of (12.23), the mass density ρ^α, linear momentum density $\rho^\alpha(\mathbf{v} + \Delta \mathbf{v}^\alpha)$, angular momentum density $\rho^\alpha \boldsymbol{\psi}^\alpha$, internal energy density $\rho^\alpha e^\alpha$, interatomic force density $\mathbf{f}^\alpha$, external force density $\mathbf{f}^\alpha_{\text{ext}}$, the homogeneous part $\mathbf{t}^\alpha$ and inhomogeneous part $\boldsymbol{\tau}^\alpha$ of stress tensor, the homogeneous part $\mathbf{q}^\alpha$ and inhomogeneous part $\mathbf{j}^\alpha$ of heat flux, and heat source h are defined as

$$\rho^\alpha = \sum_{k=1}^{N_l} \sum_{\xi=1}^{N_a} m^\xi \delta\big(\mathbf{R}^k - \mathbf{x}\big) \tilde{\delta}\big(\Delta \mathbf{r}^{k\xi} - \mathbf{y}^\alpha\big), \tag{12.26}$$

$$\rho^{\alpha}\big(\mathbf{v}+\Delta\mathbf{v}^{\alpha}\big)=\sum_{k=1}^{N_l}\sum_{\xi=1}^{N_a}m^{\xi}\big(\mathbf{V}^{k}+\Delta\mathbf{v}^{k\xi}\big)\delta\big(\mathbf{R}^{k}-\mathbf{x}\big)\tilde{\delta}\big(\Delta\mathbf{r}^{k\xi}-\mathbf{y}^{\alpha}\big), \quad (12.27)$$

$$\rho^{\alpha}\boldsymbol{\psi}^{\alpha}=\sum_{k=1}^{N_l}\sum_{\xi=1}^{N_a}m^{\xi}\mathbf{V}^{k\xi}\times\mathbf{R}^{k\xi}\delta\big(\mathbf{R}^{k}-\mathbf{x}\big)\tilde{\delta}\big(\Delta\mathbf{r}^{k\xi}-\mathbf{y}^{\alpha}\big), \quad (12.28)$$

$$\rho^{\alpha}e^{\alpha}=\sum_{k=1}^{N_l}\sum_{\xi=1}^{N_a}\left[\frac{1}{2}m^{\xi}\big(\widetilde{\mathbf{V}}^{k\xi}\big)^{2}+U^{k\xi}\right]\delta\big(\mathbf{R}^{k}-\mathbf{x}\big)\tilde{\delta}\big(\Delta\mathbf{r}^{k\xi}-\mathbf{y}^{\alpha}\big), \quad (12.29)$$

$$\mathbf{f}^{\alpha}=\sum_{k=1}^{N_l}\sum_{\xi=1}^{N_a}\mathbf{F}^{k\xi}\delta\big(\mathbf{R}^{k}-\mathbf{x}\big)\tilde{\delta}\big(\Delta\mathbf{r}^{k\xi}-\mathbf{y}^{\alpha}\big), \quad (12.30)$$

$$\mathbf{f}^{\alpha}_{\mathrm{ext}}=\sum_{k=1}^{N_l}\sum_{\xi=1}^{N_a}\mathbf{F}^{k\xi}_{\mathrm{ext}}\delta\big(\mathbf{R}^{k}-\mathbf{x}\big)\tilde{\delta}\big(\Delta\mathbf{r}^{k\xi}-\mathbf{y}^{\alpha}\big), \quad (12.31)$$

$$\begin{aligned}\mathbf{t}^{\alpha}=&-\sum_{k=1}^{N_l}\sum_{\xi=1}^{N_a}m^{\xi}\widetilde{\mathbf{V}}^{k}\otimes\widetilde{\mathbf{V}}^{k\xi}\delta\big(\mathbf{R}^{k}-\mathbf{x}\big)\tilde{\delta}\big(\Delta\mathbf{r}^{k\xi}-\mathbf{y}^{\alpha}\big)\\&-\frac{1}{2}\sum_{k,l=1}^{N_l}\sum_{\xi,\eta=1}^{N_a}\big(\mathbf{R}^{k}-\mathbf{R}^{l}\big)\otimes\mathbf{F}^{k\xi}B\big(k,\xi,l,\eta,\mathbf{x},\mathbf{y}^{\alpha}\big), \quad (12.32)\end{aligned}$$

$$\begin{aligned}\boldsymbol{\tau}^{\alpha}=&-\sum_{k=1}^{N_l}\sum_{\xi=1}^{N_a}m^{\xi}\Delta\widetilde{\mathbf{v}}^{k\xi}\otimes\widetilde{\mathbf{V}}^{k\xi}\delta\big(\mathbf{R}^{k}-\mathbf{x}\big)\tilde{\delta}\big(\Delta\mathbf{r}^{k\xi}-\mathbf{y}^{\alpha}\big)\\&-\frac{1}{2}\sum_{k,l=1}^{N_l}\sum_{\xi,\eta=1}^{N_a}\big(\Delta\mathbf{r}^{k\xi}-\Delta\mathbf{r}^{l\eta}\big)\otimes\mathbf{F}^{k\xi}B\big(k,\xi,l,\eta,\mathbf{x},\mathbf{y}^{\alpha}\big), \quad (12.33)\end{aligned}$$

$$\begin{aligned}\mathbf{q}^{\alpha}=&-\sum_{k=1}^{N_l}\sum_{\xi=1}^{N_a}\widetilde{\mathbf{V}}^{k}\left[\frac{1}{2}m^{\xi}\big(\widetilde{\mathbf{V}}^{k\xi}\big)^{2}+U^{k\xi}\right]\delta\big(\mathbf{R}^{k}-\mathbf{x}\big)\tilde{\delta}\big(\Delta\mathbf{r}^{k\xi}-\mathbf{y}^{\alpha}\big)\\&-\frac{1}{2}\sum_{k,l=1}^{N_l}\sum_{\xi,\eta=1}^{N_a}\big(\mathbf{R}^{k}-\mathbf{R}^{l}\big)\widetilde{\mathbf{V}}^{k\xi}\cdot\mathbf{F}^{k\xi}B\big(k,\xi,l,\eta,\mathbf{x},\mathbf{y}^{\alpha}\big), \quad (12.34)\end{aligned}$$

$$\begin{aligned}\mathbf{j}^{\alpha}=&-\sum_{k=1}^{N_l}\sum_{\xi=1}^{N_a}\Delta\widetilde{\mathbf{v}}^{k\xi}\left[\frac{1}{2}m^{\xi}\big(\widetilde{\mathbf{V}}^{k\xi}\big)^{2}+U^{k\xi}\right]\delta\big(\mathbf{R}^{k}-\mathbf{x}\big)\tilde{\delta}\big(\Delta\mathbf{r}^{k\xi}-\mathbf{y}^{\alpha}\big)\\&-\frac{1}{2}\sum_{k,l=1}^{N_l}\sum_{\xi,\eta=1}^{N_a}\big(\Delta\mathbf{r}^{k\xi}-\Delta\mathbf{r}^{l\eta}\big)\widetilde{\mathbf{V}}^{k\xi}\cdot\mathbf{F}^{k\xi}B\big(k,\xi,l,\eta,\mathbf{x},\mathbf{y}^{\alpha}\big), \quad (12.35)\end{aligned}$$

$$h^{\alpha}=\sum_{k=1}^{N_l}\sum_{\xi=1}^{N_a}\widetilde{\mathbf{V}}^{k\xi}\cdot\mathbf{F}^{k\xi}_{\mathrm{ext}}\delta\big(\mathbf{R}^{k}-\mathbf{x}\big)\tilde{\delta}\big(\Delta\mathbf{r}^{k\xi}-\mathbf{y}^{\alpha}\big), \quad (12.36)$$

where $\widetilde{\mathbf{V}}^{k\xi} = \mathbf{V}^{k\xi} - (\mathbf{v} + \Delta\mathbf{v}^{\xi})$, $\widetilde{\mathbf{V}}^{k} = \mathbf{V}^{k} - \mathbf{v}$ and $\Delta\widetilde{\mathbf{v}}^{k\xi} = \Delta\mathbf{v}^{k\xi} - \Delta\mathbf{v}^{\xi}$ are the differences between phase space velocities and physical space velocities; $\mathbf{F}^{k\xi}_{\text{ext}}$ is the body force, such as gravitational force and Lorentz force, acting on the $k\xi$th atom; $U^{k\xi}$ is the potential energy of the $k\xi$th atom; $\mathbf{F}^{k\xi}$ is the interatomic force acting on the $k\xi$th atom with the understanding that the total potential energy U is additive, i.e.,

$$U = \sum_{k=1}^{N_l}\sum_{\xi=1}^{N_a} U^{k\xi}, \qquad \mathbf{F}^{k\xi} = -\frac{\partial U}{\partial \mathbf{R}^{k\xi}} = -\frac{\partial U^{k\xi}}{\partial \mathbf{R}^{k\xi}} \tag{12.37}$$

and $B(k, \xi, l, \eta, \mathbf{x}, \mathbf{y}^{\alpha})$ is defined as

$$B \equiv \int_0^1 \delta\big(\mathbf{R}^{k}\lambda + \mathbf{R}^{l}(1-\lambda) - \mathbf{x}\big)\tilde{\delta}\big(\Delta\mathbf{r}^{k\xi}\lambda + \Delta\mathbf{r}^{l\eta}(1-\lambda) - \mathbf{y}^{\alpha}\big)\,\mathrm{d}\lambda. \tag{12.38}$$

Based on (12.25), a lengthy but straightforward process leads to the local balance laws of mass, linear momentum, angular momentum, and energy for each atom $\alpha \in [1, 2, 3, \ldots, N_a]$ at any point in the field $(\mathbf{x}, t)$ as [4]

$$\frac{\mathrm{d}\rho^{\alpha}}{\mathrm{d}t} + \rho^{\alpha}\nabla_{\mathbf{x}}\cdot\mathbf{v} + \rho^{\alpha}\nabla_{\mathbf{y}^{\alpha}}\cdot\Delta\mathbf{v}^{\alpha} = 0, \tag{12.39}$$

$$\rho^{\alpha}\frac{\mathrm{d}(\mathbf{v} + \Delta\mathbf{v}^{\alpha})}{\mathrm{d}t} = \nabla_{\mathbf{x}}\cdot\mathbf{t}^{\alpha} + \nabla_{\mathbf{y}^{\alpha}}\cdot\boldsymbol{\tau}^{\alpha}, + \mathbf{f}^{\alpha}_{\text{ext}} \tag{12.40}$$

$$\mathbf{t}^{\alpha} + \boldsymbol{\tau}^{\alpha} = \big(\mathbf{t}^{\alpha} + \boldsymbol{\tau}^{\alpha}\big)^{T}, \tag{12.41}$$

$$\rho^{\alpha}\frac{\mathrm{d}e^{\alpha}}{\mathrm{d}t} = \mathbf{t}^{\alpha} : \nabla_{\mathbf{x}}\big(\mathbf{v} + \Delta\mathbf{v}^{\alpha}\big) + \boldsymbol{\tau}^{\alpha} : \nabla_{\mathbf{y}^{\alpha}}\big(\mathbf{v} + \Delta\mathbf{v}^{\alpha}\big) + \nabla_{\mathbf{x}}\cdot\mathbf{q}^{\alpha} + \nabla_{\mathbf{y}^{\alpha}}\cdot\mathbf{j}^{\alpha} + h^{\alpha}, \tag{12.42}$$

where the material time-rate of A^{α} is defined as

$$\frac{\mathrm{d}A^{\alpha}}{\mathrm{d}t} \equiv \frac{\partial A^{\alpha}}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}}A^{\alpha} + \Delta\mathbf{v}^{\alpha}\cdot\nabla_{\mathbf{y}^{\alpha}}A^{\alpha}. \tag{12.43}$$

Similar to the situation in classical field theory, the balance of angular momentum leads to the symmetry of stress tensor $\mathbf{t}^{\alpha} + \boldsymbol{\tau}^{\alpha}$. It is seen that, from (12.32), (12.33), the symmetry of the stress tensor is automatically satisfied.

12.4 Discussions

If the point particle in micromorphic theory is reduced to a geometrical point, i.e., infinitesimal in size, then one can easily verify that $\mathbf{m} = \mathbf{l} = \boldsymbol{\upsilon} = \mathbf{i} = \boldsymbol{\varphi} = 0$, $\mathbf{t} = \mathbf{s} = \mathbf{t}^{T}$, and the balance laws of micromorphic theory become exactly the same as in classical continuum theory.

Each point particle in micromorphic theory has 12 degrees of freedom, i.e., 3 translational degrees of freedom for the centroid and 9 degrees of freedom for the micromotion, (12.5). In this sense, each unit cell in the multiscale concurrent atomistic/continuum theory has $3N_a$ degrees of freedom, where N_a is the number of atoms in a unit cell. The multiscale theory is a theory in physical space $(\mathbf{x}, t)$; (12.38), (12.39), (12.41) are the balance laws of mass, linear momentum, and energy for each and every atom in the unit cell; unlike classical continuum theories, the constitutive equations for the internal energy density $\rho^\alpha e^\alpha$, stress tensors $\mathbf{t}^\alpha$ and $\boldsymbol{\tau}^\alpha$, heat fluxes $\mathbf{q}^\alpha$ and $\mathbf{j}^\alpha$, (12.29), (12.32)–(12.35), for each and every atom are explicitly obtained; the only constitutive relation needed is the interatomic potential energy $U^{k\xi}$. In other words, although this theory that we derived is a field theory, we never lose the sight of atoms. This is the fundamental difference between this work and many other multiscale theories.

It is worthwhile to note that, from (12.29), the summation of internal energy density over all the atoms in a unit cell gives the internal energy per volume of a unit cell as

$$\begin{aligned}\sum_{\alpha=1}^{N_a} \rho^\alpha e^\alpha &= \sum_{k=1}^{N_l}\sum_{\alpha=1}^{N_a}\left[\frac{1}{2}m^\alpha\big(\widetilde{\mathbf{V}}^{k\alpha}\big)^2 + U^{k\alpha}\right]\delta\big(\mathbf{R}^k - \mathbf{x}\big)\\ &= \frac{3}{2}\frac{k_B}{V}T(\mathbf{x},t) + U_{\text{pot}}(\mathbf{x},t),\end{aligned} \tag{12.44}$$

where k_B is the Boltzmann constant; $T(\mathbf{x}, t)$ is the temperature; $U_{\text{pot}}(\mathbf{x}, t)$ is the potential energy density; and V is the volume of a unit cell. Then it is seen that the summation of (12.41) essentially emerges as the governing equation for temperature.

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