

Equivalent continuum for dynamically deforming atomistic particle systems

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ABSTRACT

An equivalent continuum is defined for dynamically deforming atomistic particle systems treated with concepts of molecular dynamics. The discrete particle systems considered exhibit micropolar interatomic interactions which involve both central interatomic forces and interatomic moments. The equivalence of the continuum to discrete atomic systems includes, firstly, preservation of linear and angular momenta, secondly, conservation of internal, external and inertial work rates and, thirdly, conservation of mass. This equivalence is achieved through the definition of, firstly, continuum stress and couple stress fields that make the same contribution to motion and deformation as internal interatomic forces and couples, secondly, continuum fields of body force, body moment, surface traction and surface moment that make the same contribution to motion and deformation as external forces and moments on the atoms, thirdly, a continuum deformation field that is work conjugate to the continuum kinetic fields and consistent with the atomic deformation field and, fourthly, continuum distributions of mass and moment of inertia that preserve the linear and angular momenta as well as kinetic energy. This equivalence holds for the entire system and for volume elements defined by any subset of particles in the system; therefore, averaging and characterization across different length scales are possible and size-scale effects can be explicitly analysed. The framework of analysis provides an explicit account of arbitrary atom arrangement, admitting applications to both crystalline and amorphous structures. The analysis also applies to both homogeneous materials with identical atoms and heterogeneous materials with dissimilar atoms. For non-polar atomic systems with only central interatomic forces, the fields of couple stress, body moment and surface moment vanish. This demonstrates that, on the interatomic level, interatomic moments give rise to couple stresses of dynamically equivalent nature.

§1. INTRODUCTION

Continuum theories and molecular dynamical (MD) theories of material behaviour are two distinct classes of descriptions, the first focusing on the structural response on different size scales and the latter emphasizing the structural reality of materials and fundamental mechanisms operative at atomic dimensions. Each has its own advantages and limitations. The continuum framework is more convenient for characterizations on higher length scales and the molecular framework is important to account for nanoscale mechanisms. Explicit MD descriptions are also required to

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interface with quantum-mechanical predictions of material behaviour and material properties. Reconciliation of the differences in the two descriptions and, more importantly, the integration of the two frameworks of analyses for cross-scale characterization are a great challenge in physics, material science and mechanics. Despite their different discrete and continuous perspectives, these atomistic and continuum theories are based on the same fundamental laws, including Newton's laws of motion and conservation of mass. Moreover, work rates are fundamental incremental quantities to be reconciled in both frameworks in order to assert balance of energy and to track dissipation. These fundamental laws provide a basis for interpretations of the results of one description in the context of the other.

The continuum interpretation of results of molecular theories is an important task in the scale-up of nanoscale characterizations of material behaviour. Issues involved include continuum stress interpretation of discrete atomic force fields on nanoscales, body and surface forces due to the effects of non-local interactions, and discreteness- and non-locality-induced length scales. Apparently, such effects must be captured and quantified when a transition is made from discrete molecular dynamics to continuum mechanics. The analysis of stress is important, as it measures the intensity and nature of internal interactions in materials. The most commonly used definition is the virial stress, which is an average measure describing the momentum flow through the surface of a spatial element over which averaging is carried out (Lutsko 1988). This stress includes both kinetic and potential energy contributions. Although, the virial thermodynamic approach (Clausius 1870) of calculating the stress tensor is widely used, it has shortcomings. It smears the effect of inhomogeneities due to volume averaging. For any given set of atoms, the definition requires the identification of an appropriate volume for averaging. In atomic ensembles with irregular atom arrangement, the identification of this volume can be ambiguous. Most importantly, a work-conjugate continuum deformation field is not available for the virial stress to allow regular continuum interpretation, analysis and scaling of MD results.

In this paper, an equivalent continuum is defined for dynamically deforming MD particle systems. Not only are work-conjugate continuum stress and deformation fields defined, but also specified are all other work- and momentum-preserving kinetic quantities and mass distribution for the equivalent continuum. The continuum is equivalent to its corresponding MD system in that, at all times, it preserves the linear and angular momenta of the particle system, it conserves the internal and external mechanical work rates and it has an equal amount of kinetic energy and contains the same amount of mass as the particle system. Hence, it is a dynamical representation of the MD system rather than a less strict lower-order thermodynamic representation. Construction of the continuum fields follows a process in reverse to finite-element discretization and weighted superposition. The momentum and work equivalence is achieved by virtue of the principle of virtual work for fully dynamic conditions. This equivalence holds for the entire system and, for volume elements defined by any subset of particles in the system, therefore, averaging and characterization across different length scales are possible and size-scale effects can be explicitly analysed.

Interatomic interactions occur in a variety of forms. Non-polar materials have interatomic interactions that involve linear central forces. These forces are derived from potentials that depend on interatomic distances between atoms. The Lennard-Jones potential accounts for simple pair interactions. For fcc metals, the embedded-

atom method accounting for multibody interactions has been developed and used (Daw and Baskes 1983). The modified embedded-atom method (MEAM) has also been developed to account for the angular dependence of interatomic central force interactions (Baskes 1987, Baskes *et al.* 1989). This kind of angular dependence has nothing to do with the rotational degree of freedom for individual atoms but rather reflects ordered lattice interactions within a potential with limited cut-off radius. An extensive review of potentials describing many-body interactions has been given by Carlsson (1990). As distinguished from pure central force systems, micropolar (on an atomic scale, perhaps ‘nanopolar’ would be more accurate) materials exhibit both interatomic moment interactions and central force interactions (Evans and Murad 1977, 1989). Such situations may arise, for example, in united atom approaches (Ogilvie 1988, Nath *et al.* 2001) in which molecules consisting of multiple atoms are treated as single particles that interact through central forces and moments. Interparticle moments are also manifested on polarized atomic particles in electric fields. A discussion on interatomic moments can be found in the book by Allen and Tildesley (1992). The central forces in these materials depend on interatomic distances. The moments, however, depend on interatomic distances as well as angular positions of the particles. Although the development of atomic potentials is a challenging task and is still in an early stage, the need for more accurate characterizations of atomistic behaviour and the advances in first-principles calculations can be expected to bring about realistic potentials accounting for both central force and moment interactions in the future.

A general framework of analysis is used here, accounting for both central force and moment interactions between atomic particles. The particles can be regarded as representing either individual atoms or collections of atoms, depending on the context. The results are readily specialized to the case of non-polar materials by setting the interatomic moments to zero. A separate account of the non-polar case can also be found in the paper by Zhou (2001). The framework of analysis provides an explicit account of arbitrary atom arrangement, facilitating applications to either crystalline or amorphous structures. The analysis also applies to both homogeneous materials with identical atoms and heterogeneous materials with dissimilar atoms.

§2. EQUIVALENT CONTINUUM

2.1. Continuum–particle system equivalence

Consider a dynamically deforming system of N particles which occupies space V and has an envelope of surface S as illustrated in figure 1. At time t , particle i has position \mathbf{r}_i , displacement \mathbf{u}_i and velocity $\dot{\mathbf{r}}_i = \dot{\mathbf{u}}_i = d\mathbf{u}_i/dt$. The corresponding angular displacement from a reference state is θ_i and angular velocity is $\dot{\theta}_i$. The additional degrees θ_i of freedom facilitate treatment of interparticle moment interactions. When the atomic interaction can be described by a potential, the energy of the atomic ensemble is

$$E = \Phi(r_{ij}, \theta_{ij}) \quad (1)$$

where $r_{ij} = |\mathbf{r}_{ij}| = |\mathbf{r}_j - \mathbf{r}_i|$ is the central distance between particle i and particle j and $\theta_{ij} = \theta_j - \theta_i$ is the corresponding difference in angular displacements. Equation (1) is a general form and fully admits many-body interactions in addition to pairwise interactions. Interparticle force and moment applied on particle i by particle j are

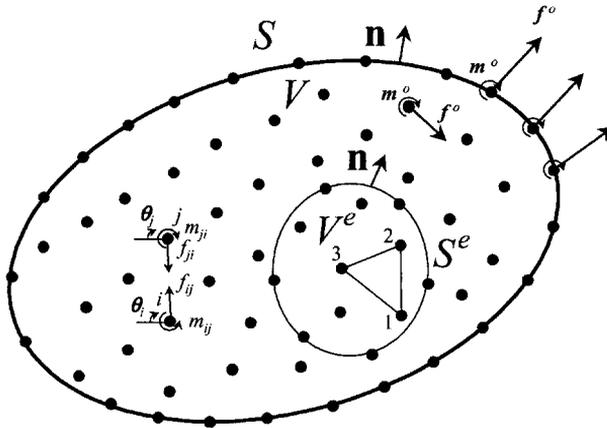


Figure 1. Particle system and equivalent continuum.

\mathbf{f}_{ij} and \mathbf{m}_{ij} respectively. Note that Newton’s third law requires that $\mathbf{f}_{ij} = -\mathbf{f}_{ji}$ and $\mathbf{m}_{ij} = -\mathbf{m}_{ji}$. Obviously,

$$\begin{aligned} \mathbf{f}_{ij} &= \frac{1}{2} \frac{\partial \Phi(r_{ij}, \theta_{ij})}{\partial r_{ij}} \frac{\mathbf{r}_{ij}}{r_{ij}}, \\ \mathbf{m}_{ij} &= \frac{1}{2} \frac{\partial \Phi(r_{ij}, \theta_{ij})}{\partial \theta_{ij}}. \end{aligned} \tag{2}$$

The force and moment on particle i due to atoms or agents that are *external* to the system under consideration are \mathbf{f}_i^0 and \mathbf{m}_i^0 respectively. The total force and moment respectively on i are

$$\begin{aligned} \mathbf{f}_i &= \sum_j \mathbf{f}_{ij} + \mathbf{f}_i^0 = \mathbf{f}_i^{\text{int}} + \mathbf{f}_i^{\text{ext}}, \\ \mathbf{m}_i &= \sum_j \mathbf{m}_{ij} + \mathbf{m}_i^0 = \mathbf{m}_i^{\text{int}} + \mathbf{m}_i^{\text{ext}}. \end{aligned} \tag{3}$$

Here, the summation is over those particles inside the system of N being considered that interact directly with particle i . It is worthwhile to point out that, owing to non-local interactions, the external force \mathbf{f}_i^0 and external moment \mathbf{m}_i^0 can exist for particles both in the interior of V and on the surface S . Note that the concepts of internal and external forces are specific to the particular subvolume V^e of V considered. So, in general, $\mathbf{f}_i^{\text{int}} \neq \sum_j \mathbf{f}_{ij}$, $\mathbf{m}_i^{\text{int}} \neq \sum_j \mathbf{m}_{ij}$, $\mathbf{f}_i^{\text{ext}} \neq \mathbf{f}_i^0$, and $\mathbf{m}_i^{\text{ext}} \neq \mathbf{m}_i^0$, except for $V^e = V$.

The continuum equivalent to the particle ensemble has volume V and surface S . A material point in the continuum initially at \mathbf{X} has position \mathbf{x} (or \mathbf{r}) in the current configuration, so that the displacement and velocity functions are $\mathbf{u} = \mathbf{x} - \mathbf{X}$ and $\dot{\mathbf{x}} = \dot{\mathbf{u}}$ respectively. The stress tensor $\boldsymbol{\sigma}$ is related to the surface traction \mathbf{t} through $\mathbf{t} = \mathbf{n} \cdot \boldsymbol{\sigma}$, and the couple stress $\boldsymbol{\mu}$ is related to the surface moment \mathbf{m}^S through $\mathbf{m}^S = \mathbf{n} \cdot \boldsymbol{\mu}$, where \mathbf{n} is the outward unit normal to any internal surface S^e or surface envelope of the body S . Body forces and body moments can result from non-local effects of atoms or agents external to the system under consideration. Let \mathbf{b} and \mathbf{m}^b denote the densities of the continuum body forces and body moments respectively in

V . In the following analyses, all kinetic and kinematic quantities are evaluated on the current deformed configuration. In general, however, $\boldsymbol{\mu} \neq \boldsymbol{\mu}^T$ and $\boldsymbol{\sigma} \neq \boldsymbol{\sigma}^T$ when $\boldsymbol{\mu} \neq \mathbf{0}$. Also, the continuum has mass density $\rho(\mathbf{x})$ and moment of inertia density $\mathbf{I}(\mathbf{x})$ (mass and moment of inertia per unit volume) in the current configuration. The continuum that we seek to occupy V should be dynamically equivalent to the particle system. This requires that, at all times,

- (i) the stress and couple stress fields over the continuum defined by a discrete particle aggregate have the same work rate as the *internal* interatomic force fields,
- (ii) the body force, body moment, surface traction and surface moment fields produce the same external work rate as that of the external interatomic force fields and
- (iii) the kinetic energy of the continuum be the same as that of the discrete atomic ensemble.

Requirement (i) ensures that the contribution of the continuum stress and couple stress fields to the motion and deformation of continuum (or the particle system) is the same as that of the original interparticle force field. Requirement (ii) ensures that the continuum external force and moment fields provide the same input to the motion and deformation of the continuum (or the particle system) as the discrete particle forces due to external atoms and agents. Requirement (iii) ensures that the contributions of material inertia to motion and deformation are the same for the equivalent continuum and the particle system. These separate requirements for the internal and external work rates and kinetic energy can be satisfied through the dynamic principle of virtual work, allowing definition of work-preserving fields of continuum stress $\boldsymbol{\sigma}$ and couple stress $\boldsymbol{\mu}$, work-preserving continuum traction \mathbf{t} , surface moment \mathbf{m}^S , body force \mathbf{b} and body moment \mathbf{m}^b , and continuum mass density $\rho(\mathbf{x})$ and moment of inertia density $\mathbf{I}(\mathbf{x})$.

For the entire ensemble with N particles, the above requirements can be written in terms of the dynamic principle of virtual work, that is

$$\begin{aligned}
 & - \int_V \boldsymbol{\sigma} : \delta \mathbf{D} dV - \int_V \boldsymbol{\mu} : \delta \mathbf{w} dV + \int_V \mathbf{b} \cdot \delta \dot{\mathbf{u}} dV + \int_V \mathbf{m}^b \cdot \delta \omega dV + \int_S \mathbf{t} \cdot \delta \dot{\mathbf{u}} dS \\
 & \quad + \int_S \mathbf{m}^S \cdot \delta \omega dS \\
 & = \sum_{i=1}^N \mathbf{f}_i \cdot \delta \dot{\mathbf{r}}_i + \sum_{i=1}^N \mathbf{m}_i \cdot \delta \dot{\boldsymbol{\theta}}_i \\
 & = \int_V \rho \dot{\mathbf{u}} \cdot \delta \dot{\mathbf{u}} dV + \int_V (\mathbf{I} \cdot \ddot{\boldsymbol{\theta}}) \cdot \delta \dot{\boldsymbol{\theta}} dV \\
 & = \sum_{i=1}^N m_i \ddot{\mathbf{r}}_i \cdot \delta \dot{\mathbf{r}}_i + \sum_{i=1}^N (\mathbf{I}_i \cdot \ddot{\boldsymbol{\theta}}_i) \cdot \delta \dot{\boldsymbol{\theta}}_i, \tag{4}
 \end{aligned}$$

where the symbol δ in $\delta \mathbf{D}$, $\delta \mathbf{w}$, $\delta \dot{\mathbf{u}}$, $\delta \dot{\boldsymbol{\theta}}$, $\delta \omega$, $\delta \dot{\mathbf{r}}_i$ and $\delta \dot{\boldsymbol{\theta}}_i$ denotes any kinematically admissible functional representations of the corresponding quantities. Superimposed double dots represent second-order material time derivative, that is $\ddot{\mathbf{u}} = d^2 \mathbf{u} / dt^2$; \mathbf{D} is the symmetric continuum rate of deformation, $\boldsymbol{\sigma} : \delta \mathbf{D} = \sigma_{\alpha\beta} \delta D_{\beta\alpha} = \text{sym } \boldsymbol{\sigma} : \delta \mathbf{D}$, with $\text{sym } \boldsymbol{\sigma} = (\boldsymbol{\sigma} + \boldsymbol{\sigma}^T) / 2$ being the symmetric part

of $\boldsymbol{\sigma}$, $\mathbf{b} \cdot \delta \dot{\mathbf{u}} = b_\alpha \delta \dot{u}_\alpha$ ($\alpha, \beta = 1, 2, 3$; summation over repeated indices α and β is implied); \mathbf{w} is the spatial gradient of the angular velocity $\boldsymbol{\omega}$ of the continuum rotation field, that is $\mathbf{w} = \partial \boldsymbol{\omega} / \partial \mathbf{x}$. Note that

$$\boldsymbol{\omega} = \text{dual } \mathbf{W} + \dot{\boldsymbol{\theta}}, \tag{5}$$

with the first part due to the vorticity or spin of the particle velocity field and the second part due to the self-spin of the atoms. \mathbf{W} is the spin tensor or the skew-symmetric part of the spatial gradient of velocity $\partial \dot{\mathbf{u}} / \partial \mathbf{x}$, dual \mathbf{W} denotes the dual vector of \mathbf{W} , and $\dot{\boldsymbol{\theta}}(\mathbf{x})$ is a continuum interpretation (through interpolation) of the self-spin rate $\dot{\boldsymbol{\theta}}_i$ of the atoms. More details on this quantity will be given later. Also, in the above equation, m_i is the mass and \mathbf{l}_i is the moment of inertia of particle i . If the mass distribution of i is spherically symmetric around its centre \mathbf{r}_i , \mathbf{l}_i is isotropic, that is $\mathbf{l}_i = l_i \mathbf{I}$, where \mathbf{I} is the second-order identity tensor. Here, the need to use the rate $\delta \mathbf{D}$ of deformation or the symmetric part of the spatial gradient of virtual velocity $\partial(\delta \dot{\mathbf{u}}) / \partial \mathbf{x}$ without its skew-symmetric part $\delta \mathbf{W}$ to evaluate the virtual work rate results from the coupling between the stress and couple stress (Malvern 1969). The relevance of the skew-symmetric part of $\boldsymbol{\sigma}$, or skew $\boldsymbol{\sigma} = (\boldsymbol{\sigma} - \boldsymbol{\sigma}^T) / 2$, will be discussed later.

To develop a scalable representation of the equivalent continuum, consider a volume element V^e with closed surface S^e associated with a subset of M ($\leq N$) particles in the ensemble. Assume that M_S out of the M particles ($M_S \leq M$) are on surface S^e , therefore defining it. The remaining $M - M_S$ particles are in the interior of V^e and are considered as internal particles for V^e . To define the momentum- and work-conserving stress $\boldsymbol{\sigma}^{(e)}$, couple stress $\boldsymbol{\mu}^{(e)}$, surface traction $\mathbf{t}^{(e)}$, surface moment $\mathbf{m}^{S(e)}$, body force $\mathbf{b}^{(e)}$, body moment $\mathbf{m}^{b(e)}$, mass density $\rho^{(e)}(\mathbf{x})$ and moment of inertia density $\mathbf{l}^{(e)}(\mathbf{x})$ over V^e , the variational principle of (4) is applied to this portion of the system, yielding

$$\begin{aligned} & - \int_{V^e} \boldsymbol{\sigma}^{(e)} : \delta \mathbf{D}^{(e)} dV - \int_{V^e} \boldsymbol{\mu}^{(e)} : \delta \mathbf{w}^{(e)} dV + \int_{V^e} \mathbf{b}^{(e)} \cdot \delta \dot{\mathbf{u}}^{(e)} dV + \int_{V^e} \mathbf{m}^{b(e)} \cdot \delta \boldsymbol{\omega}^{(e)} dV \\ & \quad + \int_{S^e} \mathbf{t}^{(e)} \cdot \delta \dot{\mathbf{u}}^{(e)} dS + \int_{S^e} \mathbf{m}^{S(e)} \cdot \delta \boldsymbol{\omega}^{(e)} dS \\ & = \sum_{I=1}^M \mathbf{f}_I^{\text{int}} \cdot \delta \dot{\mathbf{u}}_I + \sum_{I=1}^M \mathbf{f}_I^{\text{ext}} \cdot \delta \dot{\mathbf{u}}_I + \sum_{I=1}^M \mathbf{m}_I^{\text{int}} \cdot \delta \dot{\boldsymbol{\theta}}_I + \sum_{I=1}^M \mathbf{m}_I^{\text{ext}} \cdot \delta \dot{\boldsymbol{\theta}}_I \\ & = \int_{V^e} \rho^{(e)} \dot{\mathbf{u}}^{(e)} \cdot \delta \dot{\mathbf{u}}^{(e)} dV + \int_{V^e} \mathbf{l}^{(e)} \cdot \ddot{\boldsymbol{\theta}}^{(e)} \cdot \delta \dot{\boldsymbol{\theta}}^{(e)} dV \\ & = \sum_{I=1}^M \varsigma_I m_I \ddot{\mathbf{r}}_I \cdot \delta \dot{\mathbf{r}}_I + \sum_{I=1}^M \varsigma_I \mathbf{l}_I \cdot \ddot{\boldsymbol{\theta}}_I \cdot \delta \dot{\boldsymbol{\theta}}_I. \end{aligned} \tag{6}$$

Here, the subscript I denotes particle index *internal* to the volume element V^e ($1 \leq I \leq M$). Each atom inside V^e is given two indices, one is the local index I ($1 \leq I \leq M$) and the other is its global index i ($1 \leq i \leq N$) as the atom is also part of the complete system V . Since a unique correspondence between I and its global counterpart i can be established, we use them interchangeably here for convenience of discussion. Under this notation, ‘ $j \neq I$ ’ and ‘ $j = I$ ’ should be interpreted, as ‘ $j \neq i$ ’ and ‘ $j = i$ ’ respectively. For example, ‘ $j = I$ ’ should be read as ‘the particle with

global index j and the particle with local index I (and therefore global index i) are the same particle'.

This notation is used here to delineate the total force $\mathbf{f}_I^{\text{int}}$ and total moment $\mathbf{m}_I^{\text{int}}$ on atom I in V^e exerted by other atoms *also inside* V^e (either in the interior of V^e or on the surface S^e) and the force $\mathbf{f}_I^{\text{ext}}$ and moment $\mathbf{m}_I^{\text{ext}}$ that are exerted by atoms or agents *outside* V^e . A distinction must be made between these internal and external interactions. Note that the total force and moment on I are $\mathbf{f}_I = \mathbf{f}_I^{\text{int}} + \mathbf{f}_I^{\text{ext}}$ and $\mathbf{m}_I = \mathbf{m}_I^{\text{int}} + \mathbf{m}_I^{\text{ext}}$ respectively, and

$$\begin{aligned}
 \mathbf{f}_I^{\text{int}} &= \sum_{J \neq I}^M \eta_{IJ} \mathbf{f}_{IJ}, \\
 \mathbf{f}_I^{\text{ext}} &= \sum_{j, (J \neq 1, 2, \dots, M)}^N \mathbf{f}_{Ij} + \mathbf{f}_I^0, \\
 \mathbf{m}_I^{\text{int}} &= \sum_{J \neq I}^M \eta_{IJ} \mathbf{m}_{IJ}, \\
 \mathbf{m}_I^{\text{ext}} &= \sum_{j, (J \neq 1, 2, \dots, M)}^N \mathbf{m}_{Ij} + \mathbf{m}_I^0.
 \end{aligned}
 \tag{7}$$

Here, η_{IJ} is the fraction of the atomic bond that is spatially within element V^e . It pertains to the bond between atoms I and J that are both inside V^e . In general, when atoms are randomly distributed, η_{IJ} is determined by the dihedral angle of the element as a fraction of the sum of such angles (360° or less) of all elements associated with the particular bond. Consider, for example, the bcc lattice in figure 2. The bond between atoms 1 and 3 is shared by four tetrahedral cells (each of the four tetrahedral cells is considered a volume element V^e with $M = 4$). Therefore, for the tetrahedral element defined by atoms 1, 2, 3 and 4 (and for each of the other three cells) $\eta = 90^\circ/360^\circ = 0.25$ for this bond. For bonds on surface S^e (both atoms of the bond are on S^e), the sum of such angles is less than 360° . ς_I in equation (6) is the fraction of atom I that is attributed to element V^e . For example, atom 1 in figure 2 is shared by 24 tetrahedral elements; therefore, $\varsigma = 1/24$ for each element.

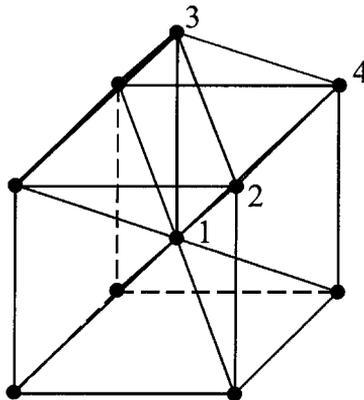


Figure 2. Atomic bonds shared by neighbouring cells.

The continuum quantities $\boldsymbol{\sigma}^{(e)}$, $\boldsymbol{\mu}^{(e)}$, $\mathbf{t}^{(e)}$, $\mathbf{m}^{S^{(e)}}$, $\mathbf{b}^{(e)}$, $\mathbf{m}^{b^{(e)}}$, $\dot{\mathbf{u}}^{(e)}$, $\mathbf{D}^{(e)}$, $\boldsymbol{\omega}^{(e)}$, $\mathbf{w}^{(e)}$, $\dot{\boldsymbol{\theta}}^{(e)}$, $\ddot{\boldsymbol{\theta}}^{(e)}$, $\rho^{(e)}$ and $\mathbf{l}^{(e)}$ in equation (4) are associated with element V^e . It is important to point out that non-local effects, multiple interactions, and the need to maintain momentum and work equivalence, in general, will cause different volume elements V^e to overlap partly. This issue necessitates proper superposition of these elemental quantities to obtain the total fields for $\boldsymbol{\sigma}$, $\boldsymbol{\mu}$, \mathbf{t} , \mathbf{m}^S , \mathbf{b} , \mathbf{m}^b , $\dot{\mathbf{u}}$, \mathbf{D} , $\boldsymbol{\omega}$, \mathbf{w} , $\dot{\boldsymbol{\theta}}$, $\ddot{\boldsymbol{\theta}}$, ρ and \mathbf{l} . More details will be given in §§2.2–2.4. In the limit that V^e is taken to be V , the global fields are obtained directly and no superposition is needed. The use of $V^e < V$ has two clear benefits. One is that it allows size effects to be analysed. The other is that the analysis with a smaller V^e is more computationally efficient, and simpler shape functions can be used.

With the above notation, the requirements that the virtual work rates of internal, external and inertial forces and moments are equal can then be written as

$$\begin{aligned}
 - \int_{V^e} \boldsymbol{\sigma}^{(e)} : \delta \mathbf{D}^{(e)} dV - \int_{V^e} \boldsymbol{\mu}^{(e)} : \delta \mathbf{w}^{(e)} dV &= \sum_{I=1}^M \mathbf{f}_I^{\text{int}} \cdot \delta \dot{\mathbf{u}}_I + \sum_{I=1}^M \mathbf{m}_I^{\text{int}} \cdot \delta \dot{\boldsymbol{\theta}}_I, \\
 \int_{S^e} \mathbf{t}^{(e)} \cdot \delta \dot{\mathbf{u}}^{(e)} dS + \int_{S^e} \mathbf{m}^{S^{(e)}} \cdot \delta \boldsymbol{\omega}^{(e)} dS &= \sum_{I=1}^{M_S} (1 - \kappa_I) \mathbf{f}_I^{\text{ext}} \cdot \delta \dot{\mathbf{u}}_I + \sum_{I=1}^{M_S} (1 - \kappa_I) \mathbf{m}_I^{\text{ext}} \cdot \delta \dot{\boldsymbol{\theta}}_I, \\
 \int_{V^e} \mathbf{b}^{(e)} \cdot \delta \dot{\mathbf{u}}^{(e)} dV + \int_{V^e} \mathbf{m}^{b^{(e)}} \cdot \delta \boldsymbol{\omega}^{(e)} dV &= \sum_{I=1}^M \kappa_I \mathbf{f}_I^{\text{ext}} \cdot \delta \dot{\mathbf{u}}_I + \sum_{I=1}^M \kappa_I \mathbf{m}_I^{\text{ext}} \cdot \delta \dot{\boldsymbol{\theta}}_I, \\
 \int_{V^e} \rho^{(e)} \dot{\mathbf{u}}^{(e)} \cdot \delta \dot{\mathbf{u}}^{(e)} dV + \int_{V^e} \left(\mathbf{l}^{(e)} \cdot \ddot{\boldsymbol{\theta}}^{(e)} \right) \cdot \delta \dot{\boldsymbol{\theta}}^{(e)} dV &= \sum_{I=1}^M \varsigma_I m_I \dot{\mathbf{r}}_I \cdot \delta \dot{\mathbf{r}}_I + \sum_{I=1}^M \varsigma_I (\mathbf{l}_I \cdot \ddot{\boldsymbol{\theta}}_I) \cdot \delta \dot{\boldsymbol{\theta}}_I.
 \end{aligned} \tag{8}$$

The second relation concerns the surface traction and surface moment. The corresponding summation is over only the M_S particles on surface S^e . The third relation concerns the body force and body moment due to external forces and moments. External forces on atoms in *the interior* of V^e contribute only to the body force density $\mathbf{b}^{(e)}$; therefore, the factor κ_I is always taken as unity ($\kappa_I = 1$) for atoms in the interior of V^e . The external forces exerted on atoms on surface S^e are considered to contribute solely to the surface traction $\mathbf{t}^{(e)}$; therefore, $\kappa_I = 0$ for atoms on S^e . This partition is somewhat arbitrary and, indeed, any choice $0 \leq \kappa_I \leq 1$ for surface atoms (together with $\kappa_I = 1$ for interior atoms) will allow external work rate to be preserved. However, the choice of $\kappa_I = 0$ for surface atoms (together with $\kappa_I = 1$ for interior atoms) has the clear advantage of yielding zero body force density and zero body moment density as non-local external forces become zero. This outcome is consistent with local continuum theories.

The above delineation of external forces and moments is related to non-local interatomic interactions and is important for the definition of $\boldsymbol{\sigma}^{(e)}$, $\boldsymbol{\mu}^{(e)}$, $\mathbf{b}^{(e)}$, $\mathbf{m}^{b^{(e)}}$, $\mathbf{t}^{(e)}$ and $\mathbf{m}^{S^{(e)}}$. It allows the length scale dependence of nanoscale atomic behaviour due to non-local interatomic interactions to be quantified as the size of V^e (and therefore the number M of atoms contained) is increased or decreased.

2.2. Stress and couple stress fields

We first focus the discussion on the internal work rate and the first relation of equation (8) for stress and couple stress. To evaluate the continuum version of the

virtual work, an interpolation for the virtual velocity and virtual angular velocity associated with the self-spin of atoms in V^e is needed. Many possible methods for the interpolation are available. One utilizes the shape functions of finite elements, that is

$$\begin{aligned} \delta \dot{\mathbf{u}}^{(e)}(\mathbf{x}) &= \sum_{I=1}^M N_I(\mathbf{x}) \delta \dot{\mathbf{u}}_I, \\ \delta \dot{\boldsymbol{\theta}}^{(e)}(\mathbf{x}) &= \sum_{I=1}^M N_I(\mathbf{x}) \delta \dot{\boldsymbol{\theta}}_I, \end{aligned} \tag{9}$$

where $N_I(\mathbf{x})$ are the shape functions and should be interpreted as $N_I^{(e)}(\mathbf{x})$. The superscript (e) is omitted for brevity. Details regarding these shape functions can be found in finite-element method texts. The corresponding virtual velocity gradient and virtual angular velocity gradient contributions respectively associated with the self-spin of atoms are

$$\begin{aligned} \frac{\partial \delta(\dot{\mathbf{u}}^{(e)})}{\partial \mathbf{x}} &= \sum_{I=1}^M \delta \dot{\mathbf{u}}_I \otimes \frac{\partial N_I}{\partial \mathbf{x}} = \sum_{I=1}^M \delta \dot{\mathbf{u}}_I \otimes \mathbf{B}_I, \\ \frac{\partial (\delta \dot{\boldsymbol{\theta}}^{(e)})}{\partial \mathbf{x}} &= \sum_{I=1}^M \delta \dot{\boldsymbol{\theta}}_I \otimes \frac{\partial N_I}{\partial \mathbf{x}} = \sum_{I=1}^M \delta \dot{\boldsymbol{\theta}}_I \otimes \mathbf{B}_I. \end{aligned} \tag{10}$$

Here, $\mathbf{B}_I = \partial N_I(\mathbf{x})/\partial \mathbf{x}$ are gradients of the shape functions and \otimes denotes the tensor product of two vectors. The virtual rate of deformation and spin tensor respectively associated with the particle velocity field are

$$\begin{aligned} \delta \mathbf{D}^{(e)} &= \frac{1}{2} \left[\frac{\partial (\delta \dot{\mathbf{u}}^{(e)})}{\partial \mathbf{x}} + \left(\frac{\partial (\delta \dot{\mathbf{u}}^{(e)})}{\partial \mathbf{x}} \right)^T \right] = \frac{1}{2} \sum_{I=1}^M (\delta \dot{\mathbf{u}}_I \otimes \mathbf{B}_I + \mathbf{B}_I \otimes \delta \dot{\mathbf{u}}_I), \\ \delta \mathbf{W}^{(e)} &= \frac{1}{2} \left[\frac{\partial (\delta \dot{\mathbf{u}}^{(e)})}{\partial \mathbf{x}} - \left(\frac{\partial (\delta \dot{\mathbf{u}}^{(e)})}{\partial \mathbf{x}} \right)^T \right] = \frac{1}{2} \sum_{I=1}^M (\delta \dot{\mathbf{u}}_I \otimes \mathbf{B}_I - \mathbf{B}_I \otimes \delta \dot{\mathbf{u}}_I). \end{aligned} \tag{11}$$

The virtual work rate of the stress tensor with respect to the virtual rate of deformation is given by

$$\begin{aligned} \int_{V^e} \boldsymbol{\sigma}^{(e)} : \delta \mathbf{D}^{(e)} \, dV &= \int_{V^e} \frac{1}{2} (\boldsymbol{\sigma}^{(e)T} + \boldsymbol{\sigma}^{(e)}) : \sum_{I=1}^M (\mathbf{B}_I \otimes \delta \dot{\mathbf{u}}_I) \, dV \\ &= \sum_{I=1}^M \int_{V^e} (\text{sym } \boldsymbol{\sigma}^{(e)} \cdot \mathbf{B}_I) \cdot \delta \dot{\mathbf{u}}_I \, dV. \end{aligned} \tag{12}$$

In order to calculate the virtual work rate of the couple stress $\boldsymbol{\mu}^{(e)} : \delta \mathbf{w}^{(e)}$, note that $\delta \mathbf{w} = \partial(\delta \boldsymbol{\omega})/\partial \mathbf{x} = \partial[\text{dual } \delta \mathbf{W} + \delta \dot{\boldsymbol{\theta}}(\mathbf{x})]/\partial \mathbf{x}$, with the first part arising from the rotation of the particle velocity field and the second part due to the self-spin of the atoms. In component form,

$$\begin{aligned}
 \delta w_{\alpha\lambda}^{(e)} &= \left(\frac{\partial \delta \boldsymbol{\omega}^{(e)}}{\partial \mathbf{x}} \right)_{\alpha\lambda} \\
 &= \frac{1}{2} \varepsilon_{\alpha\beta\gamma} \delta W_{\gamma\beta,\lambda}^{(e)} + \left(\frac{\partial (\delta \dot{\boldsymbol{\theta}}^{(e)})}{\partial \mathbf{x}} \right)_{\alpha\lambda} \\
 &= \frac{1}{2} \sum_{I=1}^M \frac{1}{2} \varepsilon_{\alpha\beta\gamma} (\delta u_{\gamma}^I B_{\beta,\lambda}^I - \delta u_{\beta}^I B_{\gamma,\lambda}^I) + \left(\sum_{I=1}^M \delta \dot{\boldsymbol{\theta}}_I \otimes \mathbf{B}_I \right)_{\alpha\lambda} \\
 &= \frac{1}{2} \sum_{I=1}^M \varepsilon_{\alpha\beta\gamma} \delta u_{\gamma}^I B_{\beta,\lambda}^I + \sum_{I=1}^M \delta \dot{\theta}_{\alpha}^I B_{\lambda}^I = \sum_{I=1}^M H_{\alpha\lambda\gamma}^I \delta u_{\gamma}^I + \delta \dot{\theta}_{\alpha}^I B_{\lambda}^I, \tag{13}
 \end{aligned}$$

where the Greek subscripts range from 1 to 3, denoting components associated with the three Cartesian coordinates. Summation is implied on repeated Greek indices. The subscript following a comma denotes partial differentiation with respect to the corresponding spatial coordinate, that is $\delta W_{\gamma\beta,\lambda}^{(e)} = \partial (\delta W_{\gamma\beta}^{(e)}) / \partial x_{\lambda}$. Although it has so far been and will continue to be written as a subscript, the index I is interchangeably written as a superscript in a few terms in the above equation. This temporary interchange in index positions is used to avoid confusion, without altering its meaning. The virtual work rate of the couple stress is

$$\boldsymbol{\mu}^{(e)} : \delta \mathbf{w}^{(e)} = \mu_{\lambda\alpha}^{(e)} \delta w_{\alpha\lambda}^{(e)} = \left(\boldsymbol{\mu}^{(e)} : \mathbf{H}_I \right) \cdot \delta \dot{\mathbf{u}}_I + \left(\boldsymbol{\mu}^{(e)\text{T}} \cdot \mathbf{B}_I \right) \cdot \delta \dot{\boldsymbol{\theta}}_I, \tag{14}$$

where \mathbf{H}_I ($I = 1, 2, \dots, M$) are third-order tensors which involve a second-order spatial differentiation. They measure the rotation effects of shape functions. The components of \mathbf{H}_I are $H_{\alpha\lambda\gamma}^I = \varepsilon_{\alpha\beta\gamma} B_{\beta,\lambda}^I$, with $\varepsilon_{\alpha\beta\gamma}$ being the permutation symbol.

Since $\delta \dot{\boldsymbol{\theta}}_I$ and $\delta \dot{\mathbf{u}}_I$ are completely arbitrary and independent degrees of freedom, the first relations of equations (8), equation (12) and equation (14) lead to

$$\begin{aligned}
 \int_{V^e} \left(\text{sym } \boldsymbol{\sigma}^{(e)} \cdot \mathbf{B}_I \right) dV + \int_{V^e} \left(\boldsymbol{\mu}^{(e)} : \mathbf{H}_I \right) dV &= -\mathbf{f}_I^{\text{int}}, \\
 \int_{V^e} \left(\boldsymbol{\mu}^{(e)\text{T}} \cdot \mathbf{B}_I \right) dV &= -\mathbf{m}_I^{\text{int}}.
 \end{aligned} \tag{15}$$

Since $\mathbf{f}_I^{\text{int}}$ and $\mathbf{m}_I^{\text{int}}$ are internal forces, Newton’s third law implies that

$$\sum_{I=1}^M \mathbf{f}_I^{\text{int}} = \mathbf{0}, \quad \sum_{I=1}^M \mathbf{r}_I \times \mathbf{f}_I^{\text{int}} = \mathbf{0}, \quad \sum_{I=1}^M \mathbf{m}_I^{\text{int}} = \mathbf{0}. \tag{16}$$

Note that one of the basic requirements for shape functions is $\sum_{I=1}^M N_I = 1$; therefore, $\sum_{I=1}^M \mathbf{B}_I = \mathbf{0}$ and $\sum_{I=1}^M \mathbf{H}_I = \mathbf{0}$. In general, for an element V^e with M atoms, equations (15) and (16) yield $6M - 9$ independent equations. Since the number of independent components in $\text{sym } \boldsymbol{\sigma}^{(e)}$ is six and the number of independent components in $\boldsymbol{\mu}$ is nine, the problem of finding the *constant average* $\text{sym } \boldsymbol{\sigma}^{(e)}$ and $\boldsymbol{\mu}^{(e)}$ is overspecified for any choice of M greater than four. Consequently, it is impossible to find the *average* work-equivalent stress and couple stress over the volume associated with an arbitrary subset of the particle ensemble. Although it may be desirable to do so, such a task is not possible because of the disparate number of degrees of freedom (DOFs) for the discrete particle subset and the fixed dimensional order of the stress and couple stress tensors. Parity in the DOFs and the order of the stress tensor

occurs (15 equations and 15 unknown stress and couple stress components) only for the simplest three-dimensional (3D) cell, the tetrahedron which is associated with four particles. In two dimensions, triangles associated with three atoms are the only possible choice (seven equations and seven independent unknown stress and couple stress components). This particular level of continuum characterization is very useful because it fully recognizes the effects of heterogeneities and steep gradients at the scale of individual atoms. This process of establishing dynamical equivalence between the continuum and MD formulations, although performed on interatomic scales, is also very important because it yields the lowest-scale continuum fields that may be subsequently subjected to various treatments of continuum averaging, including those of statistical mechanics.

It is important to point out that, for $M > 4$ in three dimensions and $M > 3$ in two dimensions, equation (15) requires, in general, spatially varying stress and couple stress fields for which quadratic or higher-order shape functions should be used in equation (9). The determination of $\sigma^{(e)}$ and $\mu^{(e)}$ for V^e with such higher numbers M of atoms necessitates proper choice of integration points in V^e for appropriate numbers of unknowns. Although somewhat more computationally involved, such a pursuit would be quite useful and important since it permits scaling and allows size effects to be quantified through the variation of the size of V^e .

Note that for central force systems, $\mathbf{m}_I^{\text{int}} = \mathbf{0}$, therefore, the second relation of equations (15) becomes a system of homogeneous equations, yielding $\mu^{(e)} = \mathbf{0}$. Under such conditions, $\sigma^{(e)} = \sigma^{(e)\text{T}}$ and the more commonly used non-polar stress theory is recovered. This result demonstrates that, at the atomic level, couple stress is the manifestation of interatomic moment interaction. The atomistic origin of couple stress requires the existence of interatomic couples. A material with interatomic couples should be considered as intrinsically endowed with couple stress on all length scales at or above interatomic levels. It is worthwhile to point out that the introduction of couple stress based on higher length scale considerations, such as the example by Kröner (1963) of spatially uniform arrays of edge dislocations of like sign, is a result of interactions of heterogeneities as depends on their mesoscopic arrangement. The length scale associated with these couples is associated with the dislocation spacing in Kröner's example. The couple stresses are determined from higher-order moments of the surface traction acting on periodic unit cells representing a uniform array of dislocations. Of course the scale over which such couple stresses are generated is relatively large compared with the interatomic spacing, in general, and they arise in Kröner's setting independent of considerations of interatomic moments. They can exist even for materials that are non-polar on the interatomic scale. It is worthwhile to point out that the introduction of couple stress based on such higher-length-scale considerations represents averaging and reinterpretation of non-polar stress fields. Such averaging is conducted over finite volumes whose size scales arise from considerations unrelated to the atomistic origin of the couple stress. Although useful above their respective length scales where the primal effects of couple stress are realized, such theories invariably do not consider the question of whether the atomistic force field of a material induces *distributed* moments. Clearly, for non-polar materials, the use of such theories is not supported by the atomistic work equivalence consideration here. Rather, they should be considered as higher-scale theories motivated by independent scaling considerations. The interpretation of their results should be maintained on or above the size scale over which average moments are evaluated.

So far, only the symmetric part of $\sigma^{(e)}$ has been specified. To obtain the skew-symmetric part, we invoke the balance of angular momentum for micropolar continua, which relates skew $\sigma^{(e)}$ with $\mu^{(e)}$, in the form (Malvern 1969)

$$(\text{skew } \sigma^{(e)})_{\alpha\beta} = \frac{1}{2} \varepsilon_{\gamma\alpha\beta} (I_{\gamma\lambda}^{(e)} \check{\theta}_{\lambda}^{(e)} - \mu_{\lambda\gamma,\lambda}^{(e)} - m_{\gamma}^{b(e)}), \tag{17}$$

where summation is implied over repeated indices. $\check{\theta}_{\lambda}^{(e)}$, $\mu_{\lambda\gamma,\lambda}^{(e)}$, $I_{\gamma\lambda}^{(e)}$ and $m_{\gamma}^{b(e)}$ are components of $\check{\theta}^{(e)}(\mathbf{x}) = \sum_{I=1}^M N_I(\mathbf{x}) \check{\theta}_I, \nabla \cdot \mu^{(e)}, \mathbf{I}^{(e)}$ and $\mathbf{m}^{b(e)}$ respectively. The first two of these four have been specified already. The continuum body moment density $\mathbf{m}^{b(e)}$ will be specified in §2.3 and the relations for the moment $\mathbf{I}^{(e)}$ of inertia will be given in §2.4.

Different volume elements V^e chosen for stress and couple stress calculation occupy different spatial regions and are of different shapes and sizes. In general, owing to multiple and non-local atomic interactions, these elements partly overlap. A two-dimensional (2D) illustration of this issue is given in figure 3. Assume that the cut-off radius (the interatomic distance beyond which direct interaction between two atoms is essentially negligible) for the material is R_c . For atom A in figure 3(a), interactions with eight other atoms must be considered. Specifically, forces on A due to atoms B, C and D give rise to elements ABC and ACD among other elements (note that only a portion of the forces may be considered in each triangle, as indicated in equation (7)). For atom D, a similar cut-off circle must be drawn and triangles DAB and DBC must be analysed among others. Since these four elements partly overlap and do not coincide, the superposition of the stress subfields varies for each spatial location in V .

In equation (4), the summation for the virtual work must be performed over all interatomic bonds ($i = 1, 2, \dots, N$) on the discrete side and over all elements on the continuum side to ensure equality of virtual work. The elemental stress $\sigma^{(e)}(\mathbf{x})$ and couple stress $\mu^{(e)}(\mathbf{x})$ at a position \mathbf{x} combine to give rise to the Cauchy stress field $\sigma(\mathbf{x})$ and couple stress field $\mu(\mathbf{x})$ respectively in V , as

$$\sigma(\mathbf{x}) = \sum_e \sigma^{(e)}(\mathbf{x}), \quad \mu(\mathbf{x}) = \sum_e \mu^{(e)}(\mathbf{x}), \tag{18}$$

where the superposition is carried out for each \mathbf{x} with all elements that contain that point.

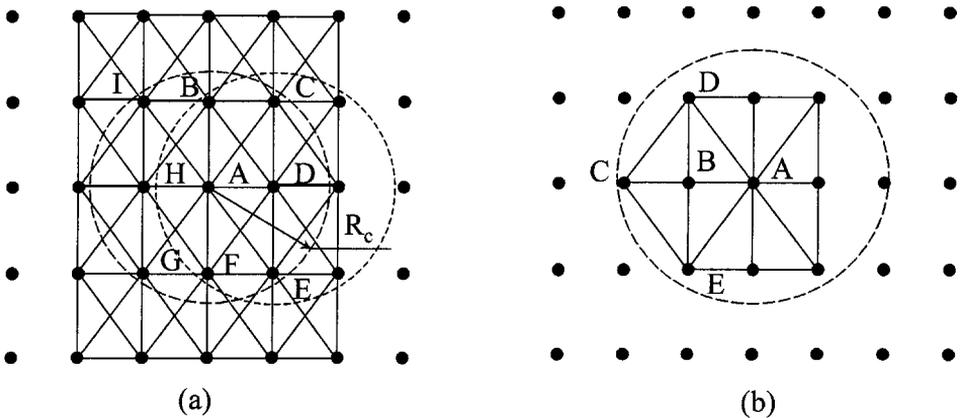


Figure 3. Superposition of stress subfields in overlapping elements.

The deformation field quantities that are work conjugate to the stress and couple stress fields in equation (18) are given by

$$D_{\beta\alpha} = \frac{\sum_e \text{sym } \sigma_{\alpha\beta}^{(e)} D_{\beta\alpha}^{(e)}}{\sum_e \text{sym } \sigma_{\alpha\beta}^{(e)}}, \quad W_{\beta\alpha} = \frac{\sum_e \text{skew } \sigma_{\alpha\beta}^{(e)} W_{\beta\alpha}^{(e)}}{\sum_e \text{skew } \sigma_{\alpha\beta}^{(e)}}, \quad w_{\beta\alpha} = \frac{\sum_e \mu_{\alpha\beta}^{(e)} W_{\beta\alpha}^{(e)}}{\sum_e \mu_{\alpha\beta}^{(e)}}, \quad (19)$$

where summation is not implied over repeated indices α and β . In the limit when $V^e = V$, there is only one element and $\sigma^{(e)}(\mathbf{x}) = \sigma(\mathbf{x})$, $\mu^{(e)}(\mathbf{x}) = \mu(\mathbf{x})$, $(\partial \dot{\mathbf{u}} / \partial \mathbf{x})^{(e)} = \partial \dot{\mathbf{u}} / \partial \mathbf{x}$ and $\mathbf{w}^{(e)} = \mathbf{w}$, therefore, no superposition is needed.

A discussion is in order for situations involving multiple atoms lying on a radial line within the cut-off sphere, as illustrated in figure 3(b). Although such situations may warrant a different treatment of the interatomic interactions in quantum physics, classical interatomic potentials do not afford a special treatment of the interatomic forces. The equivalence of continuum-particle system virtual work can be maintained through a simple redefinition of the elements. For example, in figure 3(b) the consistency can be maintained through the consideration of elements ABD, ABE, ACD and ACE together with proper sharing of the forces and moments between AD and AE.

2.3. Traction, surface moment, body force and body moment

To obtain the traction over the surface area S^e (S) of V^e (V), consider a surface element $\Delta S \subset S^e$ (or $\Delta S \subset S$) defined by L particles. The virtual velocity and virtual angular velocity respectively over ΔS are

$$\begin{aligned} \delta \dot{\mathbf{u}}^{(e)}(\mathbf{x}) &= \sum_{I=1}^L N_I(\mathbf{x}) \delta \dot{\mathbf{u}}_I, \\ \delta \boldsymbol{\omega}^{(e)}(\mathbf{x}) &= \sum_{I=1}^L [\mathbf{R}_I \cdot \delta \dot{\mathbf{u}}_I + N_I(\mathbf{x}) \delta \dot{\boldsymbol{\theta}}_I], \end{aligned} \quad (20)$$

where \mathbf{R}_I is a skew-symmetric tensor with $R_{\alpha\gamma} = \varepsilon_{\alpha\beta\gamma} B_\beta$ (summation is implied over repeated index β). Substitution into the second relation of equation (8) yields

$$\begin{aligned} & \sum_{I=1}^L \int_{\Delta S} N_I(\mathbf{x}) \mathbf{t}^{(e)}(\mathbf{x}) \cdot d\mathbf{S} \cdot \delta \dot{\mathbf{u}}_I + \sum_{I=1}^L \int_{\Delta S} \mathbf{m}^{S(e)}(\mathbf{x}) \cdot \mathbf{R}_I \cdot d\mathbf{S} \cdot \delta \dot{\mathbf{u}}_I \\ & + \sum_{I=1}^L \int_{\Delta S} N_I(\mathbf{x}) \mathbf{m}^{S(e)}(x) \cdot d\mathbf{S} \cdot \delta \dot{\boldsymbol{\theta}}_I \\ & = \sum_{I=1}^L \xi_I (1 - \kappa_I) \mathbf{f}_I^{\text{ext}} \cdot \delta \dot{\mathbf{u}}_I + \sum_{I=1}^L \xi_I (1 - \kappa_I) \mathbf{m}_I^{\text{ext}} \cdot \delta \dot{\boldsymbol{\theta}}_I, \end{aligned} \quad (21)$$

where ξ_I is the fraction of $(1 - \kappa_I) \mathbf{f}_I^{\text{ext}}$ and $(1 - \kappa_I) \mathbf{m}_I^{\text{ext}}$ that can be attributed to ΔS , since ΔS may be only a portion of S^e and particle I may be on the boundary of ΔS (shared by the rest of S^e). Again, the arbitrariness of $\delta \dot{\mathbf{u}}_I$ and $\delta \dot{\boldsymbol{\theta}}_I$ requires that

$$\int_{\Delta S} N_I(\mathbf{x}) \mathbf{t}^{(e)}(\mathbf{x}) dS + \int_{\Delta S} \mathbf{m}^{S(e)}(\mathbf{x}) \cdot \mathbf{R}_I dS = \xi_I(1 - \kappa_I) \mathbf{f}_I^{\text{ext}}, \quad (22)$$

$$\int_{\Delta S} N_I(\mathbf{x}) \mathbf{m}^{S(e)}(\mathbf{x}) dS = \xi_I(1 - \kappa_I) \mathbf{m}_I^{\text{ext}},$$

with $I = 1, 2, \dots, L$. The solution to the above is

$$\mathbf{t}^{(e)}(\mathbf{x}) = \sum_{J=1}^L N_J(\mathbf{x}) \lambda_J, \quad (23)$$

$$\mathbf{m}^{S(e)}(\mathbf{x}) = \sum_{J=1}^L N_J(\mathbf{x}) \chi_J;$$

where λ_J and χ_J are vector solutions of the linear systems of equations in the forms

$$\sum_{J=1}^L c_{IJ} \lambda_J = \xi_I(1 - \kappa_I) \mathbf{f}_I^{\text{ext}} - \int_{\Delta S} \mathbf{m}^{S(e)}(\mathbf{x}) \cdot \mathbf{R}_I dS, \quad (24)$$

$$\sum_{J=1}^L c_{IJ} \chi_J = \xi_I(1 - \kappa_I) \mathbf{m}_I^{\text{ext}}.$$

In the above equations, $c_{IJ} = \int_{\Delta S} N_I(\mathbf{x}) N_J(\mathbf{x}) dS$, with $I, J = 1, 2, \dots, L$. The simplest case is that of triangular surface areas with $L = 3$.

If ΔS resides on the surfaces of two or more elements, the total traction and moment respectively are

$$\mathbf{t}(\mathbf{x}) = \sum_e \mathbf{t}^{(e)}, \quad (25)$$

$$\mathbf{m}^S(\mathbf{x}) = \sum_e \mathbf{m}^{S(e)}.$$

To obtain the body force density \mathbf{b} and body moment density \mathbf{m}^b , consider the volume element V^e defined by M particles. The equations are

$$\int_{V^e} N_I(\mathbf{x}) \mathbf{b}^{(e)}(\mathbf{x}) dV + \int_{V^e} \mathbf{m}^{b(e)}(\mathbf{x}) \cdot \mathbf{R}_I dV = \kappa_I \mathbf{f}_I^{\text{ext}}, \quad (26)$$

$$\int_{V^e} N_I(\mathbf{x}) \mathbf{m}^{b(e)}(\mathbf{x}) dV = \kappa_I \mathbf{m}_I^{\text{ext}},$$

where $\kappa_I = 1$ for atoms in the interior of V^e and $\kappa_I = 0$ for particles on the surface S^e of V^e . The solutions are

$$\mathbf{b}^{(e)}(\mathbf{x}) = \sum_{J=1}^M N_J(\mathbf{x}) \xi_J, \quad (27)$$

$$\mathbf{m}^{b(e)}(\mathbf{x}) = \sum_{J=1}^M N_J(\mathbf{x}) \pi_J;$$

where ξ_J and π_J are the vector solutions of the linear system of equations in the forms of

$$\sum_{J=1}^M d_{IJ} \xi_J = \kappa_I \mathbf{f}_I^{\text{ext}} - \int_{\Delta V} \mathbf{m}^{b(e)}(\mathbf{x}) \cdot \mathbf{R}_I dV, \tag{28}$$

$$\sum_{J=1}^M d_{IJ} \pi_J = \kappa_I \mathbf{m}_I^{\text{ext}}.$$

In the above relations, $d_{IJ} = \int_{V^e} N_I(\mathbf{x}) N_J(\mathbf{x}) dV$, with $I, J = 1, 2, \dots, M$. The simplest case is tetrahedral regions with $M = 4$.

Because of the same considerations as in equation (18), the elemental body force and moment of inertia contributions obtained above combine to yield the total body force density and body moment density respectively as

$$\mathbf{b}(\mathbf{x}) = \sum_e \mathbf{b}^{(e)}(\mathbf{x}), \quad \mathbf{m}^b(\mathbf{x}) = \sum_e \mathbf{m}^{b(e)}(\mathbf{x}). \tag{29}$$

The deformation field quantities that are work conjugate to the above quantities are

$$\dot{\mathbf{u}}_\alpha = \frac{\sum_e b_\alpha^{(e)} \dot{\mathbf{u}}_\alpha^{(e)}}{\sum_e b_\alpha^{(e)}}, \quad \omega_\alpha = \frac{\sum_e m_\alpha^{b(e)} \omega_\alpha^{(e)}}{\sum_e m_\alpha^{b(e)}}, \tag{30}$$

where summation is *not* implied over repeated index α .

2.4. Mass and moment of inertia distributions of equivalent continuum

The equality of the continuum virtual work and atomic virtual work associated with inertia forces in the last relation of equations (8) specifies the distributions of mass and moment of inertia of the equivalent continuum. We can express these elemental densities in terms of the shape functions as

$$\rho^{(e)}(\mathbf{x}) = \sum_{K=1}^M N_K(\mathbf{x}) g_K, \tag{31}$$

$$\mathbf{l}^{(e)}(\mathbf{x}) = \sum_{K=1}^M N_K(\mathbf{x}) \mathbf{h}_K,$$

where g_K and \mathbf{h}_K ($K = 1, 2, \dots, M$) are scalar and tensorial constants respectively to be determined. Substitution of

$$\delta \dot{\boldsymbol{\theta}}^{(e)}(\mathbf{x}) = \sum_{I=1}^M N_I(\mathbf{x}) \delta \dot{\boldsymbol{\theta}}_I, \tag{32}$$

$$\ddot{\boldsymbol{\theta}}^{(e)}(\mathbf{x}) = \sum_{J=1}^M N_J(\mathbf{x}) \ddot{\boldsymbol{\theta}}_J,$$

into the last relation of equation (8) yields

$$\begin{aligned}
 & \sum_{I=1}^M \sum_{J=1}^M \left(\int_{V^e} \left[\rho^{(e)}(\mathbf{x}) N_I(\mathbf{x}) N_J(\mathbf{x}) \ddot{\mathbf{u}}_J \right] dV \right) \cdot \delta \dot{\mathbf{u}}_I \\
 & + \sum_{I=1}^M \sum_{J=1}^M \left(\int_{V^e} \left[\mathbf{l}^{(e)}(\mathbf{x}) N_I(\mathbf{x}) N_J(\mathbf{x}) \ddot{\boldsymbol{\theta}}_J \right] dV \right) \cdot \delta \dot{\boldsymbol{\theta}}_I \\
 & = \sum_{I=1}^M \varsigma_I m_I \ddot{\mathbf{u}}_I \cdot \delta \dot{\mathbf{u}}_I + \sum_{I=1}^M \varsigma_I \mathbf{l}_I \ddot{\boldsymbol{\theta}}_I \cdot \delta \dot{\boldsymbol{\theta}}_I.
 \end{aligned} \tag{33}$$

The arbitrariness of $\delta \dot{\mathbf{u}}_I$ and $\delta \dot{\boldsymbol{\theta}}_I$ requires that

$$\begin{aligned}
 & \sum_{J=1}^M \int_{V^e} \left[\rho^{(e)}(\mathbf{x}) N_I(\mathbf{x}) N_J(\mathbf{x}) \ddot{\mathbf{u}}_J \right] dV = \varsigma_I m_I \ddot{\mathbf{u}}_I, \\
 & \sum_{J=1}^M \int_{V^e} \left[\mathbf{l}^{(e)}(\mathbf{x}) N_I(\mathbf{x}) N_J(\mathbf{x}) \ddot{\boldsymbol{\theta}}_J \right] dV = \varsigma_I \mathbf{l}_I \ddot{\boldsymbol{\theta}}_I.
 \end{aligned} \tag{34}$$

Summation of the M equations in each of the above systems and the independence of $\rho^{(e)}$ and $\mathbf{l}^{(e)}$ on $\ddot{\mathbf{u}}_I$ and $\ddot{\boldsymbol{\theta}}_I$ yields

$$\begin{aligned}
 & \int_{V^e} \left[\rho^{(e)}(\mathbf{x}) N_I(\mathbf{x}) \right] dV = \varsigma_I m_I, \\
 & \int_{V^e} \left[\mathbf{l}^{(e)}(\mathbf{x}) N_I(\mathbf{x}) \right] dV = \varsigma_I \mathbf{l}_I,
 \end{aligned} \tag{35}$$

where summation is *not* implied over the repeated index I . Substitution of equations (31) into equations (35) gives

$$\begin{aligned}
 & \sum_{K=1}^M d_{IK} g_K = \varsigma_I m_I, \\
 & \sum_{K=1}^M d_{IK} \mathbf{h}_K = \varsigma_I \mathbf{l}_I.
 \end{aligned} \tag{36}$$

These two systems uniquely determine g_K and \mathbf{h}_K respectively, yielding the distributions of mass $\rho^{(e)}(\mathbf{x})$ and moment of inertia $\mathbf{l}^{(e)}(\mathbf{x})$ of the equivalent continuum through equations (31). Again, the simplest case corresponds to tetrahedral elements with $M = 4$ in three dimensions and triangular regions with $M = 3$ in two dimensions. Note that the requirement of conservation of mass is satisfied by equations (31) and (36).

Accounting for contributions from overlapping elements at a location \mathbf{x} , the total mass and moment of inertia densities respectively are

$$\rho(\mathbf{x}) = \sum_e \rho^{(e)}(\mathbf{x}), \quad \mathbf{l}(\mathbf{x}) = \sum_e \mathbf{l}^{(e)}(\mathbf{x}). \tag{37}$$

The deformation field quantities that are work conjugate to the above quantities, the velocity field in equation (30) and the angular velocity field $\dot{\boldsymbol{\theta}}$ are

$$\ddot{u}_\alpha = \frac{\sum_e \rho^{(e)} \ddot{u}_\alpha^{(e)} \dot{u}_\alpha^{(e)}}{\dot{u}_\alpha(\mathbf{x}) \rho(\mathbf{x})}, \quad \ddot{\theta}_\alpha = \frac{\sum_e l_{\beta\alpha}^{(e)} \ddot{\theta}_\alpha^{(e)} \dot{\theta}_\beta^{(e)}}{\dot{\theta}_\beta(\mathbf{x}) l_{\beta\alpha}(\mathbf{x})}, \quad (38)$$

where summation is *not* implied over repeated index α but *is* implied over repeated index β . The angular velocity field is $\dot{\boldsymbol{\theta}} = \boldsymbol{\omega}$ – dual \mathbf{W} with $\boldsymbol{\omega}$ being calculated from equation (30) and \mathbf{W} being calculated from equations (19).

We note that in general, for areas where overlap of elements occurs, the deformation field quantities from equations (19), (30) and (38) do not satisfy $\mathbf{D} = \text{sym}(\partial \dot{\mathbf{u}}/\partial \mathbf{x})$, $\mathbf{W} = \text{sym}(\partial \dot{\mathbf{u}}/\partial \mathbf{x})$ and $\mathbf{w} = \partial \boldsymbol{\omega}/\partial \mathbf{x}$, even though at the element level $\mathbf{D}^{(e)} = \text{sym}(\partial \dot{\mathbf{u}}^{(e)}/\partial \mathbf{x})$, $\mathbf{W}^{(e)} = \text{sym}(\partial \dot{\mathbf{u}}^{(e)}/\partial \mathbf{x})$ and $\mathbf{w}^{(e)} = \partial \boldsymbol{\omega}^{(e)}/\partial \mathbf{x}$ are indeed satisfied. This situation results from the weighted averaging used to maintain the work conjugacy of the stress, couple stress body force, body moment, traction and surface moment. The lack of full consistency with the continuum differential requirement occurs only on the size scale of the cut-off radius of the material. Such overlap affects only the boundary region of V^e inside S^e that has a thickness smaller than or equal to R_c (see figure 4 for the size of overlapping zone between elements V^1 and V^2). Locations in the interior of V^e that have distances from S^e greater than R_c are not affected by the overlap. As the size of V^e is increased, the effect of this lack of differential smoothness decreases. Full consistency is achieved in the limit of $V^e = V$. Full consistency is also maintained for loading under which the stress $\boldsymbol{\sigma}^{(e)}$, couple stress $\boldsymbol{\mu}^{(e)}$, body force density $\mathbf{b}^{(e)}$ and body moment density $\mathbf{m}^{b(e)}$ are the same in overlapping elements. It is worthwhile to point out that the use of such superimposed deformation quantities can also be avoided completely by always placing the locations of interest fully in the non-overlapping interior of an element. It will be shown in § 3 that the benefit of this weighted averaging is that the conservation of internal and external work rates, conservation of linear and angular momenta, and conservation of mass are achieved between the equivalent continuum and the discrete particle system.

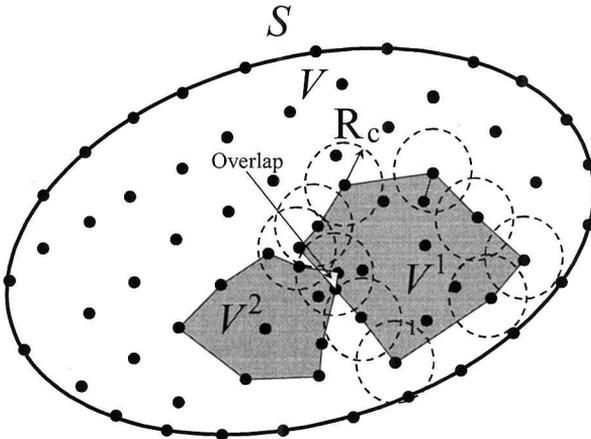


Figure 4. Size scale of element overlapping.

§3. WORK CONJUGACY AND BALANCE OF MOMENTA

To obtain the global equivalence of work rates, we replace $\delta \dot{\mathbf{u}}$ by the actual velocity $\dot{\mathbf{u}}$ and $\delta \dot{\boldsymbol{\theta}}$ by the actual angular velocity $\dot{\boldsymbol{\theta}}$. Equations (8) then become

$$-\int_V \boldsymbol{\sigma} : \mathbf{D} dV - \int_V \boldsymbol{\mu} : \mathbf{w} dV = \sum_{i=1}^N \mathbf{f}_i^{\text{int}} \cdot \dot{\mathbf{u}}_i + \sum_{i=1}^N \mathbf{m}_i^{\text{int}} \cdot \dot{\boldsymbol{\theta}}_i, \tag{39}$$

$$\begin{aligned} & \int_V \mathbf{b} \cdot \dot{\mathbf{u}} dV + \int_V \mathbf{m}^b \cdot \boldsymbol{\omega} dV + \int_S \mathbf{t} \cdot \dot{\mathbf{u}} dS + \int_S \mathbf{m}^S \cdot \boldsymbol{\omega} dS \\ & = \sum_{i=1}^N \mathbf{f}_i^{\text{ext}} \cdot \dot{\mathbf{u}}_i + \sum_{i=1}^N \mathbf{m}_i^{\text{ext}} \cdot \dot{\boldsymbol{\theta}}_i. \end{aligned} \tag{40}$$

These relations show that the equivalent continuum indeed has the same the internal, external and inertial work rates.

The equivalent continuum also has the same global linear and angular momenta as the original particle system. It can be shown that equations (22), (23), (25)–(27), (29) and (34)–(38) yield

$$\begin{aligned} & \int_S \mathbf{t} dS + \int_V \mathbf{b} dV = \sum_{i=1}^N \mathbf{f}_i^{\text{ext}} = \sum_{i=1}^N \mathbf{f}_i = \int_V \rho \dot{\mathbf{u}} dV = \sum_{i=1}^N m_i \ddot{\mathbf{r}}_i, \\ & \int_S \mathbf{r} \times \mathbf{t} dS + \int_V \mathbf{r} \times \mathbf{b} dV + \int_S \mathbf{m}^S dS + \int_V \mathbf{m}^b dV \\ & = \sum_{i=1}^N \mathbf{r}_i \times \mathbf{f}_i^{\text{ext}} + \sum_{i=1}^N \mathbf{m}_i^{\text{ext}} \\ & = \sum_{i=1}^N \mathbf{r}_i \times \mathbf{f}_i + \sum_{i=1}^N \mathbf{m}_i \\ & = \int_V \rho \mathbf{r} \times \dot{\mathbf{u}} dV + \int_V \mathbf{l} \cdot \dot{\boldsymbol{\theta}} dV \\ & = \sum_{i=1}^N m_i \mathbf{r}_i \times \ddot{\mathbf{r}}_i + \sum_{i=1}^N \mathbf{l}_i \cdot \dot{\boldsymbol{\theta}}_i. \end{aligned} \tag{41}$$

Therefore, using the dynamic principle of virtual work, we have defined an equivalent continuum which is dynamically consistent with atomic ensembles exhibiting micropolar interatomic interactions as set forth in MD idealizations of actual atomistic systems. The consistency is in the conservation of internal work rate, external work rate and work rate due to inertial forces. The fields of work-conserving stress, couple stress, surface traction, surface moment, body force density, body moment density, mass density and the moment of inertia density are determined together with a work-conjugate deformation field. The continuum–particle assembly work equality and momentum equivalence ensure that the continuum interpretation of the discrete force field maintains the physical effects of the particle system at all times. It is important to point out that the continuum fields defined here reflect an interpretation of the particle force, moment and deformation over the entire spatial region and surface occupied by the particle system. The advantage is that regular continuum averaging, scaling and interpretation are fully allowed. Furthermore, the equivalence of work rates, kinetic energy, linear momentum and angular momentum holds for

any finite volume element V^e as well as for the entire system. The formulation, algorithm and results allow a consistent transition from the MD framework to the continuum framework. The length scale effects due to non-local interatomic interactions can be accounted for in this framework of analysis. Since full fields of all fundamental kinetic and kinematic quantities are given, scaling and averaging can be carried out.

§ 4. DISCUSSION

The entire analysis here is carried out on the current deformed configuration; therefore, $\boldsymbol{\sigma}, \boldsymbol{\mu}, \mathbf{b}, \mathbf{m}^b, \mathbf{t}$ and \mathbf{m}^S represent force (moment) per unit area or per unit volume in the deformed configuration. In particular, $\boldsymbol{\sigma}$ is the Cauchy stress in the general context of micropolar continuum. This is both convenient and necessary. The evaluation of the corresponding kinetic quantities (e.g. the first Piola–Kirchhoff stress) in any non-deforming reference configuration is, in general, not possible owing to the rearrangement of discrete atoms. This difficulty results from a fundamental difference between discrete particle models and continuum models. Specifically, particle rearrangement renders the determinant of the deformation gradient $\mathbf{F} = \partial \mathbf{x} / \partial \mathbf{X}$ to be non-positive ($\det \mathbf{F} \leq 0$), a situation not permitted in continuum mechanics. Also, since \mathbf{x} is the current position of the particles, the shape functions N_I , their gradients \mathbf{B}_I , and tensors \mathbf{H}_I must be evaluated at each time step for which the equivalent continuum is to be determined.

The framework of analysis taken here admits an explicit account of arbitrary atomic arrangement. Hence, applications to crystalline or amorphous structures are equally valid. The analysis also applies to both homogeneous materials with identical atoms and heterogeneous materials with dissimilar atoms, under the condition that appropriate atomic potentials of the form in equation (1) are used.

§ 5. NON-POLAR MATERIALS

For non-polar materials (materials that do not contain electric dipoles at the individual atom level), the dependence on θ_{ij} of E in equation (1) vanishes; therefore, $\mathbf{m}_{ij} = \mathbf{0}$, $\mathbf{m}_i = \mathbf{0}$, $\mathbf{m}_I^{\text{int}} = \mathbf{0}$ and $\mathbf{m}_I^{\text{ext}} = \mathbf{0}$ and, consequently, only the central forces \mathbf{f}_{ij} and \mathbf{f}_i exist. Under such conditions, the second relation of equations (15) specifies that $\boldsymbol{\mu} = \mathbf{0}$, equations (23) and (24) yield $\mathbf{m}^S(\mathbf{x}) = \mathbf{0}$, and equations (27) and (28) yield $\mathbf{m}^b(\mathbf{x}) = \mathbf{0}$. The absence of interatomic moment interactions also removes the coupling between linear and angular momenta. Although self-spins of atoms may still exist, they are totally decoupled from atom to atom, from the central force interactions and from the effects of central forces due to external atoms or other external agents and are, therefore, inconsequential to the theory in their case. The angular velocity of atoms will remain unchanged throughout the history of deformation. These materials do not possess moments of inertia at the continuum level, that is $\mathbf{I}(\mathbf{x}) = \mathbf{0}$. Under such conditions, the equations for determining elemental stress $\boldsymbol{\sigma}^{(e)}$ (note that $\boldsymbol{\sigma}^{(e)} = \boldsymbol{\sigma}^{(e)\text{T}}$ for non-polar materials in the absence of $\boldsymbol{\mu}^{(e)}$), traction $\mathbf{t}^{(e)}$, body force density \mathbf{b} and mass density $\rho^{(e)}(\mathbf{x})$ are as follows.

(i) *Stress over V^e containing M atoms:*

$$\int_{V^e} \boldsymbol{\sigma}^{(e)} \cdot \mathbf{B}_I \, dV = -\mathbf{f}_I^{\text{int}}, \quad I = 1, 2, \dots, M. \quad (42)$$

(ii) *Traction over ΔS^e defined by L atoms on a surface:*

$$\mathbf{t}^{(e)}(\mathbf{x}) = \sum_{J=1}^L N_J(\mathbf{x})\lambda_J, \tag{43}$$

where λ_J are the vector solutions of

$$\sum_{J=1}^L c_{IJ}\lambda_J = \xi_I(1 - \kappa_I)\mathbf{f}_I^{\text{ext}}, \quad c_{IJ} = \int_{\Delta S} N_I(\mathbf{x})N_J(\mathbf{x}) \, dS, \quad I, J = 1, 2, \dots, L. \tag{44}$$

(iii) *Body force density over V^e containing M atoms:*

$$\mathbf{b}^{(e)}(\mathbf{x}) = \sum_{J=1}^M N_J(\mathbf{x})\xi_J, \tag{45}$$

where ξ_J are the solutions of

$$\sum_{J=1}^M d_{IJ}\xi_J = \kappa_I\mathbf{f}_I^{\text{ext}}, \quad d_{IJ} = \int_{V^e} N_I(\mathbf{x})N_J(\mathbf{x}) \, dV, \quad I, J = 1, 2, \dots, M. \tag{46}$$

(iv) *Mass density over V^e containing M atoms:*

$$\rho^{(e)}(\mathbf{x}) = \sum_{K=1}^M N_K(\mathbf{x})g_K, \tag{47}$$

where g_K are solutions of

$$\sum_{K=1}^M d_{IK}g_K = c_I m_I, \quad I = 1, 2, \dots, M. \tag{48}$$

It is noted that the non-polar materials referred to here include those that admit interactions that show dependence on dihedral angles between bonds in a lattice assembly for which the MEAM was developed. Such interatomic interactions are of the central force type and no interatomic moments are involved.

§ 6. EXAMPLE: UNIFORM TENSION OF A NON-POLAR MATERIAL

Consider the uniform tension under external force \mathbf{f}^0 of a non-polar lattice in figure 5. The initial square lattice constant is a_0 . The deformed lattice has dimensions a and b in the horizontal and vertical directions respectively. The material is homogeneous and the mass of each atom is m . For simplicity, assume that the cut-off radius R_c is such that $a < R_c < 2a$ and $b < R_c < 2b$; therefore, non-local interactions do not occur. Since the couple stress is not involved and triangular elements are considered, the calculation here uses the 2D linear shape functions given in appendix A. Results of the continuum interpretation of the interatomic potential solutions are listed in table 1. The problem considered is fully dynamic; therefore, the interatomic forces can vary with time and in the vertical direction (i.e. $f_{12} = f_{12}(\mathbf{x}, t)$, $f_{13} = f_{13}(\mathbf{x}, t)$ and $f_{32} = f_{32}(\mathbf{x}, t)$) while they are uniform in the horizontal direction. At the upper boundary, $f^0 = f_{12} + 2f_{13} \cos \Theta$ and $\sigma_{22} = f^0/a = (f_{12} + 2f_{13} \cos \Theta)/a$. This is consistent with the continuum solution of traction at the boundary and the continuum expectation of uniform stress in the horizontal direction. The rate of deformation, body force density, boundary traction and mass density in table 1 are also in complete agreement with continuum mechanics expectations.

Table 1. Equivalent continuum fields for uniform tension of a non-polar lattice (m is the mass of each atom).

Element	Stress, rate of deformation, body force density and mass density
1-2-3	$\boldsymbol{\sigma}^{(e)} = \begin{pmatrix} (f_{32}/2 + f_{13} \sin \Theta)/b & (-f_{13} \sin \Theta)/a \\ -(f_{13} \sin \Theta)/a & (f_{12}/2 + f_{13} \cos \Theta)/a \end{pmatrix}$ $\mathbf{D}^{(e)} = \begin{pmatrix} \dot{a}/a & 0 \\ 0 & \dot{b}/b \end{pmatrix}, \mathbf{W}^{(e)} = \mathbf{0}$ $\mathbf{b}^{(e)}(\mathbf{x}) = \mathbf{0}$ $\rho^{(e)}(\mathbf{x}) = m/2ab$
1-3-4	$\boldsymbol{\sigma}^{(e)} = \begin{pmatrix} (f_{32}/2 + f_{13} \sin \Theta)/b & (-f_{13} \sin \Theta)/a \\ (-f_{13} \sin \Theta)/a & (f_{12}/2 + f_{13} \cos \Theta)/a \end{pmatrix}$ $\mathbf{D}^{(e)} = \begin{pmatrix} \dot{a}/a & 0 \\ 0 & \dot{b}/b \end{pmatrix}, \mathbf{W}^{(e)} = \mathbf{0}$ $\mathbf{b}^{(e)}(\mathbf{x}) = \mathbf{0}$ $\rho^{(e)}(\mathbf{x}) = m/2ab$
1-2-4	$\boldsymbol{\sigma}^{(e)} = \begin{pmatrix} (f_{32}/2 + f_{13} \sin \Theta)/b & (f_{13} \sin \Theta)/a \\ (f_{13} \sin \Theta)/a & (f_{12}/2 + f_{13} \cos \Theta)/a \end{pmatrix},$ $\mathbf{D}^{(e)} = \begin{pmatrix} \dot{a}/a & 0 \\ 0 & \dot{b}/b \end{pmatrix}, \mathbf{W}^{(e)} = \mathbf{0}$ $\mathbf{b}^{(e)}(\mathbf{x}) = \mathbf{0}, \rho^{(e)}(\mathbf{x}) = m/2ab$
2-3-4	$\boldsymbol{\sigma}^{(e)} = \begin{pmatrix} (f_{32}/2 + f_{13} \sin \Theta)/b & (f_{13} \sin \Theta)/a \\ (f_{13} \sin \Theta)/a & (f_{12}/2 + f_{13} \cos \Theta)/a \end{pmatrix},$ $\mathbf{D}^{(e)} = \begin{pmatrix} \dot{a}/a & 0 \\ 0 & \dot{b}/b \end{pmatrix}, \mathbf{W}^{(e)} = \mathbf{0}$ $\mathbf{b}^{(e)}(\mathbf{x}) = \mathbf{0}$ $\rho^{(e)}(\mathbf{x}) = m/2ab$
Overall	$\boldsymbol{\sigma} = \begin{pmatrix} (f_{32} + 2f_{13} \sin \Theta)/b & 0 \\ 0 & (f_{12} + 2f_{13} \cos \Theta)/a \end{pmatrix}$ $\mathbf{D} = \begin{pmatrix} \dot{a}/a & 0 \\ 0 & \dot{b}/b \end{pmatrix}, \mathbf{W} = \mathbf{0},$ $\mathbf{b}(\mathbf{x}) = \mathbf{0}$ $\mathbf{t}(\mathbf{x} = \text{upper and lower boundaries}) = \pm \mathbf{t}^0 = \pm \mathbf{f}^0/a$ $\rho(\mathbf{x}, t) = m/ab$

The virial stress (Tsai 1979, Rowlinson and Widom 1982) at \mathbf{r}_i is

$$\boldsymbol{\Pi} = \frac{1}{\Omega} \left(-m_i \dot{\mathbf{u}}_i \otimes \dot{\mathbf{u}}_i + \frac{1}{2} \sum_{j(\neq i)} \mathbf{r}_{ij} \otimes \mathbf{f}_{ij} \right). \quad (49)$$

Here, tensile stresses are defined as positive, therefore, $\partial\Phi/\partial r_{ij} > 0$ if \mathbf{f}_{ij} is attractive in equation (2). Ω is a proper choice of volume associated with atom i and summation is *not* implied over repeated indices. For atomic ensembles with irregular atom positions, the choice of Ω is not obvious and can be ambiguous. In the current example, however, the regular shape and periodicity of the rectangular lattice allows Ω to be identified as the volume (or area) of the unit cell, that is $\Omega = ab$. The mechanical part (second term) of the virial stress for the problem in figure 5 matches the solution in table 1. This agreement occurs because of the simple geometry of the problem, the uniformity of loading and the absence of non-local interactions.

A proper perspective is in order here. In general, the current stress and the virial stress do not coincide because of their clearly different definitions. Both stresses are measured relative to the equilibrium configuration of a particle system. The stress defined here always makes the same work contribution to deformation as the interparticle force system over any finite volume element while the virial stress does not. Indeed, the virial stress is defined without regard to any possible work-conjugate deformation field. A detailed discussion on the virial stress has been given by Zhou (2001). The calculation of the current stress does not involve *ad hoc* specification of a relevant volume. The evaluation of the virial stress for any set of atoms requires the identification of a proper Ω whose extent is not always obvious. In the example in figure 5, the overall deformation is homogeneous across different unit cells and periodicity of the lattice is maintained. In addition, locality of interatomic forces is assumed through the choice of the relatively small cut-off radius. Therefore, Ω can be taken as the volume of the unit cell. Under conditions of arbitrary and inhomogeneous deformations, the identification of Ω is ambiguous and somewhat uncertain. The virial stress contains a kinetic energy term (the first term in equation (49)). This term represents a statistical mechanics characterization of the effects of kinetic energy of atomic particles on the *apparent* traction on a spatial plane that is external to the particle system. It is not related to the *internal* mechanical interaction between particles (or material points). Clearly, it should not have (and, indeed, it does not

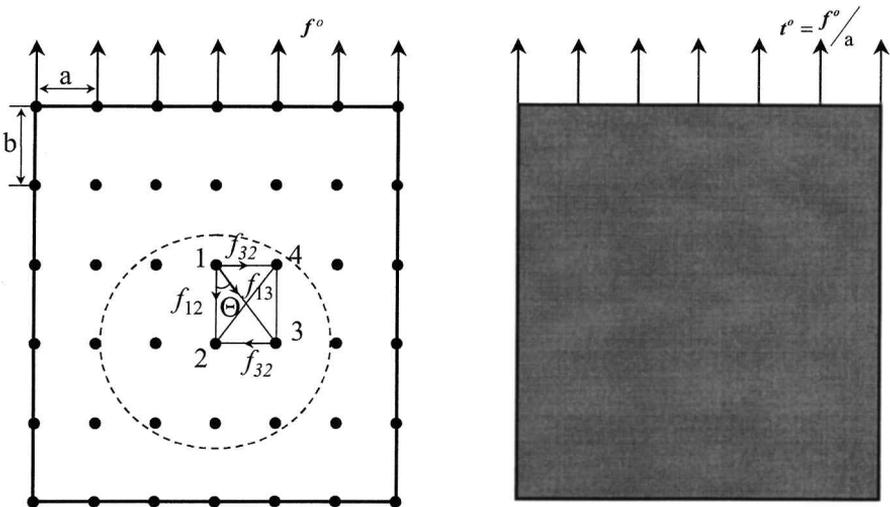


Figure 5. Uniform tension of a 2D lattice and continuum equivalent.

have) a part in the dynamically work- and momentum-conserving definition of stress which is a measure of *internal* interactions between material points. More detailed analyses of the virial stress are given in Zhou (2001, 2002). In the current analysis, the effects of kinetic energy on motion and deformation are properly accounted for by the continuum deformation fields and by the mass distribution. In summary, the virial stress does not represent the dynamically equivalent medium in the same sense as the Cauchy stress in this paper. Moreover, it is relatively insensitive to local heterogeneity if computed over some substantial volume.

§7. CONCLUSION

An equivalent polar continuum has been defined for dynamically deforming atomistic systems. For non-polar materials, the resulting Cauchy stress is contrasted with the commonly used virial stress. It is shown that the Cauchy stress has certain advantages in specificity and rigour. The equivalent continuum fields here represent a reinterpretation of the result of a MD calculation. In their present form, these fields have exactly the same number of independent degrees of freedom as the discrete fields in the MD system. In the context of multiscale characterization of material response, this paper may be regarded as offering a theoretical basis for ‘continuum-ization’ which is the first step in a rigorous averaging process. Subsequent steps should include ‘averaging’ and ‘scaling’. Another potential application of the theoretical framework developed here is multiscale computational modelling of material behaviour which combines both MD and continuum descriptions in the development of constitutive relations at different scales. This is facilitated by the work-conjugate deformation and stress fields that can be calculated on any desired scale. The equivalent continuum developed here has certain implications. Firstly, it is computationally quite intensive to obtain the fields through a large ensemble of atoms because elements must be constructed and weighting must be applied. Secondly, the fields thus determined are piecewise continuous, leading to potentially large fluctuations among small groups of atoms. This is an intrinsic feature of dynamic equivalence on interatomic scales and is also a reflection of the effects of atomic-scale material heterogeneity. The resolution of such interatomic features is important for problems involving heterogeneity and steep gradients of the fields, such as interfaces and crack tips. The fields obtained are amenable to continuum treatment, including averaging. Future work will address the principles of averaging these fields over larger scales in a manner that delivers useful information across length scales. Such averaging procedures should strive to preserve the dynamical work equivalence and the attendant statistical mechanics features of the MD solution.

It is worth noting that the approach taken here fully admits non-local atomistic interactions. The continuum fields obtained reflect the non-local characteristics of the MD solutions. For this reason, the superposed solution embodied in equations (18), (19), (25), (29), (30), (37) and (38) and the solution obtained by taking $V = V^e$ are not identical except for conditions of uniform deformation or uniform loading. The former preserves global work rates and momenta but lacks general differential compatibility of the kinematic quantities. The latter fully preserves the global work rates and momenta and satisfies the requirements of kinematic differential compatibility. Moreover, such full consistency is also achieved for the V^e defined by any subset of an atomistic system. This consistency on any size scale allows the effects of non-locality and scaling to be quantified within the context of a continuum framework.

To achieve the dynamic equivalence between the continuum and the particle system on any size scale, the analysis here involves a systematic delineation of internal and external interatomic interactions, delineation of surface and body forces, sharing of a bond by neighbouring elements and distribution of atomic mass to elements connected to an atom. These processes use the parameters ς (equation (6)), η (equation (7)), κ (equation (8)) and ξ (equation (21)). It is important to point out that values for these parameters are independent of the dynamic principle of virtual work (PVW); therefore, they cannot be determined by the PVW beyond the extent that the sum of each of these parameters be unity for the corresponding bond or atom. Any value in the ranges given earlier for these parameters will allow the work and momentum equivalence to be maintained. Realistic determination of the values should depend on material structure, symmetry, quantum-mechanical description of the spatial shape of the interatomic bonds, and consistency with continuum mechanics expectations on higher scales. The macroscopic continuum expectation that mass be uniformly distributed ($\rho(\mathbf{x}) = \text{constant}$) for uniform periodic lattices consisting of identical atoms such as that in figure 5 dictates that, for 3D tetrahedral and 2D triangular elements, $\varsigma_I^e = V^e / \sum_e^k V^e$, with k being the number of elements connected to atom I . The determination of ξ should use a similar consideration for uniform traction distributions on planar surfaces for the type of shape functions used. Considerations for the determination of κ are fully given in §2. It is important to point out that, in the limit of $V^e = V$ and $S^e = S$, the parameters ς , η and ξ become unnecessary and irrelevant.

The issue of obtaining a continuum characterization of plasticity due to atomic rearrangement or configuration change should not be obscured by the conservative nature (nonlinear elastic) of interatomic potentials used in molecular dynamics. The reversibility of atomic reordering and restorability of broken atomic bonds must not be perceived as to prevent MD models to account for plasticity and dissipation in the continuum sense. MD and continuum theories have vastly different resolutions for defects or atomic structure changes. While MD models fully resolve atomic processes, continuum formulations typically employ far too few state variables to be able to capture the dynamical atomic state of the system. Instead, they opt to characterize the thermodynamic state of the system, a much less ambitious exercise. Note that defect generation through atomic rearrangement (e.g. dislocations) is the source of plasticity or dissipation at the continuum level, even though such defects can be reversed at the atomic level if the right conditions are made available. Such conditions to return the defect structure to any particular state are very hard to arrange, owing to the large number of degrees of freedom at the atomic level. They do not occur under deformations which continuum theories are formulated to describe. In other words, macroscopic plasticity theories describe processes that involve changes in defect structures not explicitly accounted for by strain alone. Such processes do not return a body's defect structure to its original state even though the macroscopic strain returns to zero, giving rise to the continuum phenomenological dissipation. A cycle of macroscopic plastic strain must not be equated with the return of atomic structures at the MD level. Realistic MD models on the size and time scales of processes considered by continuum plasticity theories should capture evolution and irreversibility of defect structures. The equivalent continuum is a faithful representation of the MD system, in terms of work rates, momentum, mass as well as energy. It naturally characterizes dissipation embedded in the MD models. One of the issues in the grand challenge of multiscale modeling of material behaviour is to

devise continuum representations of MD results on different time and length scales with appropriately reduced numbers of DOFs. One requirement for such developments is accurate reflection of dissipation embedded in the MD results and the equivalent continuum representation.

The equivalence that we introduce here is defined at each time in the Eulerian sense using the current configuration and therefore is not affected by atomic rearrangement. The geometry of the continuum always follows that of the atomic system, in essence an updated Lagrangian approach. Full work, momentum, and mass equivalence is maintained in this process. Additional analysis is needed for a delineation of the phenomena of elasticity and plasticity as expressed in the continuum setting, but of course they are fully embedded within the MD analyses. The generation and motion of defects in the MD calculations are highly non-equilibrium dissipative processes and are eventually to be cast in the continuum setting in appropriate constitutive laws. The equivalent continuum stress or couple stress and deformation fields directly reflect the effects of interatomic constitutive laws in the MD formulation. As is the case for experimental measurements of deformation and stress obtained from laboratory tests, these fields can be used to extract appropriate continuum constitutive relations. This is an application of the theory advanced here. It is not an objective of this paper.

The issue of couple stress is intrinsically tied to length scale, and for all scales above the interatomic is related to a homogenization process in which the heterogeneous medium is replaced by an effective continuum imbued with additional microrotational DOFs. Such effective media representations are valid only on scales at or above the characteristic length over which couples or microrotations could occur as equivalent force or moment distributions as determined from higher-order moments of the surface traction. Such couple stresses differ fundamentally from those associated with interatomic couples. The former can arise from collective defect distributions by considering higher-order moments of the surface traction information even for a dynamically equivalent continuum over some finite volume shown in figure 1 that is non-polar ($\mu^{(e)} = \mathbf{0}$) on the interatomic scale. However, it is unclear whether such higher-scale couple stresses can have a work conjugate micro-rotation field that is consistent with the principle of dynamic equivalence applied to a set of discrete particles as set forth in this paper. In particular, the couple stress and Cauchy stress in most continuum theories are not defined out of the consideration that they produce an equal amount of internal work on material deformation as exerted by the original non-polar stress field. It is therefore doubtful that they have a close connection to results of atomistic solutions.

It is important to recognize that a complete continuum representation for evolution of point and line defects within the material must also be consistent with the rate of dissipation, or rate of reduction in free energy density due to irreversible microstructure rearrangement. The dynamically equivalent continuum fields that we derive in this paper fully and explicitly embed effects of mass and momentum exchange of defects with the lattice, based on molecular dynamics as the underlying ‘constitutive relation’, and hence offer a dynamically consistent treatment that also reconciles dissipation. The volume-averaged stress and deformation fields in this case completely reflect the statistical aspects of lattice–defect interactions. However, in practice we often desire to formulate continuum constitutive relations that reflect MD results. When the stress and deformation fields are expressed as averages over much higher length scales, the resulting measures must be augmented in the continuum constitu-

tive relations by additional variables that represent the collective effects of defects, sometimes called state variables or internal state variables (ISVs). These variables are either explicit or implicit representations of defect distribution in the higher-scale continuum setting and evolve with generation and motion of defects or by other means of microstructure rearrangement (e.g. phase transformations) in a manner consistent with dissipation over the characteristic averaging volume considered. It is therefore clear that the need to introduce ISVs arises from scaling considerations of the dynamically equivalent fields, and that additional ISVs are unnecessary in atomistic models because in this case the configuration of defects is completely prescribed by the position of atoms, and the dissipation by their rate of irreversible rearrangement. By disposing of the very large number of atomistic DOFs in the process of averaging the continuum stress and deformation fields, and representing the explicit defect fields by lower-order field variables, one would effectively move from a fully dynamic representation of lattice-defect interactions to a weaker, thermodynamically consistent representation. The order of the statistical representation of the evolving defect population in the continuum constitutive relations is invariably reduced. This scaling consideration is significant, as it affects the capability of the continuum constitutive relations to mimic path history dependence of non-equilibrium microstructure evolution obtained from MD simulations, for example. One then must choose between various representations of the defect fields and their evolution in order to model material response; there is always a ‘criterion of choice’ involved for the analyst. At the same time it becomes necessary to decompose rate of deformation, for example, into elastic and inelastic parts. Development of principles for establishing these criteria are yet another fertile area of future development. This is why we emphasize the distinction between the concept of a dynamically equivalent continuum and the related but separate issue of multiscale modelling or scale transition.

Finally, in passing, it is noted that the same formulation can be applied directly to higher-length-scale discrete particle systems without loss of generality, in analogy to other theories of polar continua. Such applications will allow an account of couple stress effects that arise either owing to interparticle polarity (e.g. friction) or owing to lower scale force dipoles (e.g. magnetodielectricity) that are incorporated into the particle description. For such higher-scale systems, however, non-local interactions with second- and higher-nearest-neighbour particles may be negligible; this may simplify the equivalence arguments set forth here.

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APPENDIX A SHAPE FUNCTIONS

In general, for polar materials, calculation of the couple stress involves a second spatial differentiation. Therefore, quadratic or even higher-order shape functions are

required. Higher-order shape functions are also needed when spatial regions V^e with $M > 4$ (three dimensions) and $M > 3$ (two dimensions) are considered. However, many analyses concern non-polar materials. If attention is focused on formulating a continuum representation using 3D tetrahedral elements or 2D triangular elements for solution convenience, linear shape functions can be used.

For 3D tetrahedral elements, the linear shape function is

$$N_1(\mathbf{r}) = \frac{|(\mathbf{r} - \mathbf{r}_2) \times (\mathbf{r} - \mathbf{r}_3) \cdot (\mathbf{r} - \mathbf{r}_4)|}{|(\mathbf{r}_1 - \mathbf{r}_2) \times (\mathbf{r}_1 - \mathbf{r}_3) \cdot (\mathbf{r}_1 - \mathbf{r}_4)|}, \quad (\text{A } 1)$$

where $\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}$. Expressions for N_2 , N_3 and N_4 can be obtained by even permutations of the indices. These functions and their gradients have the following properties.

$$N_I(\mathbf{r}_J) = \begin{cases} 1, & I = J, \\ 0, & I \neq J, \end{cases} \quad \sum_{I=1}^4 N_I = 1, \quad \int_{V^e} N_I dV = \frac{V^e}{4}, \quad \sum_{I=1}^4 \mathbf{B}_I = \mathbf{0}, \quad (\text{A } 2)$$

where $V^e = \frac{1}{6}|(\mathbf{r}_1 - \mathbf{r}_2) \times (\mathbf{r}_1 - \mathbf{r}_3) \cdot (\mathbf{r}_1 - \mathbf{r}_4)|$ is the volume of the tetrahedron. For 2D triangular elements and on 3D surfaces,

$$N_1(\mathbf{r}) = \frac{|(\mathbf{r} - \mathbf{r}_2) \times (\mathbf{r} - \mathbf{r}_3)|}{|(\mathbf{r}_1 - \mathbf{r}_2) \times (\mathbf{r}_1 - \mathbf{r}_3)|}. \quad (\text{A } 3)$$

Expressions for N_2 and N_3 can be obtained by even permutations of the indices. These functions have properties similar to those in equations (A 2), that is

$$N_I(\mathbf{r}_J) = \begin{cases} 1, & I = J, \\ 0, & I \neq J, \end{cases} \quad \sum_{I=1}^3 N_I = 1, \quad \int_{A^e} N_I dV = \frac{A^e}{3}, \quad \sum_{I=1}^3 \mathbf{B}_I = \mathbf{0}, \quad (\text{A } 4)$$

where $A^e = \frac{1}{2}|(\mathbf{r}_1 - \mathbf{r}_2) \times (\mathbf{r}_1 - \mathbf{r}_3)|$ is the area of the triangular element. When 2D triangular elements are used, only three of the six relations of equations (42) are independent and they can be chosen to be three of the following six, where the choice is arbitrary as long as not all three are for the same (x or y) direction:

$$\begin{aligned} (\sigma_{11}^{(e)} B_{11} + \sigma_{12}^{(e)} B_{12}) A^e &= p_{11}, \\ (\sigma_{21}^{(e)} B_{11} + \sigma_{22}^{(e)} B_{12}) A^e &= p_{12}, \\ (\sigma_{11}^{(e)} B_{21} + \sigma_{12}^{(e)} B_{22}) A^e &= p_{21}, \\ (\sigma_{21}^{(e)} B_{21} + \sigma_{22}^{(e)} B_{22}) A^e &= p_{32}, \\ (\sigma_{11}^{(e)} B_{31} + \sigma_{12}^{(e)} B_{32}) A^e &= p_{21}, \\ (\sigma_{21}^{(e)} B_{31} + \sigma_{22}^{(e)} B_{32}) A^e &= p_{32}; \end{aligned} \quad (\text{A } 5)$$

where p_{11} and p_{12} are the x and y components respectively of $\mathbf{f}_1^{\text{int}}$. In general, the first subscript of $p_{\alpha\beta}$ and $B_{\alpha\beta}$ refers to the atom with which the vectors are associated and the second subscript refers to the component of the vector. Note that $\alpha = 1, 2, 3$ and $\beta = 1, 2$ here. Also, $\sigma_{12}^{(e)} = \sigma_{21}^{(e)}$.

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