

SAND REPORT

SAND2002-8608

Unlimited Release

Printed December 2002

Continuum Definitions for Stress in Atomistic Simulation

J. A. Zimmerman, R. E. Jones, P. A. Klein, D. J. Bammann, E.B. Webb III, J.J. Hoyt

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

Approved for public release; further dissemination unlimited.



Sandia National Laboratories

Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.

NOTICE: This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof, or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof, or any of their contractors.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone: (865)576-8401
Facsimile: (865)576-5728
E-Mail: reports@adonis.osti.gov
Online ordering: <http://www.doe.gov/bridge>

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Rd
Springfield, VA 22161

Telephone: (800)553-6847
Facsimile: (703)605-6900
E-Mail: orders@ntis.fedworld.gov
Online order: <http://www.ntis.gov/ordering.htm>



SAND2002-8608
Unlimited Release
Printed December 2002

Continuum Definitions for Stress in Atomistic Simulation

J.A. Zimmerman R.E. Jones P.A. Klein D.J. Bammann
Science-based Materials Modeling Department

Sandia National Laboratories
P.O. Box 969
Livermore, CA 94551

E.B. Webb III J.J. Hoyt
Materials & Process Modeling Department

Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87158

Abstract

This report is a collection of documents written by the group members of the Engineering Sciences Research Foundation (ESRF), Laboratory Directed Research and Development (LDRD) project titled "A Robust, Coupled Approach to Atomistic-Continuum Simulation". An essential requirement of this project is to develop definitions for continuum quantities that can be evaluated locally within an atomistic region. We are developing physical measures of stress, deformation and temperature that are calculable in an atomistic simulation and have well-defined meanings when evaluated in the continuum limit. During the course of FY02, we reviewed many articles presenting the use of definitions of stress in atomistic simulation. The key articles were identified and summarized via internal documents.

Keywords: stress; atomistic simulation; continuum mechanics; virial theorem; crystal; free surface; Cauchy stress.

This page intentionally left blank.

Contents

1	Introduction	9
2	Correspondence of atomistic and continuum boundary value problems	11
2.1	Describing material motion	11
2.2	Correspondence of continuum and atomistic boundary value problems	11
3	A Critical Review of the Virial Theorem	15
3.1	Mean stress theorem	15
3.2	Virial theorem	16
3.3	Comments	18
4	Stress Expression of Cheung and Yip	19
4.1	Cauchy's tetrahedron	19
4.2	Cheung and Yip's stress expression	20
4.3	Comments	21
5	Atomistic-Continuum Formulation of Lutsko and Cormier <i>et al.</i>	23
5.1	Particle mechanics	23
5.2	Cormier's formulation	24
5.3	Comments	27
6	Atomistic-Continuum Formulation of Robert J. Hardy	29
6.1	Review of continuum mechanics	29
6.2	Hardy's formulation	32
6.2.1	Densities and Localization	32
6.2.2	Energy and Force Assumptions	34
6.2.3	Hardy's balance laws	35
6.2.4	Macroscopic Flow and Microscopic Motion	38
6.3	Comparison of Hardy's method with Moving Least Squares	42
6.3.1	Moving Least Squares (MLS) particle methods	42
6.3.2	Comparison of Hardy's atomistic method and MLS methods	44
6.4	Evaluation of Continuum Stress in Atomistic Simulation	45
6.4.1	Stress in a crystal at zero temperature	45

6.4.2	Stress in a crystal at finite temperature	48
6.4.3	Stress in a crystal with a free surface	48
6.4.4	Remarks	49
6.5	Extending Hardy's formulation to non-central potentials	51
6.5.1	Bonds, Energies and Forces in Atomistic Mechanics	51
6.5.2	Hardy's Assumptions Revisited	53
6.5.3	Using Hardy's method for 3-body forces	56
6.6	Comments	60
7	Eringen's Micropolar Continuum Formulation	61
7.1	Motivation	61
7.2	Kinematics of a micromorphic continuum	61
7.3	Kinematics of a micropolar continuum	62
7.4	Mass and inertia	64
7.5	Balance laws	65
7.6	Preface to Hardy formulation	67
8	Bibliography	68
9	Distribution	77

List of Figures

6.1	MLS representations of a linear field.	43
6.2	Virial and Hardy stress for an atomic system at zero temperature and pressure.	45
6.3	Mean of the Hardy stress averaged over many spatial points.	47
6.4	Variance of the Hardy stress averaged over many spatial points.	47
6.5	Virial and Hardy stress for an atomic system at zero temperature and 2% uniaxial strain.	48
6.6	The force-term portions of the Virial and Hardy stresses for an atomic system at room temperature and 5% uniaxial strain.	49
6.7	Virial and Hardy stress for an atomic system at zero temperature and pressure with a free surface. The heavy, dashed line denotes the position of the top layer of atoms, both at zero, while the heavy, solid line denotes the effective position of the free surface of the crystal.	50
6.8	The normal stresses for the cubic directions parallel to the free surface for the system shown in Figure 6.7.	51

This page intentionally left blank.

Chapter 1

Introduction

This report is a collection of documents written by the group members of the Engineering Sciences Research Foundation (ESRF), Laboratory Directed Research and Development (LDRD) project titled “A Robust, Coupled Approach to Atomistic-Continuum Simulation”. With the growing focus on predictive modeling and simulation, Sandia must develop the capability to model deformation and failure in multiple scale settings. We are developing a robust approach to coupled atomistic-continuum simulation, capable of both quasi-static and finite temperature/dynamic analyses. Sandia currently does not have this simulation capability. Our methodology will simulate systems at finite temperatures correctly, which involves the transfer of energy from the continuous spectrum of vibrations in the atomistic region to the separate modes of a scalar temperature field and long elastic waves in the continuum. Current schemes in the literature make no attempt to differentiate between the exchange of thermal and elastic energy. A comprehensive framework is being created to relate the dynamic motion of atoms with the kinetics of a continuum. Our approach will introduce high-fidelity physics to capture nano-scale processes, while using continuum mechanics to model the elastic deformation for the majority of a system with micro-scale dimensions.

An essential requirement of our work is to develop definitions for continuum quantities that can be evaluated locally within an atomistic region. Currently, continuum variables are only defined in terms of equilibrium thermodynamics. The instantaneous, individual atomic contributions to these averages do not have the same physical interpretation as the corresponding point-wise continuum quantities. We are developing physical measures of stress, deformation and temperature that are calculable in an atomistic simulation and have well-defined meanings when evaluated in the continuum limit.

The first task required for the success of this project was a thorough study of current definitions of stress, deformation and temperature used in atomistic calculations. During the course of FY02, many articles were reviewed, and the key ones were identified and summarized via internal documents. This report is a collection of those documents. Chapter 2 draws a correspondence between the atomistic and continuum viewpoints of defining a boundary value problem. Chapter 3 presents a critical review of the virial theorem, the first defini-

CHAPTER 1. INTRODUCTION

tion of stress for an atomistic system that has physical meaning within a thermo-mechanical continuum. The theorem was simultaneously developed by Clausius [1] and Maxwell [2, 3] to quantify the stress or pressure field applied to fixed volume of energetically-interacting particles. Chapter 4 discusses the article by Cheung and Yip [4], a notable paper that presented the consequences of misusing the virial theorem to define a local measure of Cauchy stress. Chapter 5 summarizes the works by Lutsko [5] and Cormier *et al.* [6]. These articles attempted to define continuum fields in terms of atomistic variables, albeit with moderate success. Chapter 6 reviews the formulation of Robert J. Hardy, who makes a similar attempt as Lutsko and Cormier *et al.* This formulation was found to be preferable to all previous works, although the current version cannot be used for all types of interatomic potentials. The project group members are in the process of determining if combining Hardy's method with Eringen's micropolar elasticity [7] would generalize its usage. Chapter 7 reviews Eringen's methodology for completeness.

Chapter 2

Correspondence of atomistic and continuum boundary value problems

2.1 Describing material motion

A “motion” is a Lagrangian construct where a fixed reference configuration is mapped by a time-dependent function χ_t , the “motion”, to the configuration at any time t . A “flow”, on the other hand, is an Eulerian construct where any configuration at time s is mapped to the configuration at time t by the function $\phi_{t,s}$ called the “flow”. If the motion is invertible a flow can be constructed $\phi_{t,s} = \chi_t \circ \chi_s^{-1}$. Likewise, a motion for which the reference configuration is the initial configuration is obtained by $\chi_t = \phi_{t,0}$

In a continuum, the mapping function χ_t can be applied to a reference position vector anywhere within the domain, and maps it to some new value in the continuous deformed configuration. For a particle assemblage, the position vectors can only take on discrete values corresponding to particle positions for both the reference and deformed configurations.

2.2 Correspondence of continuum and atomistic boundary value problems

Let’s examine three nested classes of motions:

Class A. Globally polynomial :

$$\chi(\mathbf{X}) = \mathbf{C}_0 + \mathbf{C}_1\mathbf{X} + \frac{1}{2}\mathbf{C}_2(\mathbf{X} \otimes \mathbf{X}) + \dots$$

where \mathbf{C}_n is an n th order constant tensor,

Class B. Smooth :

no Burger’s vectors and all derivatives $\partial_{\mathbf{X}}^i \chi$, $i = 1, 2, \dots$ exist,

CHAPTER 2. CORRESPONDENCE OF ATOMISTIC AND CONTINUUM BOUNDARY VALUE PROBLEMS

Class C. General

Any homogeneous deformation of a body is an example of a first order Class A motion i.e. $C_n = 0, n > 1$. “Pure” beam bending is an example of a second order Class A motion. Given a bounded domain and the Stone-Weierstrass theorem, Class B motions can be approximated by Class A motions using, say, a Taylor series. Question : can Class B *boundary value problems* (BVPs) be approximated by Class A problems?

Although it is not clear how to compare stresses in continuum to forces in an atomistic simulation, it is always possible to compare the corresponding motions. This leads to the idea of “equivalent” problems, where the same motion results given the same prescribed *displacement* boundary conditions, side-stepping the atomic force-continuum stress relationship for the moment. A plausible conjecture is that only problems with no length-scale and self-similarity with scaling would have “equivalent” continuum and atomistic representations. A further conjecture is that all of the problems in Class A fall into this category, i.e. they have “equivalent” representations.

So why do we care? First of all, we would like to have an idea of when a continuum solution is also a atomistic solution and we would like to make a correspondence between atomistic material behavior and continuum constitutive models.

To get a sense of what forces are generated by the *deformation* induced by a motion governed by the balance laws (typically balance of linear and angular momentum and conservation of mass), an atomistic model of material looks at the relative motion of atoms currently neighboring a particular atom; on the other hand, a continuum model of material looks at the derivatives of the motion at a point of interest (in fact only certain parts of the derivatives affect the stress e.g. local rotations do not change the strain energy of a hyperelastic material). These models can be seen to be extracting similar information. For example, both formulations are insensitive to zeroth order Class A motions, i.e. rigid displacements. Furthermore, nearest neighbors lead to finite difference, i.e. discrete approximations, of the gradient of the local motion and, conversely, higher order gradients of the motion carry more information about the neighboring deformation state i.e. torsion as well as rotation and stretch of material (as well as smoothness requirements).

There are distinct differences between the models too. In atomistic models the use of nearest neighbors leads to the definition of a (non-local) region surrounding the point of interest from which information is drawn. Without information from neighbors in a region of a certain minimum size, the particles cannot interact and response of the particles as a material cannot be modelled. This is unlike a continuum point for which the limit as a neighborhood shrinks to a point exists, at least for classical theories like hyperelasticity. Nevertheless, in both paradigms a first order approximation of the motion in the constitutive model relating deformation to force is sufficient to generate higher order motions e.g. classical linear elasticity which only depends on the (symmetric part of the) first order gradient admits pure bending and more complicated global motions.

For atomistic models, we can expect convergence of kinematic (and hopefully kinetic) measures, e.g. strain, as the neighborhood shrinks for smooth enough (i.e. Class A) motions up to to a minimum neighborhood where not enough information is being sampled (which

2.2. CORRESPONDENCE OF CONTINUUM AND ATOMISTIC BOUNDARY VALUE PROBLEMS

usually corresponds to the neighborhood over which the force interactions are defined). The polynomial order of motion for the particular BVP together with the type representation used for the kinematic measure determine the rate and limit convergence. In an analogy with finite elements (which are effectively discrete chunks of material), we see for pure beam bending with linear elements convergence to the exact solution but with quadratic elements an exact representation of the motion determined by the BVP. So if the atomistic kinematic measure incorporates enough neighbors to reconstruct the global motion in that neighborhood and the forces generated depend on that deformation, it can be then put into correspondence with *some* continuum material model for a material region undergoing an equivalent motion. Note that this hypothetical kinematic measure might have no effect on the solution of the atomistic BVP and, like most that we've seen, may be merely a post-processing of the atomistic solution.

So, the measure/s we choose to make the correspondence between the atomistic and continuum BVPs, if it is not the motion, will determine how the corresponding constitutive models are related. In this vein we discussed the various types of continuum constitutive models used to represent metals:

- Point: only local information (and first derivatives) are used to determine material response e.g. elasticity.
- Neighborhood: inhomogeneous fields in neighborhood are sampled for the constitutive response, but no dislocations are modelled.
- Discrete dislocation: sufficiently low populations of dislocations exist so that there are not enough to generate a reasonable "density" of dislocations, and dislocations are individually represented.
- Dislocation density : a net Burger's vector for the neighborhood exists and phenomenological dislocation dynamics are employed.
- Phenomenological : e.g. classical plasticity with "plastic" gradient to represent irreversible motions.

The idea being that the correspondence between atom and continuum might require using an continuum model with more information than the classical "Point" type. This may not be true for motions restricted to Class A.

CHAPTER 2. CORRESPONDENCE OF ATOMISTIC AND CONTINUUM
BOUNDARY VALUE PROBLEMS

This page intentionally left blank.

Chapter 3

A Critical Review of the Virial Theorem

3.1 Mean stress theorem

For a continuum body occupying region Ω and in equilibrium :

$$\partial_{\mathbf{x}} \cdot \boldsymbol{\sigma} + \rho \mathbf{b} = \mathbf{0} ,$$

where $\boldsymbol{\sigma}$ is the Cauchy stress, ρ is the mass density, \mathbf{b} is the body force, and $\partial_{\mathbf{x}} \equiv \frac{\partial}{\partial \mathbf{x}}$. The mean (Cauchy) stress, $\bar{\boldsymbol{\sigma}}$, is given by

$$\begin{aligned} V_{\Omega} \bar{\boldsymbol{\sigma}} &= \int_{\Omega} \boldsymbol{\sigma} dv = \int_{\Omega} \boldsymbol{\sigma} \cdot \partial_{\mathbf{x}} \mathbf{x} dv \\ &= \int_{\Omega} -\partial_{\mathbf{x}} \cdot \boldsymbol{\sigma} \otimes \mathbf{x} dv + \int_{\partial\Omega} \mathbf{t} \otimes \mathbf{x} da \\ &= \int_{\Omega} \rho \mathbf{b} \otimes \mathbf{x} dv + \int_{\partial\Omega} \mathbf{t} \otimes \mathbf{x} da \end{aligned} \quad (3.1)$$

by way of the divergence theorem and the definition $\mathbf{t} = \boldsymbol{\sigma} \mathbf{n}$, where \mathbf{n} is the outward unit normal. A similar but more complicated expression can be derived for a continuum body that is not in equilibrium

$$\begin{aligned} V_{\Omega} \bar{\boldsymbol{\sigma}} &= \int_{\Omega} \rho (\mathbf{b} - \ddot{\mathbf{x}}) \otimes \mathbf{x} dv + \int_{\partial\Omega} \mathbf{t} \otimes \mathbf{x} da \\ &= \int_{\Omega} \rho \dot{\mathbf{x}} \otimes \dot{\mathbf{x}} dv - \frac{d}{dt} \int_{\Omega} \rho \dot{\mathbf{x}} \otimes \mathbf{x} dv + \int_{\Omega} \rho \mathbf{b} \otimes \mathbf{x} dv + \int_{\partial\Omega} \mathbf{t} \otimes \mathbf{x} da \end{aligned} \quad (3.2)$$

where the first term can be recognized as twice the tensor \mathbf{K}_{Ω} whose trace is the kinetic energy K_{Ω} for the region.

3.2 Virial theorem

The equations of motion (Newton's Law) for a system of particles $\{\alpha = 1..N\}$ are

$$m^\alpha \ddot{\mathbf{x}}^\alpha = \mathbf{F}^\alpha \quad (3.3)$$

where m^α is the particle's mass, \mathbf{x}^α is its position and \mathbf{F}^α is the force acting on it. With manipulation (3.3) becomes

$$m^\alpha \frac{d}{dt} (\dot{\mathbf{x}}^\alpha \otimes \mathbf{x}^\alpha) - m^\alpha \dot{\mathbf{x}}^\alpha \otimes \dot{\mathbf{x}}^\alpha = \mathbf{F}^\alpha \otimes \mathbf{x}^\alpha. \quad (3.4)$$

After taking a (long) time average for the set $\{\alpha = 1, 2, \dots, N\}$

$$-\left\langle \sum_{\alpha=1}^N m^\alpha \dot{\mathbf{x}}^\alpha \otimes \dot{\mathbf{x}}^\alpha \right\rangle = \left\langle \sum_{\alpha=1}^N \mathbf{F}^\alpha \otimes \mathbf{x}^\alpha \right\rangle. \quad (3.5)$$

where

$$\left\langle \sum_{\alpha=1}^N m^\alpha \frac{d}{dt} (\dot{\mathbf{x}}^\alpha \otimes \mathbf{x}^\alpha) \right\rangle := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \sum_{\alpha=1}^N m^\alpha \frac{d}{dt} (\dot{\mathbf{x}}^\alpha \otimes \mathbf{x}^\alpha) dt = 0$$

is assumed. This assumption is based on constant particle masses and the idea that the system will have a bounded total momentum-position dyad $\sum_{\alpha=1}^N m^\alpha \dot{\mathbf{x}}^\alpha \otimes \mathbf{x}^\alpha$ far in the future (as it does in the beginning $t = 0$) so that

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \sum_{\alpha=1}^N m^\alpha \frac{d}{dt} (\dot{\mathbf{x}}^\alpha \otimes \mathbf{x}^\alpha) dt = \lim_{T \rightarrow \infty} \frac{1}{T} \left(\sum_{\alpha=1}^N m^\alpha \dot{\mathbf{x}}^\alpha \otimes \mathbf{x}^\alpha \Big|_{t=T} - \sum_{\alpha=1}^N m^\alpha \dot{\mathbf{x}}^\alpha \otimes \mathbf{x}^\alpha \Big|_{t=0} \right) = 0.$$

Practically speaking, the size of the time interval $[0, T]$ must be much larger than the difference in the total momentum-position dyad at the end-points for this to be true.

Now, with forces split into those internal to the system and those external, (3.5) becomes

$$-2 \langle \mathbf{K}_N \rangle = \left\langle \sum_{\alpha=1}^N \mathbf{F}_{int}^\alpha \otimes \mathbf{x}^\alpha \right\rangle + \left\langle \sum_{\alpha=1}^N \mathbf{F}_{ext}^\alpha \otimes \mathbf{x}^\alpha \right\rangle. \quad (3.6)$$

after recognizing the LHS as twice the tensor \mathbf{K}_N whose trace is the kinetic energy, K_N , of the system. The internal forces result from the interatomic potentials and can be written $\mathbf{F}_{int}^\alpha = -\partial_{\mathbf{x}^\alpha} U_N$, where U_N is the potential energy for the system (which depends on the configuration of the system and the inter-atomic potential). Equation (3.6) is known as the dyad form of the classical *virial theorem*. Clausius' original work [1] used the dot product instead of the dyad product, and connected the time average term containing the external forces to a measurable pressure used to contain a volume of gas at finite temperature. The dyad form appearing in (3.6) was first done by Maxwell [2, 3] at approximately the same time as Clausius' effort.

Assuming that all \mathbf{F}_{ext} results from continuum surface tractions (i.e. $\mathbf{b} = \mathbf{0}$) and the same argument regarding total momentum-position dyad holds for (3.2), it is possible to compare (3.6)

$$-\left\langle \sum_{\alpha=1}^N \mathbf{F}_{int}^{\alpha} \otimes \mathbf{x}^{\alpha} \right\rangle = 2 \langle \mathbf{K}_N \rangle + \left\langle \sum_{\alpha=1}^N \mathbf{F}_{ext}^{\alpha} \otimes \mathbf{x}^{\alpha} \right\rangle .$$

with a reduced form of (3.2)

$$\langle V_{\Omega} \bar{\boldsymbol{\sigma}} \rangle = 2 \langle \mathbf{K}_{\Omega} \rangle + \left\langle \int_{\partial\Omega} \mathbf{t} \otimes \mathbf{x} da \right\rangle \quad (3.7)$$

Now, formally at least, $d\mathbf{F} = \mathbf{t}_n da$ and so it's possible to relate terms in the atomistic and continuum expressions. If the naive correspondence between the kinetic energies¹ $2 \langle \mathbf{K}_N \rangle \approx 2 \langle \mathbf{K}_{\Omega} \rangle$ is made, and the external forces are considered comparable $\left\langle \sum_{\alpha=1}^N \mathbf{F}_{ext}^{\alpha} \otimes \mathbf{x}^{\alpha} \right\rangle \approx \left\langle \int_{\partial\Omega} \mathbf{t} \otimes \mathbf{x} da \right\rangle$, then

$$\langle V_{\Omega} \bar{\boldsymbol{\sigma}} \rangle = - \left\langle \sum_{\alpha=1}^N \mathbf{F}_{int}^{\alpha} \otimes \mathbf{x}^{\alpha} \right\rangle .$$

It follows that

$$\langle V_{\Omega} \bar{\boldsymbol{\sigma}} \rangle = 2 \langle \mathbf{K}_N \rangle + \left\langle \sum_{\alpha=1}^N \mathbf{F}_{ext}^{\alpha} \otimes \mathbf{x}^{\alpha} \right\rangle .$$

This departs from traditional derivations which seem to have the obvious inconsistency that a dynamic version of Newton's momentum balance is used for the particles but a static version of the linear momentum balance is used for the continuum. (This disparate treatment may be justified, in part, by the fact that an atomistic system has momenta associated with the continuum quantity "temperature".) Also this derivation obviates the quandary of the type of boundary condition seeming to define the stress quantity being measured e.g. with frictionless boundaries only spherical stress tensors result. Clearly, the boundary conditions do still affect the motions but in actuality the material response due to U_N , which can be interpreted as strain energy, determines the mean stress.

Now, say the same procedure was not applied to an impermeable material region but to a spatially fixed "box". Unfortunately,

$$\left\langle \sum_{\alpha \in \square} m^{\alpha} \frac{d}{dt} (\dot{\mathbf{x}}^{\alpha} \otimes \mathbf{x}^{\alpha}) \right\rangle := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \sum_{\alpha \in \square} m^{\alpha} \frac{d}{dt} (\dot{\mathbf{x}}^{\alpha} \otimes \mathbf{x}^{\alpha}) dt$$

is not necessarily zero since $\sum_{\alpha \in \square}$ and $\frac{d}{dt}$ do not commute. However, recognizing this expression as the "(internal) generation" term of a discrete transport theorem :

$$\text{total change in set} = \text{generation within set} + \text{flux into set} . \quad (3.8)$$

¹This correspondence may be scale dependent and require modification to distinguish macroscopic kinetic motion from microscopic thermal motion, see Chapter 6.

Since no acceptable densities can be defined, a rate form of (3.8) is difficult to construct; consequently

$$\left\langle \frac{d}{dt} \sum_{\alpha \in \square} m^\alpha (\dot{\mathbf{x}}^\alpha \otimes \mathbf{x}^\alpha) \right\rangle = \left\langle \sum_{\alpha \in \square} m^\alpha \frac{d}{dt} (\dot{\mathbf{x}}^\alpha \otimes \mathbf{x}^\alpha) \right\rangle + \langle \mathcal{F}_{mp} \rangle \quad (3.9)$$

makes sense, where $\langle \mathcal{F}_{mp} \rangle$ is the long time average of the flux of momentum-position dyads $m^\alpha (\dot{\mathbf{x}}^\alpha \otimes \mathbf{x}^\alpha)$, but a flux rate \mathcal{F}_{mp} has only a formal definition. For bounded systems, the left hand side of equation (3.9) equals zero. So, the creation of momentum within the spatial region, *i.e.* a non-zero value for $\langle \sum_{\alpha \in \square} m^\alpha \frac{d}{dt} (\dot{\mathbf{x}}^\alpha \otimes \mathbf{x}^\alpha) \rangle$, has to be balanced by the flux $-\langle \mathcal{F}_{mp} \rangle$. With this in hand,

$$\langle V_\Omega \bar{\sigma} \rangle = 2 \langle \mathbf{K}_N \rangle - \langle \mathcal{F}_{mp} \rangle + \left\langle \sum_{\alpha=1}^N \mathbf{F}_{ext}^\alpha \otimes \mathbf{x}^\alpha \right\rangle$$

results.

3.3 Comments

The virial theorem provides the oldest, and most frequently used, expression for relating forces and motion within an atomic system to a continuum stress. As we have noted in this chapter, it does contain several deficiencies. The virial theorem only relates continuum properties to time and ensemble averages of system properties; the stress expression developed has no clear physical meaning at an arbitrary point in space and time. Some ambiguity exists with regard to how boundary conditions affect the form of the derived stress expression. Also, the naive correspondence between atomic and continuum kinetic energies may be scale dependent and may be problematic for a dynamic continuum at finite temperature. Nevertheless, the virial theorem remains the yardstick by which other expressions for stress are measured. All other derived formulations for stress will be expected to yield the virial theorem's behavior for the appropriate limits of space and time averaging.

Chapter 4

Stress Expression of Cheung and Yip

4.1 Cauchy's tetrahedron

¹By a simple geometric argument, Cauchy derived a stress tensor $\boldsymbol{\sigma}$ from a surface traction vector \mathbf{t} (\mathbf{t} is admitted *a priori*).

Take the integral statement of the balance of linear momentum for a tetrahedral material region \mathcal{T}

$$\int_{\mathcal{T}} \rho(\dot{\mathbf{v}} - \mathbf{b})dV = \int_{\partial\mathcal{T}} \mathbf{t}dA \quad (4.1)$$

where ρ is mass density, \mathbf{v} is velocity and \mathbf{b} is body force. Orient \mathcal{T} so that three of the faces have outward normals in the cardinal directions $\mathbf{e}_i, i = 1..3$ and the fourth face has an outward normal \mathbf{n} , so that

$$\int_{\partial\mathcal{T}} \mathbf{t}dA = \int_S \mathbf{t}_n dA + \sum_i \int_{S_i} \mathbf{t}_{e_i} dA$$

where S is the area of the face with normal \mathbf{n} (and \mathbf{t}_n denotes the traction vector on the surface S with normal \mathbf{n}). To be brief, as the tetrahedron is made smaller the LHS of (4.1) remains bounded since all functions are assumed continuous and limiting expression is obtained

$$\|\rho(\dot{\mathbf{v}} - \mathbf{b})\|^* \frac{1}{3}Sh \geq \|\mathbf{t}_n^* S - \sum_i \mathbf{t}_{e_i}^* S n_i\| \quad (4.2)$$

where $(\bullet)^*$ represents the mean value of the respective integrand and h is the height of the tetrahedron to the S face. Recalling $\mathbf{a} \otimes \mathbf{b} \mathbf{c} = \mathbf{a}(\mathbf{b} \cdot \mathbf{c})$, it follows that

$$\mathbf{t}_n = \sum_i \mathbf{t}_{e_i} n_i = \sum_i (\mathbf{t}_{e_i} \otimes \mathbf{e}_i) \mathbf{n} = \sum_i \sum_j \sigma_{ji} \mathbf{e}_j n_i \quad (4.3)$$

¹The development in this section follows class notes from the course taught by P.M. Naghdi at U.C. Berkeley.

where σ_{ij} are the components of $\boldsymbol{\sigma}$, which can be shown to be tensorial i.e. transform correctly with change of coordinates. Clearly, Equation (4.3) is the familiar $\mathbf{t} = \boldsymbol{\sigma} \mathbf{n}$ and, furthermore, it shows that the stress tensor $\boldsymbol{\sigma}$ can be represented by the traction vectors on three independent (in this case orthogonal) planes.

4.2 Cheung and Yip's stress expression

Seemingly in the spirit of Cauchy's construction, Cheung and Yip [4] develop an expression for stress based on the "time rate of change of momentum flux across a surface". This surface is fixed in space unlike the material surfaces in (4.1) and Cheung and Yip's expression for a stress measure

$$\boldsymbol{\sigma} = \frac{1}{A} \left[-\frac{1}{2} \sum_{\alpha \in \mathcal{C}} \frac{m_\alpha}{\Delta t} \mathbf{v}_\alpha \otimes \mathbf{n} + \sum_{(\alpha, \beta) \in \mathcal{P}} \frac{\partial \phi}{\partial \mathbf{x}^{\alpha\beta}} \frac{\mathbf{x}^{\alpha\beta} \cdot \mathbf{n}}{|\mathbf{x}^{\alpha\beta} \cdot \mathbf{n}|} \frac{1}{x^{\alpha\beta}} \mathbf{x}_{\alpha\beta} \otimes \mathbf{n} \right] \quad (4.4)$$

is immediately restricted to pair potentials. (Spatial regions are a necessity given that material surfaces are hard to define in particle systems.) The expression (4.4) appears without a derivation and a number of oddities are embedded in it. First of all, it refers to a single surface S , not three as in Cauchy's developments, with outward normal \mathbf{n} and area A . Second, the first term in (4.4) is summed over the set of particles \mathcal{C} that cross S over a time interval of length Δt and the second term is summed over different set of particles \mathcal{P} , (unique) pairs that have force interactions across S at a unspecified time. The sets \mathcal{C} and \mathcal{P} can be very different depending on the magnitude of $\mathbf{v} \cdot \mathbf{n} \Delta t$ versus the typical interaction distance. (In fact, for some of Cheung and Yip's examples \mathcal{C} is empty.) The first term is obviously some measure of momentum flux and the second term can be recognized as

$$-\frac{1}{2} \sum_{(\alpha, \beta) \in \mathcal{P}} \frac{\mathbf{x}^{\alpha\beta} \cdot \mathbf{n}}{|\mathbf{x}^{\alpha\beta} \cdot \mathbf{n}|} \mathbf{F}_{\alpha\beta} \otimes \mathbf{n} .$$

where $\mathbf{F}_{\alpha\beta}$ is the pair force between atoms α and β . Cheung and Yip explain the $\frac{\mathbf{x}^{\alpha\beta} \cdot \mathbf{n}}{|\mathbf{x}^{\alpha\beta} \cdot \mathbf{n}|}$ coefficient as a term that gives the contribution of $\mathbf{F}_{\alpha\beta}$ the same sign as $\mathbf{F}_{\alpha\beta}$ relative to the outward normal \mathbf{n} . In essence, the second term of (4.4) is

$$-\frac{1}{2} \sum_{(\alpha, \beta) \in \mathcal{P}^+} \mathbf{F}_{\alpha\beta} \otimes \mathbf{n}$$

where the sum is now over the set \mathcal{P}^+ of oriented pairs, composed of atoms α on the inward side of the surface that have pair interactions with atoms β on the outward side.

If Δt is allowed to go to its infinitesimal limit, and the assumption is made that the set \mathcal{C} coincides with the set \mathcal{P}^+ , the expression takes the form

$$\boldsymbol{\sigma} = -\frac{1}{2A} \left[\sum_{\alpha \in \mathcal{P}^+} m_\alpha \frac{d}{dt} \mathbf{v}_\alpha \otimes \mathbf{n} + \sum_{(\alpha, \beta) \in \mathcal{P}^+} \mathbf{F}_{\alpha\beta} \otimes \mathbf{n} \right]$$

which, after employing Newton's 2nd and 3rd laws, becomes

$$\boldsymbol{\sigma} = -\frac{1}{2A} \left[\sum_{\alpha \in \mathcal{P}^+} \sum_{\beta \neq \alpha} \mathbf{F}_{\alpha\beta} \otimes \mathbf{n} + \sum_{(\alpha,\beta) \in \mathcal{P}^+} \mathbf{F}_{\alpha\beta} \otimes \mathbf{n} \right].$$

This is an odd result indeed, for no other reason than the forces for pairs straddling the surface are counted with a -1 factor and all the others with $-\frac{1}{2}$ factor

$$\boldsymbol{\sigma} = \frac{1}{A} \left[\sum_{\alpha \in \mathcal{P}^+} \left(-\frac{1}{2} \sum_{\beta \neq \alpha, \beta \notin \mathcal{P}^+} \mathbf{F}_{\alpha\beta} \otimes \mathbf{n} - \sum_{\beta \neq \alpha, \beta \in \mathcal{P}^+} \mathbf{F}_{\alpha\beta} \otimes \mathbf{n} \right) \right].$$

A more rational expression could be derived by employing Cauchy's methodology for a finite tetrahedral region \mathcal{T}_h in the atomistic particle system. There is a small concern since *material* surfaces such as the boundaries of \mathcal{T}_h are not easily definable in the particle system; however, at any instant a spatial surface coincides with some material surface. So, the mean value in the finite tetrahedral region of a Cauchy-like stress $\boldsymbol{\sigma}$ could be related to the traction vectors derived from solely from the sources of momentum i.e. the potential forces

$$\mathbf{t}_{\mathbf{e}_i} = \sum_{(\alpha,\beta) \in \mathcal{P}_{\mathbf{e}_i}^+} \mathbf{F}_{\alpha\beta}$$

on the three orthogonal bounding surfaces S_i , with related sets $\mathcal{P}_{\mathbf{e}_i}^+$, using $\boldsymbol{\sigma} = \mathbf{t}_{\mathbf{e}_i} \otimes \mathbf{e}_i$; however, it's doubtful that this measure would transform tensorially with change of basis \mathbf{e}_i .

4.3 Comments

Although the effort exerted by Cheung and Yip to derive an expression for stress based on considerations of internal forces and momentum flux is admirable, the end product, equation (4.4), is ill-suited for the point-wise calculation of stress within an atomic system during molecular dynamic or static simulation. For such a calculation, the spatial planes discussed are difficult to define. The construction of their expression is ad-hoc and does not conform to any standard continuum formulation. In addition, the factor of "1/2" used for the momentum term in (4.4) is suspect as its origins are not explained, and the factor is missing in earlier work by Tsai [8].

This page intentionally left blank.

Chapter 5

Atomistic-Continuum Formulation of Lutsko and Cormier *et al.*

5.1 Particle mechanics

For a system of N particles with positions \mathbf{x}^α and momenta \mathbf{p}^α , the Hamiltonian, or total energy,

$$H = \sum_{\alpha} \frac{1}{2m^{\alpha}} \mathbf{p}^{\alpha} \cdot \mathbf{p}^{\alpha} + \Phi(\mathbf{x}^{\alpha})$$

is composed of the usual kinetic and potential energies. The resulting equations of motion are

$$\begin{aligned} \dot{\mathbf{x}}^{\alpha} &= \partial_{\mathbf{p}^{\alpha}} H = \frac{1}{m^{\alpha}} \mathbf{p}^{\alpha} \\ \dot{\mathbf{p}}^{\alpha} &= -\partial_{\mathbf{x}^{\alpha}} H = -\partial_{\mathbf{x}^{\alpha}} \Phi \end{aligned} \tag{5.1}$$

the second of which is identical to Newton's First Law or Lagrange's formulation for a system of particles. Note that the superposed dot represents the time derivative of the quantity *for the particle*, not a position in space.

Implicit in this formulation is a (trivial) conservation of mass

$$\frac{d}{dt} \sum_{\alpha} m^{\alpha} = 0$$

for the whole system, and (redundant) balance of angular momentum

$$\mathbf{x}^{\alpha} \times (\dot{\mathbf{p}}^{\alpha} + \partial_{\mathbf{x}^{\alpha}} \Phi) = \mathbf{0}$$

for individual particles. So there are no natural analogues to the corresponding balances in a continuum.

5.2 Cormier's formulation

Cormier [6] and Lutsko [5] choose to define the momentum of the system as

$$\mathbf{p} = \sum_{\alpha} \mathbf{p}^{\alpha} \delta(\mathbf{x} - \mathbf{x}^{\alpha})$$

where $\delta(\mathbf{x})$ is the Dirac delta "function". Its spatial Fourier transform, i.e. transform from \mathbf{x} space to \mathbf{k} wave vector space, is

$$\hat{\mathbf{p}} = \mathcal{F}\mathbf{p} = \int_{\Omega} d\mathbf{x} \exp(i\mathbf{k} \cdot \mathbf{x}) \mathbf{p} = \sum_{\alpha} \mathbf{p}^{\alpha} \exp(i\mathbf{k} \cdot \mathbf{x}^{\alpha})$$

where Ω is the extent of the whole system and *should be infinite* for a classical Fourier transform. An integral transform is necessary for any manipulation due to the delta function; alternate integral transforms exist e.g. the wavelet transform. The time derivative of $\hat{\mathbf{p}}$ is

$$\left. \frac{\partial}{\partial t} \right|_{\mathbf{k}} \hat{\mathbf{p}} = \sum_{\alpha} \dot{\mathbf{p}}^{\alpha} \exp(i\mathbf{k} \cdot \mathbf{x}^{\alpha}) + \mathbf{p}^{\alpha} \exp(i\mathbf{k} \cdot \mathbf{x}^{\alpha}) i\mathbf{k} \cdot \dot{\mathbf{x}}^{\alpha}. \quad (5.2)$$

Substituting Hamilton's equations of motion (5.1) for the particles and factoring out the exponential function leads to

$$\left. \frac{\partial}{\partial t} \right|_{\mathbf{k}} \hat{\mathbf{p}} = \sum_{\alpha} \left(-\partial_{\mathbf{x}^{\alpha}} \Phi + (i\mathbf{k} \cdot \frac{1}{m^{\alpha}} \mathbf{p}^{\alpha}) \mathbf{p}^{\alpha} \right) \exp(i\mathbf{k} \cdot \mathbf{x}^{\alpha}).$$

With the assumption that the system potential is composed of pair potentials

$$\Phi(\mathbf{x}^{\alpha}) = \frac{1}{2} \sum_{\alpha} \sum_{\beta \neq \alpha} \phi^{\alpha\beta}(x^{\alpha\beta}),$$

where $x^{\alpha\beta}$ is defined as the magnitude of

$$\mathbf{x}^{\alpha\beta} = \mathbf{x}^{\alpha} - \mathbf{x}^{\beta},$$

the first term in (5.2) becomes

$$\begin{aligned} \sum_{\gamma} \partial_{\mathbf{x}^{\gamma}} \Phi \exp(i\mathbf{k} \cdot \mathbf{x}^{\gamma}) &= \frac{1}{2} \sum_{\gamma} \sum_{\alpha} \sum_{\beta \neq \alpha} \frac{d\phi^{\alpha\beta}}{dx^{\alpha\beta}} \frac{dx^{\alpha\beta}}{dx^{\gamma}} \exp(i\mathbf{k} \cdot \mathbf{x}^{\gamma}) \\ &= \sum_{\alpha} \sum_{\beta \neq \alpha} \frac{d\phi^{\alpha\beta}}{dx^{\alpha\beta}} \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} (\exp(i\mathbf{k} \cdot \mathbf{x}^{\alpha}) - \exp(i\mathbf{k} \cdot \mathbf{x}^{\beta})). \end{aligned}$$

Now since

$$\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} = \frac{i\mathbf{k} \cdot \mathbf{x}^{\alpha\beta} \mathbf{x}^{\alpha\beta}}{i\mathbf{k} \cdot \mathbf{x}^{\alpha\beta} x^{\alpha\beta}} = \frac{x^{\alpha\beta}}{i\mathbf{k} \cdot \mathbf{x}^{\alpha\beta}} \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} \otimes \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} i\mathbf{k},$$

expression (5.2) becomes

$$\begin{aligned} \frac{\partial}{\partial t} \Big|_{\mathbf{k}} \hat{\mathbf{p}} = & \sum_{\alpha} \left(-\frac{1}{2} \sum_{\beta \neq \alpha} \frac{d\phi^{\alpha\beta}}{dx^{\alpha\beta}} \frac{x^{\alpha\beta}}{i\mathbf{k} \cdot \mathbf{x}^{\alpha\beta}} (\exp(i\mathbf{k} \cdot \mathbf{x}^{\alpha}) - \exp(i\mathbf{k} \cdot \mathbf{x}^{\beta})) \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} \otimes \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} \right) i\mathbf{k} \\ & + \sum_{\alpha} \left(\exp(i\mathbf{k} \cdot \mathbf{x}^{\alpha}) \frac{1}{m^{\alpha}} \mathbf{p}^{\alpha} \otimes \mathbf{p}^{\alpha} \right) i\mathbf{k}. \end{aligned} \quad (5.3)$$

Cormier *et al.* and Lutsko make a formal statement of the balance of linear momentum, ignoring body forces, for the "continuum" composed of the system of particles

$$\dot{\mathbf{p}} = \partial_{\mathbf{x}} \cdot \boldsymbol{\sigma}$$

where $\boldsymbol{\sigma}$ corresponds to the Cauchy stress and $\dot{\mathbf{p}}$ is the material time derivative of \mathbf{p} i.e. $\dot{\mathbf{p}} = \partial_t \mathbf{p}|_{\mathbf{x}^{\alpha}}$ the derivative following the particles not $\partial_t \mathbf{p}|_{\mathbf{x}}$ the partial holding the position in space fixed. (In the continuum

$$\dot{\mathbf{p}} = \partial_t \mathbf{p} + \partial_{\mathbf{x}} \mathbf{p} \left[\frac{1}{\rho} \mathbf{p} \right]$$

where $\partial_{\mathbf{x}} \mathbf{p}$ is a second order tensor acting, i.e. $\mathbf{a} \otimes \mathbf{b} \mathbf{c} = \mathbf{a} (\mathbf{b} \cdot \mathbf{c})$, on the vector $\frac{1}{\rho} \mathbf{p}$. This clearly begs the question: what is the density ρ for the system of particles.)

In the transform domain $\{\mathbf{k}, t\}$, this balance becomes

$$\frac{d}{dt} \hat{\mathbf{p}} = \hat{\boldsymbol{\sigma}}^T i\mathbf{k}.$$

Proceeding under the assumption that the (non-linear) convective term of the material derivative is negligible, i.e. small motions, it is possible to match terms with (5.3) and get an expression for the Fourier transform of stress

$$\begin{aligned} \hat{\boldsymbol{\sigma}} = & \sum_{\alpha} \left(\sum_{\beta \neq \alpha} \frac{d\phi^{\alpha\beta}}{dx^{\alpha\beta}} \frac{x^{\alpha\beta}}{i\mathbf{k} \cdot \mathbf{x}^{\alpha\beta}} (\exp(i\mathbf{k} \cdot \mathbf{x}^{\alpha}) - \exp(i\mathbf{k} \cdot \mathbf{x}^{\beta})) \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} \otimes \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} \right) \\ & + \sum_{\alpha} \left(\exp(i\mathbf{k} \cdot \mathbf{x}^{\alpha}) \frac{1}{m^{\alpha}} \mathbf{p}^{\alpha} \otimes \mathbf{p}^{\alpha} \right). \end{aligned}$$

(The necessity of this assumption to derive the above expression escapes both Lutsko and Cormier.) Transforming back to the spatial domain $\{\mathbf{x}, t\}$ requires a trick. Following Cormier

$$\begin{aligned} \mathcal{F}^{-1} \left(\frac{\exp(i\mathbf{k} \cdot \mathbf{x}^{\alpha}) - \exp(i\mathbf{k} \cdot \mathbf{x}^{\beta})}{i\mathbf{k} \cdot \mathbf{x}^{\alpha\beta}} \right) &= \frac{1}{(2\pi)^3} \int d\mathbf{k} \left\{ \int_0^1 ds \exp(-is\mathbf{k} \cdot \mathbf{x}^{\alpha\beta}) \right\} \exp(-i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}^{\alpha})) \\ &= - \int_0^1 ds \delta(\mathbf{x} - \mathbf{x}^{\alpha} - s\mathbf{x}^{\alpha\beta}). \end{aligned} \quad (5.4)$$

CHAPTER 5. ATOMISTIC-CONTINUUM FORMULATION OF LUTSKO AND CORMIER *ET AL.*

The interpretation of (5.4) is a function that is only non-zero on a line segment connecting \mathbf{x}^α and \mathbf{x}^β . Interestingly enough this is an artifact of the Fourier inversion trick, *other contours are possible* as suggested by Schofield and Henderson [9]. So the stress in the spatial domain is

$$\begin{aligned} \boldsymbol{\sigma} = & \sum_{\alpha} \left(\sum_{\beta \neq \alpha} -\frac{d\phi^{\alpha\beta}}{dx^{\alpha\beta}} x^{\alpha\beta} \left(\int_0^1 ds \delta(\mathbf{x} - \mathbf{x}^\alpha - s\mathbf{x}^{\alpha\beta}) \right) \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} \otimes \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} \right) \\ & + \sum_{\alpha} \left(\frac{1}{m^\alpha} \mathbf{p}^\alpha \otimes \mathbf{p}^\alpha \right). \end{aligned} \quad (5.5)$$

This “local” expression for stress still suffers from singularities due to the Dirac delta and non-local character due to the integral. So an average stress is put forward based on a averaging volume, say a ball B_r of radius r ,

$$\begin{aligned} \boldsymbol{\sigma}_r = & \frac{1}{Vol(B_r)} \int_{B_r} d\bar{\mathbf{x}} \boldsymbol{\sigma}(\mathbf{x} - \bar{\mathbf{x}}) \\ = & \frac{1}{Vol(B_r)} \sum_{\alpha \in B_r} \left(\sum_{\beta \neq \alpha} -\frac{d\phi^{\alpha\beta}}{dx^{\alpha\beta}} x^{\alpha\beta} l_r^{\alpha\beta} \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} \otimes \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} \right) \\ & + \frac{1}{Vol(B_r)} \sum_{\alpha \in B_r} \left(\frac{1}{m^\alpha} \mathbf{p}^\alpha \otimes \mathbf{p}^\alpha \right) \end{aligned}$$

where $l_r^{\alpha\beta}$ is the fraction of the pair bond, i.e. fraction of the line segment between \mathbf{x}^α and \mathbf{x}^β , inside the ball B_r . Literally,

$$l_r^{\alpha\beta} = \int_{B_r} \int_0^1 ds \delta(\mathbf{x} - \mathbf{x}^\alpha - s\mathbf{x}^{\alpha\beta})$$

which is similar to expression formed by other authors, notably [10].

Lutsko goes on to make the statement that the “local” stress (5.5) is derivable from an energy expression

$$e(\mathbf{x}) = \sum_{\alpha} \frac{1}{2m^\alpha} \mathbf{p}^\alpha \cdot \mathbf{p}^\alpha \delta(\mathbf{x} - \mathbf{x}^\alpha) + \frac{1}{2} \sum_{\alpha} \sum_{\beta \neq \alpha} \phi^{\alpha\beta} \left(\int_0^1 ds \delta(\mathbf{x} - \mathbf{x}^\alpha - s\mathbf{x}^{\alpha\beta}) \right)$$

by means of

$$\boldsymbol{\sigma} = \partial_{\mathbf{E}} e$$

where \mathbf{E} seems to correspond to the (continuum) Lagrange strain tensor. This is a formal claim at best, due to the fact that the deformation gradient for the atomistic system is not given a complete definition and it is the second Piola-Kirchhoff stress, and **not** the Cauchy stress, that is dual to the Lagrange strain.

5.3 Comments

Lutkso's derivation of continuum stress for an atomistic system is noteworthy because it connects atomic properties of mass and momentum directly to a standard formulation of continuum mechanics and derives an expression for continuum stress that is defined at an instant in time for either a specific point in space or a localized volume centered at such a point. The shortcomings of his work were not in the concept, but rather in the implementation. He used an incorrect form for the balance of linear momentum, $\dot{\mathbf{p}} = \partial_{\mathbf{x}} \cdot \boldsymbol{\sigma}$. Even the most optimistic interpretation of this expression as $\partial_t \mathbf{p} = \partial_{\mathbf{x}} \cdot \boldsymbol{\sigma}$ results in an expression that is not truly equivalent to Cauchy stress $\boldsymbol{\sigma}$, but rather the combined quantity of $\boldsymbol{\sigma} - \rho \mathbf{v} \otimes \mathbf{v}$. In addition, his use of Dirac delta functions and Fourier space require that the continuum exist over **all** physical space, making the validity of the resulting stress expression questionable for a bounded system. Cormier *et al.* [6] note this feature as well, but do not suggest alternatives during the derivation of their own stress expression. One such alternative is the approach by Hardy, to be discussed in the next chapter.

This page intentionally left blank.

Chapter 6

Atomistic-Continuum Formulation of Robert J. Hardy

6.1 Review of continuum mechanics

We can consider a continuum body B to go from some original, reference configuration at time zero, B_0 , to a new configuration at a later time t , B_t . A material point on B_0 is described by the vector \mathbf{X} , and its location on B_t at a later time t is given by the transformation $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$. Any property of the system can be described by a field variable which is dependent upon time and the material point at which it is being evaluated. Either the reference position of the material point or the current position can be used. The choice of the former is the Lagrangian or Material description. For a field variable A , $A = A(\mathbf{X}, t)$. The time variation of the variable A is expressed as a time derivative:

$$\dot{A} = \frac{dA}{dt} = \frac{\partial A(\mathbf{X}, t)}{\partial t}.$$

Alternatively, the field variable can be expressed as a function of time and the current position of the material point, $\tilde{A} = \tilde{A}(\mathbf{x}(\mathbf{X}, t), t) = A(\mathbf{X}, t)$. This description of the material is known as the Eulerian or Spatial description. Since the spatial position \mathbf{x} is itself a function of time, the time derivative can only be obtained using the chain-rule:

$$\dot{\tilde{A}} = \frac{d\tilde{A}}{dt} = \frac{\partial \tilde{A}(\mathbf{x}, t)}{\partial t} + \frac{\partial \tilde{A}(\mathbf{x}, t)}{\partial \mathbf{x}} \cdot \frac{\partial \mathbf{x}}{\partial t}.$$

The quantity $\frac{\partial \mathbf{x}}{\partial t}$ is the velocity \mathbf{v} of the material point at \mathbf{x} , and so

$$\frac{d\tilde{A}}{dt} = \frac{\partial \tilde{A}(\mathbf{x}, t)}{\partial t} + \mathbf{v} \cdot \partial_{\mathbf{x}} \tilde{A}, \quad (6.1)$$

where

$$\partial_{\mathbf{x}} \equiv \frac{\partial}{\partial \mathbf{x}}.$$

In some of the literature, $\frac{\partial}{\partial t}$ is known as the partial time derivative while $\frac{d}{dt}$ is known as the full or material time derivative and is also often expressed as $\frac{D}{Dt}$. One example of the above expression is the calculation of the acceleration \mathbf{a} of the material point at \mathbf{x} ,

$$\mathbf{a} = \dot{\mathbf{v}} = \frac{d\mathbf{v}}{dt} = \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \partial_{\mathbf{x}} \mathbf{v}. \quad (6.2)$$

One property of the body B that does not change with time is its total mass $m_B = m_{B_0} = m_{B_t}$. This fact can be used to relate the density of the body in the reference configuration ρ_0 with the current density ρ . Consider,

$$m_{B_0} = \int_{B_0} \rho_0 dV = m_{B_t} = \int_{B_t} \rho d\mathcal{V}. \quad (6.3)$$

Here, dV is the volume for a differential element in the reference configuration while $d\mathcal{V}$ is the the volume for the same element in the current configuration. They are related by the relation $d\mathcal{V} = JdV$, where J is the determinant of the deformation gradient tensor $F \equiv \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$. Thus,

$$\int_{B_0} \rho_0 dV = \int_{B_t} \rho d\mathcal{V} = \int_{B_0} \rho J dV, \quad (6.4)$$

and

$$\rho_0 = \rho J. \quad (6.5)$$

This relation can be used to express the conservation of mass at a point in B . Since $\rho_0 = \rho_0(\mathbf{X})$,

$$\frac{d\rho_0}{dt} = 0 = \frac{d(\rho J)}{dt} = \frac{d\rho}{dt} J + \rho \frac{dJ}{dt}.$$

Using equation (6.1),

$$0 = \left(\frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \partial_{\mathbf{x}} \rho \right) J + \rho \left(\frac{\partial J}{\partial t} + \mathbf{v} \cdot \partial_{\mathbf{x}} J \right).$$

It can be shown that $\left(\frac{\partial J}{\partial t} + \mathbf{v} \cdot \partial_{\mathbf{x}} J \right) \equiv (\partial_{\mathbf{x}} \cdot \mathbf{v}) J$, so the above expression becomes

$$0 = \left(\frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \partial_{\mathbf{x}} \rho + \rho \partial_{\mathbf{x}} \cdot \mathbf{v} \right) J,$$

and since J cannot be equal to zero, then

$$\frac{\partial \rho}{\partial t} + \partial_{\mathbf{x}} \cdot (\rho \mathbf{v}) = 0. \quad (6.6)$$

Equation (6.6) can also be stated as

$$\frac{d\rho}{dt} + \rho \partial_{\mathbf{x}} \cdot \mathbf{v} = 0 \quad (6.7)$$

using equation (6.1).

A similar mathematical exercise can be used to derive Reynold's transport theorem, which states that for any quantity $I(t)$ which describes some aspect of the body B_t and is defined as the integration of some density $\phi(\mathbf{x}, t)$ over the body's volume,

$$I(t) = \int_{B_t} \phi(\mathbf{x}, t) dV,$$

the time derivative of I can be shown to be

$$\frac{dI}{dt} = \int_{B_t} \left(\frac{\partial \phi}{\partial t} + \partial_{\mathbf{x}} \cdot (\phi \mathbf{v}) \right) dV. \quad (6.8)$$

We observe that for the case where $I = m_{B_t}$ and $\phi = \rho$, equation (6.6) is recovered.

We can also consider the linear momentum of B , making $I = \int_{B_t} \rho \mathbf{v} dV$ and $\phi = \rho \mathbf{v}$. The material time derivative of the linear momentum of a body is, by Newton's 2nd law, the sum of all forces acting on that body. Thus,

$$\sum \mathbf{F} = \int_{B_t} \left(\frac{\partial (\rho \mathbf{v})}{\partial t} + \partial_{\mathbf{x}} \cdot (\rho \mathbf{v} \otimes \mathbf{v}) \right) dV. \quad (6.9)$$

For the continuum body B , the forces exerted on that body come in the form of body forces \mathbf{b} acting per unit mass and traction acting on the surface of the body,

$$\sum \mathbf{F} = \int_{B_t} \rho \mathbf{b} dV + \oint_{\Gamma_t} \boldsymbol{\sigma} \cdot \mathbf{n} dS, \quad (6.10)$$

where Γ_t is the surface that encloses the volume B_t . Applying the divergence theorem to the second half of the RHS of equation (6.10) yields

$$\sum \mathbf{F} = \int_{B_t} (\rho \mathbf{b} + \partial_{\mathbf{x}} \cdot \boldsymbol{\sigma}) dV,$$

which, when combined with equation (6.9), produces

$$\int_{B_t} \left(\frac{\partial (\rho \mathbf{v})}{\partial t} + \partial_{\mathbf{x}} \cdot (\rho \mathbf{v} \otimes \mathbf{v}) - \rho \mathbf{b} - \partial_{\mathbf{x}} \cdot \boldsymbol{\sigma} \right) dV = 0. \quad (6.11)$$

As in the case for mass density, in order to insure a balance of momentum density for any material point in B_t , the above equation becomes

$$\frac{\partial (\rho \mathbf{v})}{\partial t} = \partial_{\mathbf{x}} \cdot (\boldsymbol{\sigma} - \rho \mathbf{v} \otimes \mathbf{v}) + \rho \mathbf{b}. \quad (6.12)$$

Using equation (6.1), the material point-wise balance of linear momentum is more commonly expressed as

$$\rho \frac{d\mathbf{v}}{dt} = \partial_{\mathbf{x}} \cdot \boldsymbol{\sigma} + \rho \mathbf{b}. \quad (6.13)$$

A similar analysis can be performed on the time derivative of the total energy of the system E_t . This total energy is comprised of body integration of potential energy \hat{u} , kinetic energy and thermal energy \hat{t} densities,

$$E_t = \int_{B_t} \hat{e} dV = \int_{B_t} \left(\hat{u} + \frac{1}{2} \rho v^2 + \hat{t} \right) dV. \quad (6.14)$$

The quantity E_t is only altered by the work done by surface traction and body forces, and by the flux of heat into or out of the body's surface. By applying Reynold's transport theorem and reducing the resulting expression to a point-wise balance of energy, one gets

$$\frac{\partial \hat{e}}{\partial t} = \partial_{\mathbf{x}} \cdot (\boldsymbol{\sigma} \cdot \mathbf{v} - \hat{e} \mathbf{v} - \mathbf{q}) + \rho \mathbf{b} \cdot \mathbf{v}. \quad (6.15)$$

Performing the same analysis on the balance of angular momentum does not result in another differential relationship, but rather the property of symmetry of the stress tensor, $\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$. This and the previous derivations do not assume the existence of couple stresses, and reformulation of the balance laws is required to include them.

6.2 Hardy's formulation

Hardy's work uses the balance equations for mass (6.6), linear momentum (6.12) and energy (6.15) derived above. He considers the body B_t to be the system of N atoms which are interacting with each other through some interatomic potential energy formulation. Each atom α is characterized by its mass m^α , its current position \mathbf{x}^α , and its velocity $\mathbf{v}^\alpha = \frac{d\mathbf{x}^\alpha}{dt}$.

Note: For the benefit of those familiar with continuum mechanics notation, a superscripted, lower-case Greek letter will denote a property associated with an atom, *e.g.* mass m^α , momentum \mathbf{p}^α , etc., whereas a subscripted, lower-case Roman letter will denote the Cartesian coordinate components of vector quantities. For example, v_i^α denotes the i -th component of the velocity vector of atom α .

6.2.1 Densities and Localization

The best way to understand Hardy's work is to consider that there are two views of the material system. One perspective is the continuum, where quantities are point-wise functions

of time and position. These quantities include mass density $\rho(\mathbf{x}, t)$, momentum density $\mathbf{p}(\mathbf{x}, t)$, and energy density $E^0(\mathbf{x}, t)$. The other perspective is that the material system contains atoms, each of which has its own mass, momentum, potential energy and kinetic energy. In order to connect the two views, Hardy uses a localization function ψ which spreads out the properties of the atoms, and allows all atoms to contribute to a continuum property at a specific position and time. His three key relations are:

$$\rho(\mathbf{x}, t) = \sum_{\alpha=1}^N m^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \quad (6.16)$$

$$\mathbf{p}(\mathbf{x}, t) = \sum_{\alpha=1}^N m^\alpha \mathbf{v}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \quad (6.17)$$

$$E^0(\mathbf{x}, t) = \sum_{\alpha=1}^N \left\{ \frac{1}{2} m^\alpha (v^\alpha)^2 + \phi^\alpha \right\} \psi(\mathbf{x}^\alpha - \mathbf{x}). \quad (6.18)$$

A few things to note:

- From the above equations, it is apparent that the localization function $\psi(\mathbf{r})$ is NOT dimensionless, but has dimensions of inverse volume,

$$\psi \sim \left[\frac{1}{L^3} \right].$$

In effect, this states that at the continuum position \mathbf{x} , the properties of mass, momentum and energy densities are influenced by all the atoms within some characteristic volume, and the weight of each atom's contribution is governed by the functional form of ψ .

- The velocity field \mathbf{v} is not determined in the same fashion as mass and momentum, but is defined by the expression

$$\mathbf{v}(\mathbf{x}, t) \equiv \frac{\mathbf{p}(\mathbf{x}, t)}{\rho(\mathbf{x}, t)}. \quad (6.19)$$

- In equation (6.18), the total potential energy density of the system is expressed as the summation of individual atomic potential energies, ϕ_α .

Hardy establishes a few rules with regard to the localization function ψ . They are:

1. $\psi(\mathbf{r})$ is a normalized function, thus

$$\iiint_{R^3} \psi(\mathbf{r}) d^3r = 1. \quad (6.20)$$

2. The spatial gradient of the localization function, $\partial_{\mathbf{x}}\psi(\mathbf{x}^\alpha - \mathbf{x}) = \frac{\partial\psi(\mathbf{x}^\alpha - \mathbf{x})}{\partial\mathbf{x}}$, is equivalent to the the negative of the gradient of ψ with respect to it's argument,

$$\frac{\partial\psi(\mathbf{r})}{\partial\mathbf{x}} = \frac{\partial\psi(\mathbf{r})}{\partial\mathbf{r}} \frac{\partial\mathbf{r}}{\partial\mathbf{x}}.$$

For $\mathbf{r} = \mathbf{x}^\alpha - \mathbf{x}$, this becomes

$$\frac{\partial\psi(\mathbf{r})}{\partial\mathbf{x}} = -\frac{\partial\psi(\mathbf{r})}{\partial\mathbf{r}}.$$

This relation can be used to show that

$$\frac{\partial\psi(\mathbf{x}^\alpha - \mathbf{x})}{\partial t} = -\mathbf{v}^\alpha \cdot \partial_{\mathbf{x}}\psi(\mathbf{x}^\alpha - \mathbf{x}). \quad (6.21)$$

3. A Bond function $B^{\alpha\beta}(\mathbf{x})$ between atoms α and β is defined by the expression

$$B^{\alpha\beta}(\mathbf{x}) \equiv \int_0^1 \psi(\lambda\mathbf{x}^{\alpha\beta} + \mathbf{x}^\beta - \mathbf{x}) d\lambda, \quad (6.22)$$

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

$$\frac{\partial\psi(\lambda\mathbf{x}^{\alpha\beta} + \mathbf{x}^\beta - \mathbf{x})}{\partial\lambda} = -\mathbf{x}^{\alpha\beta} \cdot \partial_{\mathbf{x}}\psi(\lambda\mathbf{x}^{\alpha\beta} + \mathbf{x}^\beta - \mathbf{x}), \quad (6.23)$$

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

$$\psi(\mathbf{x}^\alpha - \mathbf{x}) - \psi(\mathbf{x}^\beta - \mathbf{x}) = -\mathbf{x}^{\alpha\beta} \cdot \partial_{\mathbf{x}}B^{\alpha\beta}(\mathbf{x}). \quad (6.24)$$

6.2.2 Energy and Force Assumptions

Note: The forces discussed in this subsection do not include body forces acting on the atoms $\mathbf{f}_{\text{body}}^\alpha = m^\alpha \mathbf{b}^\alpha$.

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

$$\Phi = \sum_{\alpha=1}^N \phi^\alpha. \quad (6.25)$$

Although this is not always the case, it is usually assumed true for simulations of systems governed by empirical potentials.

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

$$\mathbf{F}^\alpha \equiv -\frac{\partial\Phi}{\partial\mathbf{x}^\alpha} = \sum_{\beta \neq \alpha}^N \mathbf{F}^{\alpha\beta}. \quad (6.26)$$

This statement can always be made, although it is not always clear what the physical meaning of $\mathbf{F}^{\alpha\beta}$ is. When Φ is the summation of pair potentials, $\phi^\alpha = \frac{1}{2} \sum_{\beta \neq \alpha}^N \phi^{\alpha\beta}(x^{\alpha\beta})$ where $x^{\alpha\beta} = \|\mathbf{x}^{\alpha\beta}\|$, or for the Embedded Atom Method, $\mathbf{F}^{\alpha\beta}$ obviously means the force exerted on atom α from atom β . However, for some multi-body potentials, such as the 3-body term in the Stillinger-Weber potential [11], the meaning is not so straight-forward.

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

$$\mathbf{F}^\alpha = - \sum_{\beta \neq \alpha}^N \sum_{\gamma=1}^N \frac{\partial \phi^\gamma}{\partial x^{\alpha\beta}} \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}. \quad (6.27)$$

This expression includes the possibility that $\alpha = \gamma$. Again, radially-symmetric potentials such as Lennard-Jones and EAM qualify for this assumption, but it is unclear whether potential energies that depend on bond orientations do.

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

$$\mathbf{F}^{\alpha\beta} = - \left\{ \frac{\partial \phi^\alpha}{\partial x^{\alpha\beta}} + \frac{\partial \phi^\beta}{\partial x^{\alpha\beta}} \right\} \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}. \quad (6.28)$$

Clearly, while pair potentials and EAM qualify for this assumption, the 3-body potential of Stillinger-Weber does not.

6.2.3 Hardy's balance laws

Conservation of Mass

Using Hardy's expression for density (6.16) and the time derivative of ψ (6.21),

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= \frac{\partial}{\partial t} \left\{ \sum_{\alpha=1}^N m^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \right\} \\ &= \sum_{\alpha=1}^N m^\alpha \frac{\partial \psi(\mathbf{x}^\alpha - \mathbf{x})}{\partial t} \\ &= \sum_{\alpha=1}^N m^\alpha (-\mathbf{v}^\alpha \cdot \partial_{\mathbf{x}} \psi(\mathbf{x}^\alpha - \mathbf{x})) \\ &= -\partial_{\mathbf{x}} \cdot \left(\sum_{\alpha=1}^N m^\alpha \mathbf{v}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \right) = -\partial_{\mathbf{x}} \cdot \mathbf{p}. \end{aligned}$$

This shows that Hardy's use of the localization function to define expressions for continuum mass density and momentum density satisfies the continuum conservation of mass.

Balance of Linear Momentum

Starting with Hardy's expression for momentum density (6.17),

$$\begin{aligned}
 \frac{\partial \mathbf{p}}{\partial t} &= \frac{\partial}{\partial t} \left\{ \sum_{\alpha=1}^N m^\alpha \mathbf{v}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \right\} \\
 &= \sum_{\alpha=1}^N \left[m^\alpha \frac{\partial \mathbf{v}^\alpha}{\partial t} \psi(\mathbf{x}^\alpha - \mathbf{x}) + m^\alpha \mathbf{v}^\alpha \frac{\partial \psi(\mathbf{x}^\alpha - \mathbf{x})}{\partial t} \right] \\
 &= \sum_{\alpha=1}^N \left[(\mathbf{F}^\alpha + m^\alpha \mathbf{b}^\alpha) \psi(\mathbf{x}^\alpha - \mathbf{x}) + m^\alpha \mathbf{v}^\alpha (-\mathbf{v}^\alpha \cdot \partial_{\mathbf{x}} \psi(\mathbf{x}^\alpha - \mathbf{x})) \right].
 \end{aligned}$$

The force term on the RHS of the above expression can be combined with Hardy's second force assumption to obtain,

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

Since α and β run over all atoms in the system, they are considered dummy indices and can be switched. By doing this, and using Newton's 3rd law, $\mathbf{F}^{\alpha\beta} = -\mathbf{F}^{\beta\alpha}$, one obtains

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

Combining this with expression (6.24), the time derivative of the momentum density becomes

$$\begin{aligned}
 \frac{\partial \mathbf{p}}{\partial t} &= \sum_{\alpha=1}^N \left\{ \frac{1}{2} \sum_{\beta \neq \alpha}^N \mathbf{F}^{\alpha\beta} (-\mathbf{x}^{\alpha\beta} \cdot \partial_{\mathbf{x}} B^{\alpha\beta}(\mathbf{x})) \right\} + m^\alpha \mathbf{b}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) + m^\alpha \mathbf{v}^\alpha (-\mathbf{v}^\alpha \cdot \partial_{\mathbf{x}} \psi(\mathbf{x}^\alpha - \mathbf{x})) \\
 &= -\partial_{\mathbf{x}} \cdot \left(\frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \mathbf{F}^{\alpha\beta} B^{\alpha\beta}(\mathbf{x}) + \sum_{\alpha=1}^N m^\alpha \mathbf{v}^\alpha \otimes \mathbf{v}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \right) + \sum_{\alpha=1}^N m^\alpha \mathbf{b}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}).
 \end{aligned} \tag{6.29}$$

Comparing equation (6.29) with the continuum balance of momentum (6.12), we observe that in order for these expressions to be consistent with one another,

$$-\boldsymbol{\sigma} + \rho \mathbf{v} \otimes \mathbf{v} = \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \mathbf{F}^{\alpha\beta} B^{\alpha\beta}(\mathbf{x}) + \sum_{\alpha=1}^N m^\alpha \mathbf{v}^\alpha \otimes \mathbf{v}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}), \tag{6.30}$$

and,

$$\rho \mathbf{b} = \sum_{\alpha=1}^N m^\alpha \mathbf{b}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}). \tag{6.31}$$

Equation (6.31) can be rearranged to define the continuum body-force field,

$$\mathbf{b}(\mathbf{x}, t) \equiv \frac{\mathbf{f}_{\text{body}}(\mathbf{x}, t)}{\rho(\mathbf{x}, t)} = \frac{\sum_{\alpha=1}^N m^{\alpha} \mathbf{b}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x})}{\sum_{\alpha=1}^N m^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x})}. \quad (6.32)$$

It is important to note for equation (6.30) that we cannot yet separate out the stress and momentum flux terms on the RHS. This is because the continuum velocity field \mathbf{v} does NOT include atomic motion characterized as thermal motion, hence the continuum term $\rho \mathbf{v} \mathbf{v}$ is not equal to the second term on the RHS of equation (6.30), but only a portion of it.

Balance of Energy

Starting with Hardy's expression for the system energy (6.18),

$$\begin{aligned} \frac{\partial E^0}{\partial t} &= \frac{\partial}{\partial t} \left\{ \sum_{\alpha=1}^N \left\{ \frac{1}{2} m^{\alpha} (v^{\alpha})^2 + \phi^{\alpha} \right\} \psi(\mathbf{x}^{\alpha} - \mathbf{x}) \right\} \\ &= \sum_{\alpha=1}^N \left[\left\{ m^{\alpha} \left(\frac{\partial \mathbf{v}^{\alpha}}{\partial t} \cdot \mathbf{v}^{\alpha} \right) + \frac{\partial \phi^{\alpha}}{\partial t} \right\} \psi(\mathbf{x}^{\alpha} - \mathbf{x}) + \left\{ \frac{1}{2} m^{\alpha} (v^{\alpha})^2 + \phi^{\alpha} \right\} \frac{\partial \psi(\mathbf{x}^{\alpha} - \mathbf{x})}{\partial t} \right] \\ &= \sum_{\alpha=1}^N \left[\left\{ (\mathbf{F}^{\alpha} + m^{\alpha} \mathbf{b}^{\alpha}) \cdot \mathbf{v}^{\alpha} + \frac{\partial \phi^{\alpha}}{\partial t} \right\} \psi(\mathbf{x}^{\alpha} - \mathbf{x}) + \left\{ \frac{1}{2} m^{\alpha} (v^{\alpha})^2 + \phi^{\alpha} \right\} (-\mathbf{v}^{\alpha} \cdot \partial_{\mathbf{x}} \psi(\mathbf{x}^{\alpha} - \mathbf{x})) \right]. \end{aligned}$$

By imposing the second and third force assumptions, Hardy combines the \mathbf{F}^{α} and $\frac{\partial \phi^{\alpha}}{\partial t}$ terms into

$$\begin{aligned} \frac{\partial E^0}{\partial t} &= \sum_{\alpha=1}^N [m^{\alpha} \mathbf{b}^{\alpha} \cdot \mathbf{v}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x})] + \partial_{\mathbf{x}} \cdot \left(\sum_{\alpha=1}^N \left[\sum_{\beta \neq \alpha}^N \left[\sum_{\gamma \neq \alpha}^N \left(\frac{\partial \phi^{\beta}}{\partial x^{\alpha \gamma}} \frac{\mathbf{x}^{\alpha \gamma}}{x^{\alpha \gamma}} \cdot \mathbf{v}^{\alpha} \right) \mathbf{x}^{\alpha \beta} B_{\alpha \beta}(\mathbf{x}) \right] \right] \right) \\ &\quad - \partial_{\mathbf{x}} \cdot \left(\sum_{\alpha=1}^N \left\{ \frac{1}{2} m^{\alpha} (v^{\alpha})^2 + \phi^{\alpha} \right\} \mathbf{v}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x}) \right). \end{aligned} \quad (6.33)$$

By comparing equation (6.33) with (6.15), we see that

$$\begin{aligned} \boldsymbol{\sigma} \cdot \mathbf{v} - \hat{\mathbf{e}} \mathbf{v} - \mathbf{q} &= \sum_{\alpha=1}^N \left[\sum_{\beta \neq \alpha}^N \left[\sum_{\gamma \neq \alpha}^N \frac{\partial \phi^{\beta}}{\partial x^{\alpha \gamma}} \frac{\mathbf{x}^{\alpha \gamma} \otimes \mathbf{x}^{\alpha \beta}}{x^{\alpha \gamma}} B^{\alpha \beta}(\mathbf{x}) \right] \right] \cdot \mathbf{v}^{\alpha} \\ &\quad - \sum_{\alpha=1}^N \left\{ \frac{1}{2} m^{\alpha} (v^{\alpha})^2 + \phi^{\alpha} \right\} \mathbf{v}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x}), \end{aligned} \quad (6.34)$$

and

$$\rho \mathbf{b} \cdot \mathbf{v} = \sum_{\alpha=1}^N m^{\alpha} \mathbf{b}^{\alpha} \cdot \mathbf{v}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x}). \quad (6.35)$$

As before, expressions (6.34) and (6.35) are in their simplest forms since we have not yet addressed the issue of atomic motion versus continuum motion and thermal energy flow.

6.2.4 Macroscopic Flow and Microscopic Motion

In order to separate atomic motion into continuum dynamics and thermal energy, Hardy splits the atomic velocities \mathbf{v}^α into the continuum velocity $\mathbf{v}(\mathbf{x}, t)$ and a *relative* velocity $\mathbf{u}^\alpha(\mathbf{x}, t)$,

$$\mathbf{v}^\alpha = \mathbf{v}(\mathbf{x}, t) + \mathbf{u}^\alpha(\mathbf{x}, t). \quad (6.36)$$

As Hardy shows, this relative velocity field has zero net momentum. Hardy now goes on to reformulate the balance laws for momentum and energy in terms of \mathbf{v} and \mathbf{u}^α .

Balance of Linear Momentum - Revisited

Starting with equation (6.30),

$$\begin{aligned} -\boldsymbol{\sigma} + \rho \mathbf{v} \otimes \mathbf{v} &= \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \mathbf{F}^{\alpha\beta} B^{\alpha\beta}(\mathbf{x}) + \sum_{\alpha=1}^N m^\alpha \mathbf{v}^\alpha \otimes \mathbf{v}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \\ &= \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \mathbf{F}^{\alpha\beta} B^{\alpha\beta}(\mathbf{x}) + \sum_{\alpha=1}^N m^\alpha (\mathbf{u}^\alpha + \mathbf{v}) \otimes (\mathbf{u}^\alpha + \mathbf{v}) \psi(\mathbf{x}^\alpha - \mathbf{x}) \\ &= \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \mathbf{F}^{\alpha\beta} B^{\alpha\beta}(\mathbf{x}) + \sum_{\alpha=1}^N m^\alpha \mathbf{u}^\alpha \otimes \mathbf{u}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \\ &\quad + \left(\sum_{\alpha=1}^N m^\alpha \mathbf{u}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \right) \otimes \mathbf{v} + \mathbf{v} \otimes \left(\sum_{\alpha=1}^N m^\alpha \mathbf{u}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \right) \\ &\quad + \left(\sum_{\alpha=1}^N m^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \right) \mathbf{v} \otimes \mathbf{v}. \end{aligned}$$

As stated previously, the net momentum of the relative velocity field is zero by the definition of \mathbf{v} , found in (6.19). This makes the third and fourth terms on the RHS of the above expression both equal zero. Also, we can re-use Hardy's definition of the mass density field (6.16),

$$-\boldsymbol{\sigma} + \rho \mathbf{v} \otimes \mathbf{v} = \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \mathbf{F}^{\alpha\beta} B^{\alpha\beta}(\mathbf{x}) + \sum_{\alpha=1}^N m^\alpha \mathbf{u}^\alpha \otimes \mathbf{u}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) + \rho \mathbf{v} \otimes \mathbf{v}. \quad (6.37)$$

Obviously, we can now isolate the expression for the stress tensor,

$$\boldsymbol{\sigma} = - \left\{ \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \mathbf{F}^{\alpha\beta} B^{\alpha\beta}(\mathbf{x}) + \sum_{\alpha=1}^N m^\alpha \mathbf{u}^\alpha \otimes \mathbf{u}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \right\}. \quad (6.38)$$

Balance of Energy - Revisited

Starting with equation(6.34),

$$\begin{aligned}
 \boldsymbol{\sigma} \cdot \mathbf{v} - \hat{e}\mathbf{v} - \mathbf{q} &= \sum_{\alpha=1}^N \left[\sum_{\beta \neq \alpha}^N \left[\sum_{\gamma \neq \alpha}^N \frac{\partial \phi^\beta}{\partial x^{\alpha\gamma}} \frac{\mathbf{x}^{\alpha\gamma} \otimes \mathbf{x}^{\alpha\beta}}{x^{\alpha\gamma}} B^{\alpha\beta}(\mathbf{x}) \right] \right] \cdot \mathbf{v}^\alpha \\
 &\quad - \sum_{\alpha=1}^N \left\{ \frac{1}{2} m^\alpha (v^\alpha)^2 + \phi^\alpha \right\} \mathbf{v}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \\
 \boldsymbol{\sigma} \cdot \mathbf{v} - \hat{e}\mathbf{v} - \mathbf{q} &= \sum_{\alpha=1}^N \left[\sum_{\beta \neq \alpha}^N \left[\sum_{\gamma \neq \alpha}^N \frac{\partial \phi^\beta}{\partial x^{\alpha\gamma}} \frac{\mathbf{x}^{\alpha\gamma} \otimes \mathbf{x}^{\alpha\beta}}{x^{\alpha\gamma}} B^{\alpha\beta}(\mathbf{x}) \right] \right] \cdot (\mathbf{u}^\alpha + \mathbf{v}) \\
 &\quad - \sum_{\alpha=1}^N \left\{ \frac{1}{2} m^\alpha ((u^\alpha)^2 + 2\mathbf{u}^\alpha \cdot \mathbf{v} + v^2) + \phi^\alpha \right\} (\mathbf{u}^\alpha + \mathbf{v}) \psi(\mathbf{x}^\alpha - \mathbf{x}).
 \end{aligned}$$

Rearranging terms on the RHS of the above expression, we obtain

$$\begin{aligned}
 \boldsymbol{\sigma} \cdot \mathbf{v} - \hat{e}\mathbf{v} - \mathbf{q} &= \left(\sum_{\alpha=1}^N \left[\sum_{\beta \neq \alpha}^N \left[\sum_{\gamma \neq \alpha}^N \frac{\partial \phi^\beta}{\partial x^{\alpha\gamma}} \frac{\mathbf{x}^{\alpha\gamma} \otimes \mathbf{x}^{\alpha\beta}}{x^{\alpha\gamma}} B^{\alpha\beta}(\mathbf{x}) \right] \right] - \sum_{\alpha=1}^N m^\alpha \mathbf{u}^\alpha \otimes \mathbf{u}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \right) \cdot \mathbf{v} \\
 &\quad - \left(\sum_{\alpha=1}^N \left\{ \frac{1}{2} m^\alpha ((u^\alpha)^2 + v^2) + \phi^\alpha \right\} \psi(\mathbf{x}^\alpha - \mathbf{x}) \right) \mathbf{v} \\
 &\quad + \sum_{\alpha=1}^N \left[\sum_{\beta \neq \alpha}^N \left[\sum_{\gamma \neq \alpha}^N \frac{\partial \phi^\beta}{\partial x^{\alpha\gamma}} \frac{\mathbf{x}^{\alpha\gamma} \otimes \mathbf{x}^{\alpha\beta}}{x^{\alpha\gamma}} B^{\alpha\beta}(\mathbf{x}) \right] \right] \cdot \mathbf{u}^\alpha \\
 &\quad - \sum_{\alpha=1}^N \left\{ \frac{1}{2} m^\alpha ((u^\alpha)^2 + v^2) + \phi^\alpha \right\} \mathbf{u}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}).
 \end{aligned} \tag{6.39}$$

The second term on the RHS of (6.39) can be simplified by using the Hardy's definition of mass density (6.16), and the zero net momentum property of the relative velocity field is

used to simplify the fourth term. The resulting expression is

$$\begin{aligned}
 \boldsymbol{\sigma} \cdot \mathbf{v} - \hat{e}\mathbf{v} - \mathbf{q} &= \left(\sum_{\alpha=1}^N \left[\sum_{\beta \neq \alpha}^N \left[\sum_{\gamma \neq \alpha}^N \frac{\partial \phi^\beta}{\partial x^{\alpha\gamma}} \frac{\mathbf{x}^{\alpha\gamma} \otimes \mathbf{x}^{\alpha\beta}}{x^{\alpha\gamma}} B^{\alpha\beta}(\mathbf{x}) \right] \right] - \sum_{\alpha=1}^N m^\alpha \mathbf{u}^\alpha \otimes \mathbf{u}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \right) \cdot \mathbf{v} \\
 &\quad - \left(\frac{1}{2} \rho v^2 + \sum_{\alpha=1}^N \left\{ \frac{1}{2} m^\alpha (u^\alpha)^2 + \phi^\alpha \right\} \psi(\mathbf{x}^\alpha - \mathbf{x}) \right) \mathbf{v} \\
 &\quad + \sum_{\alpha=1}^N \left[\sum_{\beta \neq \alpha}^N \left[\sum_{\gamma \neq \alpha}^N \frac{\partial \phi^\beta}{\partial x^{\alpha\gamma}} \frac{\mathbf{x}^{\alpha\gamma} \otimes \mathbf{x}^{\alpha\beta}}{x^{\alpha\gamma}} B^{\alpha\beta}(\mathbf{x}) \right] \right] \cdot \mathbf{u}^\alpha \\
 &\quad - \sum_{\alpha=1}^N \left\{ \frac{1}{2} m^\alpha (u^\alpha)^2 + \phi^\alpha \right\} \mathbf{u}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}).
 \end{aligned} \tag{6.40}$$

The first term on the RHS of equation (6.40) does APPEAR to match up with the continuum term of $\boldsymbol{\sigma} \cdot \mathbf{v}$, provided that for atom α ,

$$-\frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \mathbf{F}^{\alpha\beta} B^{\alpha\beta}(\mathbf{x}) = \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \left[\sum_{\gamma \neq \alpha}^N \frac{\partial \phi^\beta}{\partial x^{\alpha\gamma}} \frac{\mathbf{x}^{\alpha\gamma} \otimes \mathbf{x}^{\alpha\beta}}{x^{\alpha\gamma}} B^{\alpha\beta}(\mathbf{x}) \right]. \tag{6.41}$$

This is the reason for Hardy's fourth force assumption, which restricts the value of β to equal only α or γ to provide non-zero terms on the RHS of the above expression. It follows that,

$$\begin{aligned}
 \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \left[\sum_{\gamma \neq \alpha}^N \frac{\partial \phi^\beta}{\partial x^{\alpha\gamma}} \frac{\mathbf{x}^{\alpha\gamma} \otimes \mathbf{x}^{\alpha\beta}}{x^{\alpha\gamma}} B^{\alpha\beta}(\mathbf{x}) \right] &= \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \left[\sum_{\gamma \neq \alpha}^N \frac{\partial \phi^\beta}{\partial x^{\alpha\gamma}} (\delta_{\alpha\beta} + \delta_{\beta\gamma}) \frac{\mathbf{x}^{\alpha\gamma} \otimes \mathbf{x}^{\alpha\beta}}{x^{\alpha\gamma}} B^{\alpha\beta}(\mathbf{x}) \right] \\
 &= \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \frac{\partial \phi^\beta}{\partial x^{\alpha\beta}} \frac{\mathbf{x}^{\alpha\beta} \otimes \mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} B^{\alpha\beta}(\mathbf{x}) \\
 &= \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \left\{ \frac{\partial \phi^\alpha}{\partial x^{\alpha\beta}} + \frac{\partial \phi^\beta}{\partial x^{\alpha\beta}} \right\} \frac{\mathbf{x}^{\alpha\beta} \otimes \mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} B^{\alpha\beta}(\mathbf{x}).
 \end{aligned} \tag{6.42}$$

The last line shown above confirms that the two expressions are equivalent by equation (6.28). As stated previously, this restriction is violated for empirical potentials such as Stillinger-Weber [11]. S-W has a 3-body energy term that gets split three ways among the interacting atoms, but is a function of all three interatomic distances. As such, a non-zero term will occur for $\beta \neq \alpha, \gamma$.

By comparing the second term in (6.40) with the definition of continuum energy density \hat{e} found in (6.14), we can isolate the potential energy density,

$$\hat{u} = \sum_{\alpha=1}^N \phi^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}), \tag{6.43}$$

and the thermal energy density,

$$\hat{t} = \sum_{\alpha=1}^N \frac{1}{2} m^{\alpha} (u^{\alpha})^2 \psi(\mathbf{x}^{\alpha} - \mathbf{x}). \quad (6.44)$$

Finally, the remaining third and fourth terms comprise the heat flux per unit volume \mathbf{q} ,

$$\mathbf{q} = - \sum_{\alpha=1}^N \left[\sum_{\beta \neq \alpha}^N \left[\sum_{\gamma \neq \alpha}^N \frac{\partial \phi^{\beta}}{\partial x^{\alpha \gamma}} \frac{\mathbf{x}^{\alpha \gamma} \otimes \mathbf{x}^{\alpha \beta}}{x^{\alpha \gamma}} B^{\alpha \beta}(\mathbf{x}) \right] \right] \cdot \mathbf{u}^{\alpha} + \sum_{\alpha=1}^N \left\{ \frac{1}{2} m^{\alpha} (u^{\alpha})^2 + \phi^{\alpha} \right\} \mathbf{u}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x}). \quad (6.45)$$

This relation can be simplified by Hardy's fourth assumption,

$$\mathbf{q} = - \sum_{\alpha=1}^N \left[\sum_{\beta \neq \alpha}^N \frac{\partial \phi^{\beta}}{\partial x^{\alpha \beta}} \frac{\mathbf{x}^{\alpha \beta} \otimes \mathbf{x}^{\alpha \beta}}{x^{\alpha \beta}} B^{\alpha \beta}(\mathbf{x}) \right] \cdot \mathbf{u}^{\alpha} + \sum_{\alpha=1}^N \left\{ \frac{1}{2} m^{\alpha} (u^{\alpha})^2 + \phi^{\alpha} \right\} \mathbf{u}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x}). \quad (6.46)$$

One remaining task is to revisit the body force term derived during the balance of energy in equation (6.35). Starting with this equation, we obtain

$$\begin{aligned} \rho \mathbf{b} \cdot \mathbf{v} &= \sum_{\alpha=1}^N m^{\alpha} \mathbf{b}^{\alpha} \cdot \mathbf{v}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x}) \\ &= \sum_{\alpha=1}^N m^{\alpha} \mathbf{b}^{\alpha} \cdot (\mathbf{u}^{\alpha} + \mathbf{v}) \psi(\mathbf{x}^{\alpha} - \mathbf{x}) \\ &= \sum_{\alpha=1}^N m^{\alpha} \mathbf{b}^{\alpha} \cdot \mathbf{u}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x}) + \left(\sum_{\alpha=1}^N m^{\alpha} \mathbf{b}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x}) \right) \cdot \mathbf{v} \\ &= \sum_{\alpha=1}^N m^{\alpha} \mathbf{b}^{\alpha} \cdot \mathbf{u}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x}) + \rho \mathbf{b} \cdot \mathbf{v}. \end{aligned}$$

Clearly this is only true if

$$\sum_{\alpha=1}^N m^{\alpha} \mathbf{b}^{\alpha} \cdot \mathbf{u}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x}) = 0. \quad (6.47)$$

This does NOT automatically seem to be satisfied. However, for the case of the same body force on each atom, $\mathbf{b}^1 = \mathbf{b}^2 = \dots = \mathbf{b}^N$, the zero net momentum property of the relative velocity field does make it true. This extra term can be thought of as "fine scale work" done by the body force field on the relative atomic velocity field that is neglected by the continuum formulation.

6.3 Comparison of Hardy's method with Moving Least Squares

6.3.1 Moving Least Squares (MLS) particle methods

A group of methods for representing a continuum with computational points or "particles" variously named : Smooth Particle Hydrodynamics (SPH) [12], Moving Least Squares (MLS) [13], Element Free Galerkin Method (EFG) [14] and Reproducing Kernel Particle Method (RKPM) [15] , fall into a common framework. All the methods are derived from the linear transformation of a field $u(\mathbf{y})$

$$u_h = \int_{\Omega} \varphi_h(\mathbf{x}, \mathbf{x} - \mathbf{y})u(\mathbf{y})d\mathbf{y} \quad (6.48)$$

through convolution with a smoothing (or kernel) function $\varphi_h(\mathbf{x}, \mathbf{x} - \mathbf{y})$. The function φ_h is sometimes called a 'window' function since it typically approaches zero as the magnitude of the second argument approaches a characteristic distance h , i.e. as \mathbf{y} gets further than h away from the center point \mathbf{x} . Various authors propose a number restrictions on the form of the kernel function:

1. compact support, $\varphi_h(\mathbf{x}, \mathbf{x} - \mathbf{y}) = 0$ outside a finite region that includes \mathbf{x} ,
2. positiveness, $\varphi_h(\mathbf{x}, \mathbf{x} - \mathbf{y}) \geq 0$ everywhere,
3. centeredness, $\varphi_h(\mathbf{x}, \mathbf{x} - \mathbf{y})$ monotonically decreases as $\|\mathbf{x} - \mathbf{y}\|$ increases,
4. Dirac delta property, $\lim_{h \rightarrow 0} \varphi_h(\mathbf{x}, \mathbf{x} - \mathbf{y})$ approaches the Dirac delta,
5. normality, $\int_{\Omega} \varphi_h(\mathbf{x}, \mathbf{x} - \mathbf{y})d\mathbf{y} = 1$

Item 1 is useful for computational reasons, much like how most implementations of atomistic potentials have a finite interaction distance. The other properties regulate the behavior of the transformation, but item 5 is the only property that is necessary for the transformation (6.48) to be able to reproduce (constant) fields.

For illustration, examine the RKPM window functions

$$\varphi_h(\mathbf{x}, \mathbf{x} - \mathbf{y}) = \mathbf{b}(\mathbf{x}) \cdot \mathbf{P}(\mathbf{x} - \mathbf{y})\bar{\varphi}_h(\mathbf{x} - \mathbf{y}),$$

here $\mathbf{b}(\mathbf{x}) \cdot \mathbf{P}(\mathbf{x} - \mathbf{y})$ forms a multiplicative correction to the simple window function $\bar{\varphi}_h$. The quantity $\mathbf{P}(\mathbf{x})$ is a vector of polynomial basis functions (in one dimension, a basis of order k would be $\mathbf{P}^T(x) = (1, x, x^2, \dots, x^k)$) and \mathbf{b} is a vector whose components are determined by the consistency condition, which, with manipulation, is equivalent to

$$\mathbf{P}(0) = \int \mathbf{b}(\mathbf{x}) \cdot \mathbf{P}(\mathbf{x} - \mathbf{y})\bar{\varphi}_h(\mathbf{x} - \mathbf{y})\mathbf{P}(\mathbf{x} - \mathbf{y})d\mathbf{y} \quad (6.49)$$

6.3. COMPARISON OF HARDY'S METHOD WITH MOVING LEAST SQUARES

so that

$$\mathbf{b} = \left[\int \mathbf{P}(\mathbf{x} - \mathbf{y}) \otimes \mathbf{P}(\mathbf{x} - \mathbf{y}) \bar{\varphi}_h(\mathbf{x} - \mathbf{y}) d\mathbf{y} \right]^{-1} \mathbf{P}(0) . \quad (6.50)$$

This consistency condition allows the RKPM to represent signals u up to the order of the polynomial basis $\mathbf{P}(\mathbf{x})$ exactly. Notice that the first equation of the system of equations (6.49) is precisely the normality condition. For a uniform grid in one dimension the correction function only differs from unity at the boundary of the domain; however, for a non-uniform distribution of particles, the function $\mathbf{b}(x) \cdot \mathbf{P}(\mathbf{x} - \mathbf{y})$ needs values away from unity almost everywhere in order to correct the simple window function $\bar{\varphi}_h(\mathbf{x} - \mathbf{y})$. To see the difference between a MLS representation of a linear field using corrected RKPM kernels and uncorrected kernels examine Figure 6.1.

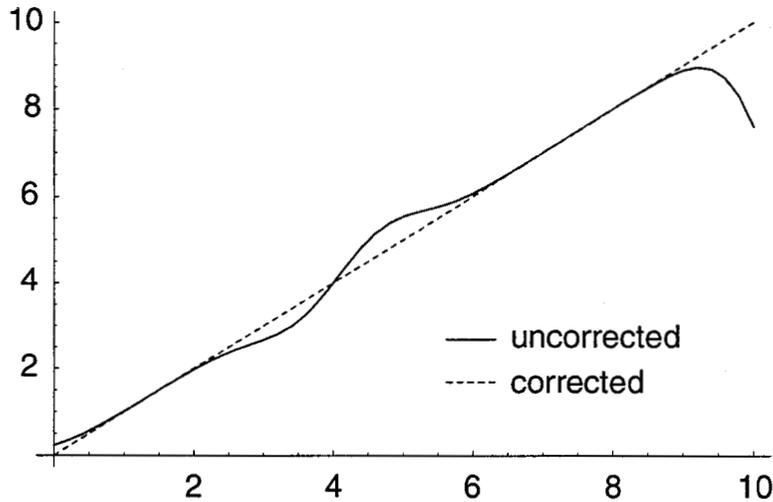


Figure 6.1: MLS representations of a linear field.

By evaluating the integral in equation (6.48) with quadrature, an approximation

$$u_h = \sum_I \mathbf{b}(\mathbf{x}) \cdot \mathbf{P}(\mathbf{x} - \mathbf{x}_I) \bar{\varphi}_h(\mathbf{x} - \mathbf{x}_I) u(\mathbf{x}_I) \Delta V_I = \sum_I \varphi_h(\mathbf{x}, \mathbf{x} - \mathbf{x}_I) \Delta V_I u_I = \sum_I \Phi_I(\mathbf{x}) u_I \quad (6.51)$$

to the original field u can be made. This approximation relies on the existence of the inverse in equation (6.50), which, in turn, requires that the quadrature involve enough points in the support of $\varphi(\mathbf{x}, \mathbf{x} - \mathbf{x}_I)$ so that the matrix being inverted has full rank. With this in hand, it is possible to identify the approximant functions

$$\Phi_I = \mathbf{b}(\mathbf{x}) \cdot \mathbf{P}(\mathbf{x} - \mathbf{x}_I) \bar{\varphi}_h(\mathbf{x} - \mathbf{x}_I) \Delta V_I .$$

This representation clearly implies that the function $\bar{\varphi}_h$ has the inverse units of the tributary volumes ΔV_I .

6.3.2 Comparison of Hardy's atomistic method and MLS methods

To make a meaningful comparison between Hardy's continuum interpretation of atomistic particle methods and MLS continuum particle methods, first the positions \mathbf{x}_I of the integration points of the MLS method need to be identified with the positions \mathbf{x}_α of the atoms. Although, in some sense, they carry different information: the MLS quadrature points are samplings of what is assumed to be an underlying continuum field, whereas the atoms' information is inherently discrete in space. Basically this is what Hardy is trying to resolve; his method is giving a prescription of how to take the so-called "continuum limit" where there are enough particles in the region being examined to construct a continuous field from the discrete values.

For his analysis, Hardy chooses density, momentum and energy to be his primary fields, which are derived from the fundamental atomistic quantities of particle mass m_α , particle position \mathbf{x}_α , and the time derivatives of its position. To see the correlation between MLS and Hardy, consider u in equation (6.51) to be linear momentum

$$\mathbf{p}_h = \sum_I \rho_I \mathbf{v}_I \varphi(\mathbf{x}, \mathbf{x} - \mathbf{x}_I) \Delta V_I .$$

Hardy's expression is

$$\mathbf{p} = \sum_I m_I \mathbf{v}_I \psi(\mathbf{x} - \mathbf{x}_I),$$

where $\psi(\mathbf{x} - \mathbf{x}_I)$ is his window function. Clearly, in the continuum the (reference) density is known *a priori* and in the atomistic system the particle masses are known at the outset. This leads to a volume weighted versus a mass weighted quadrature where either $\sum_I \Delta V_I$ equals the volume of the body or $\sum_I m_I$ equals the mass of the system. With tributary volumes assigned to Hardy's atomic quadrature i.e.

$$\mathbf{p} = \sum_I m_I \mathbf{v}_I \psi(\mathbf{x} - \mathbf{x}_I) = \sum_I \frac{1}{\Delta V_I} m_I \mathbf{v}_I \psi(\mathbf{x} - \mathbf{x}_I) \Delta V_I ,$$

its easy to see that $\varphi(\mathbf{x}, \mathbf{x} - \mathbf{x}_I)$ and $\psi(\mathbf{x} - \mathbf{x}_I)$ do essentially the same job. So, if one wanted Hardy's method to represent linear (as in a patch test) or higher order fields well, it would require the use of corrected RKPM window functions.

It is interesting that in Hardy's formulation other fields like velocity and stress are defined in a way that makes them consistent with the continuum balance of linear momentum. Unlike MLS, where a smoothing approximation would be applied first and then a constitutive law based on the continuum displacement or velocity would be applied to obtain stress, Hardy derives his stress ultimately from the interatomic energy potentials and the atomic velocity trajectories. It seems that Hardy's method is a post-processing step, but given that he makes his derived quantities consistent with continuum balance laws, an outside observer could not tell whether continuum quantities were derived from atomistic balance of linear momentum (Newton's 2nd law) or the continuum version (perhaps with internal variables). This is ideal for atom-continuum coupling.

6.4 Evaluation of Continuum Stress in Atomistic Simulation

In this section, we compare stress for atomistic systems as described by the virial theorem to results obtained using an expression for the Cauchy stress derived by R.J. Hardy. As a function of increasing cutoff radius for the stress analysis volume, the Hardy description of stress displays a quicker convergence to values expected from continuum theory than volume averages of the local virial stress. Furthermore, the behavior of Hardy's expression near a free surface is consistent with the mechanical definition for stress.

6.4.1 Stress in a crystal at zero temperature

For our simulations, we used the embedded atom potentials for Ni and Cu by Foiles, Baskes and Daw [16] and a constant localization function within a spherical volume of radius R_c . With this choice of ψ , $B^{\alpha\beta}$ has the simple geometric interpretation of the fraction of bond length between atoms α and β (normalized by $\frac{4}{3}\pi R_c^3$) that lies within the localization volume.

Our first simulations were quasi-static for a bulk Cu lattice comprised of 3,072 atoms with periodic boundary conditions on all sides at zero temperature and pressure. The size of the computational box was $8 \times 8 \times 12$ unit cells. For this system, the stress at any spatial point should equal zero. However, this was not observed, as shown in Figure 6.2. Figure 6.2 shows

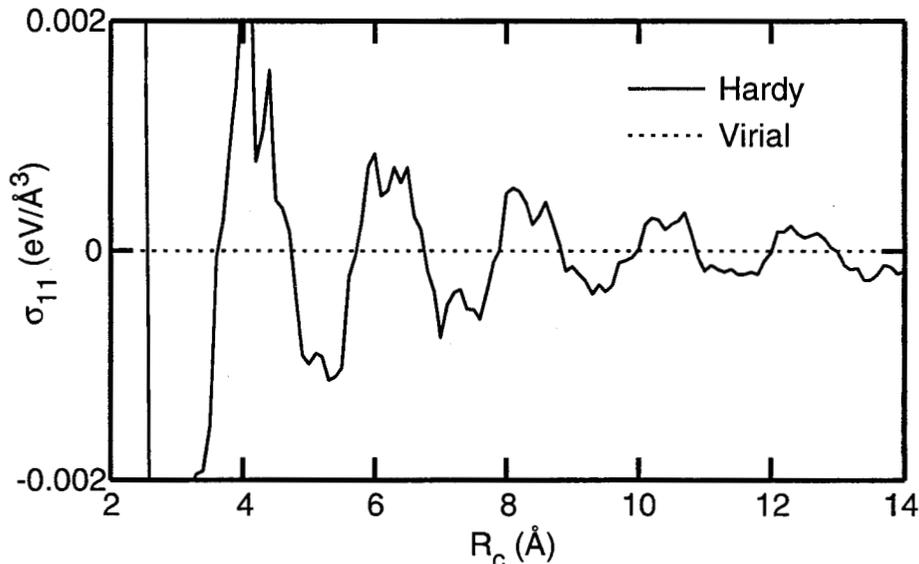


Figure 6.2: Virial and Hardy stress for an atomic system at zero temperature and pressure.

that the Hardy stress evaluated at a randomly chosen point contains a small fluctuation that diminishes in magnitude as R_c increases. Figure 6.2 also shows the volume average of the local virial stress for a spherical volume of radius R_c . This volume average can be expressed

by the relation

$$\bar{\pi} = -\frac{1}{V_c} \left\{ \frac{1}{2} \sum_{\alpha \in V_c} \sum_{\beta \neq \alpha} \mathbf{x}^{\alpha\beta} \otimes \mathbf{F}^{\alpha\beta} + \sum_{\alpha \in V_c} m^\alpha \dot{\mathbf{x}}^\alpha \otimes \dot{\mathbf{x}}^\alpha \right\}, \quad (6.52)$$

where $V_c = \frac{4}{3}\pi R_c^3$ and the symbol π is used to denote the local virial stress in order to differentiate it from the Hardy expression for stress. For quasi-static analysis, the second term in the above expression vanishes. Figure 6.2 shows that the value of $\bar{\pi}_{11}$ is exactly zero for all values of R_c , an expected result since all local virial stresses are zero for this case. We attribute the behavior of the Hardy stress to differing amounts of force contribution for each interacting atomic pair as the localization volume changes. As the averaging volume increases, the bond function B changes its value only for those atomic pairs that have at least one of the atoms lying outside the volume. As R_c increases, the magnitude of these force contributions become much less significant than the force contributions from atomic pairs interior to the volume. In fact, since the number of bonds lying completely within the volume increases as R_c^3 and the number that partially contribute to the stress increases as R_c^2 , one would expect the amplitude of fluctuations to decay as roughly R_c^{-1} . Hardy, Root and Swanson [17] themselves noticed the correlation between fluctuations in stress and the size of the localization volume.

The curve shown in Figure 6.2 was for the normal stress evaluated at a single spatial point chosen at random. Examination of the mean of this curve averaged over many such randomly chosen points, shown in Figure 6.3, reveals that the magnitude of these fluctuations becomes vanishingly small as the number of averaging points increases. The fluctuations decrease in magnitude by a factor of 10 when stress is averaged over 10 or 100 points, and decrease by a factor of 50 or greater when stress is averaged over 1000 points. This behavior is consistent with the mathematical definition of the Hardy stress, equation (6.38). As more spatial points are used for averaging, we are, in-effect, integrating (6.38) over all space. This integration results in recovery of the expression for the virial stress for the system, which is zero for this case. We can also examine the *variance* of these averaging distributions, shown in Figure 6.4. The variance, or standard deviation, is defined by the relation

$$\text{var}(\sigma_{11}) \equiv \sqrt{\frac{1}{N_p - 1} \sum_{p=1}^{N_p} (\sigma_{11}(\mathbf{x}_p) - \bar{\sigma}_{11})^2}, \quad (6.53)$$

where N_p is the number of spatial points averaged over. Not only does Figure 6.4 show that this variance approaches zero as R_c increases, but it also reveals that the behavior of the variance as a function of R_c is virtually the same whether 100 or 1000 spatial points are used for averaging. This may indicate some limiting behavior in the functional dependence of the variance on R_c as $N_p \rightarrow \infty$.

The impact of these fluctuations is less significant for cases of non-zero values of stress, as shown in Figure 6.5 for a system under 2% uniaxial strain. The Hardy stress fluctuates around the expected value of $0.02 \text{ eV}/\text{\AA}^3$, with the magnitude of the fluctuation decaying

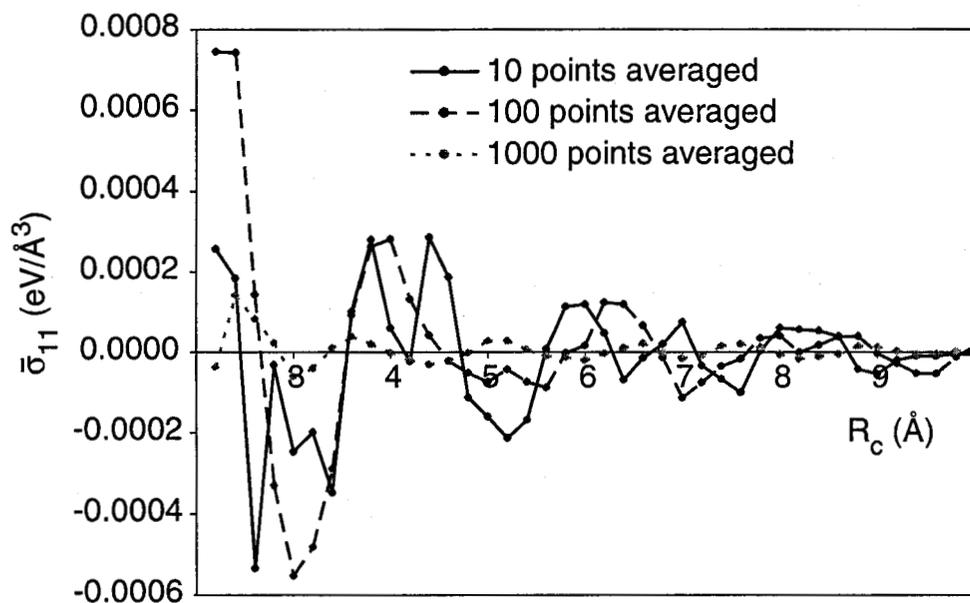


Figure 6.3: Mean of the Hardy stress averaged over many spatial points.

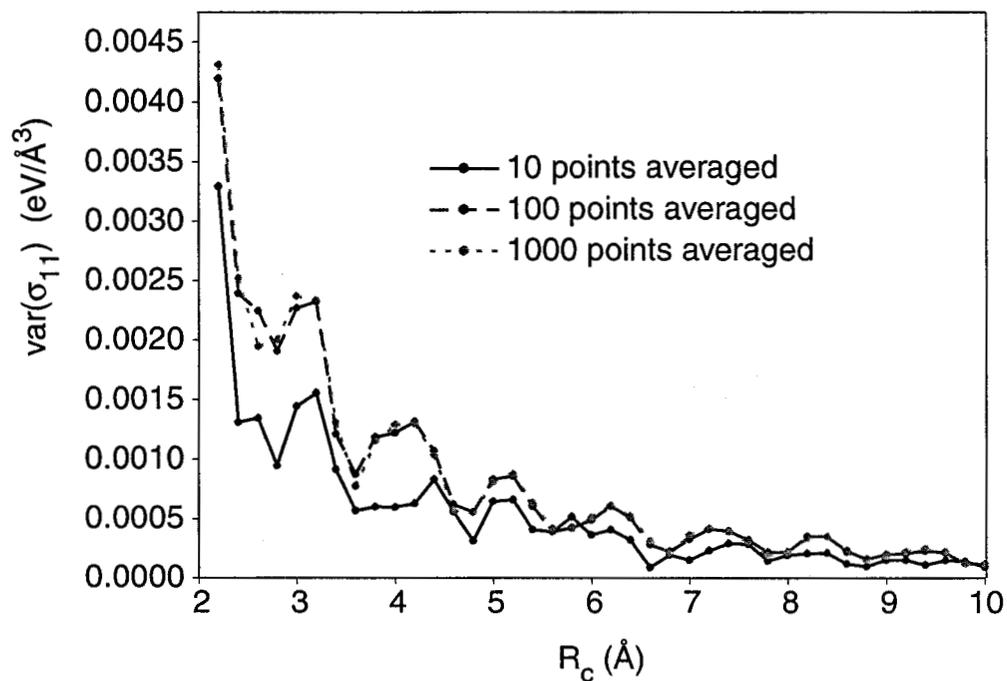


Figure 6.4: Variance of the Hardy stress averaged over many spatial points.

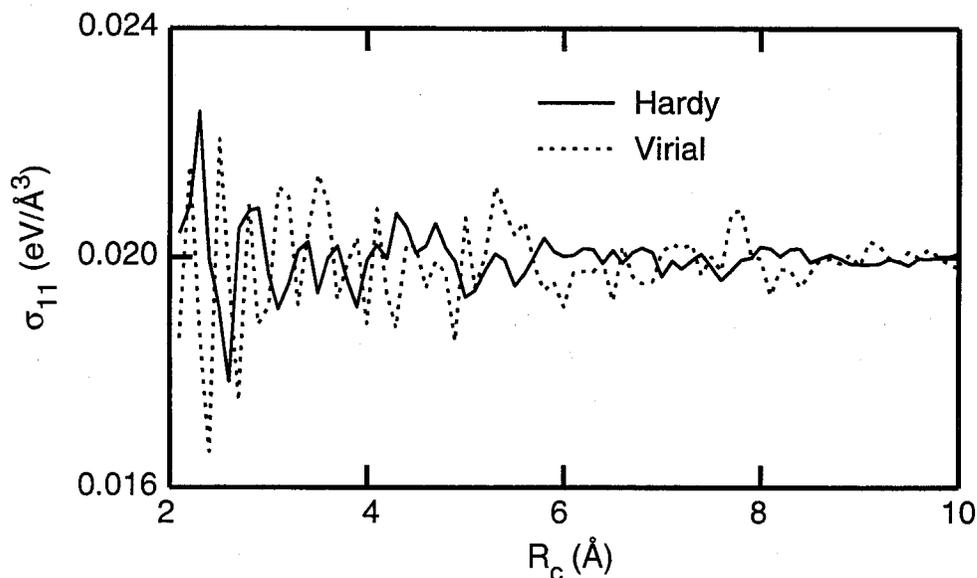


Figure 6.5: Virial and Hardy stress for an atomic system at zero temperature and 2% uniaxial strain.

with increased R_c . The error is acceptably low, only 4% at $R_c = 6 \text{ \AA}$. The virial stress also fluctuates about the expected value due to the minor changes in volume that alter all continuum densities. The error in the averaged virial stress does not decay as quickly as for the Hardy stress, and is significant even up to distances of 8 \AA .

6.4.2 Stress in a crystal at finite temperature

Stress within a system at finite temperature was also evaluated. Figure 6.6 shows the stress for a system that was equilibrated to be at zero pressure at room temperature, then uniaxially strained by 5%. Only the force-term portion of the stresses is shown in Figure 6.6, as the kinetic term is the same for both Hardy and virial expressions and contributes less than 10% of the total stress. In Figure 6.6, all data points are calculated for a localization volume centered at the same particular spatial point at a given instant in time. While both Hardy and virial stresses show oscillations that converge to the same limit, 0.0738 eV/\AA^3 , the Hardy formulation smoothes the fluctuations more effectively than the virial. Notice that the magnitude of these thermal fluctuations overwhelms those noticed at zero temperature.

6.4.3 Stress in a crystal with a free surface

Differing causes of fluctuations for the two stresses impacts stress evaluation for regions with inhomogeneous structure, such as at a free surface. Figure 6.7 shows the stress within a crystal as a function of distance from a free surface for two values of R_c , 6 and 10 \AA . Within a distance R_c of the top atomic layer, the magnitude of fluctuations is comparable for both

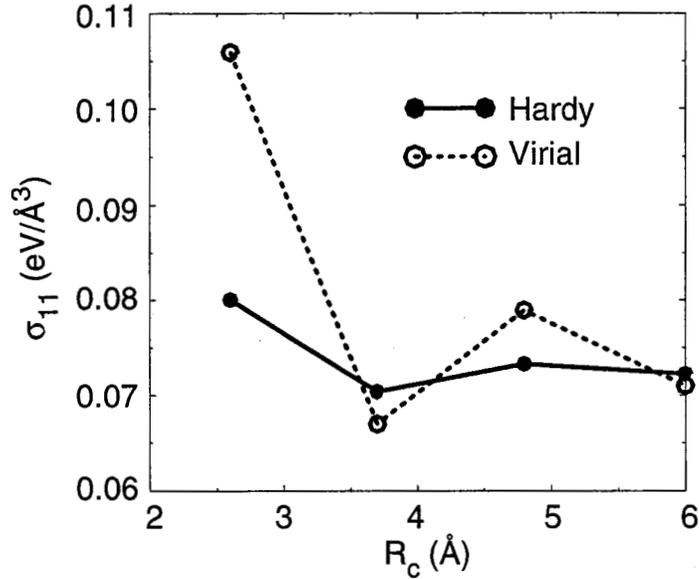


Figure 6.6: The force-term portions of the Virial and Hardy stresses for an atomic system at room temperature and 5% uniaxial strain.

expressions. However, the wavelength of the virial fluctuation is clearly tied to the size of the averaging volume, *i.e.* it equals twice the value of R_c . This result shows a ‘smearing’ of the oscillation in local virial stress noticed by Cheung and Yip [4]. In contrast, the wavelength for the Hardy stress fluctuations is considerably smaller than for the virial, and is roughly the same for both values of R_c . Also, the Hardy value decays within the region between the top atomic layer and the “effective” surface of the crystal, located at a distance equal to R_c , while the virial stress increases in magnitude, only dropping to zero within 0.5 Å of the effective surface.

We also examined the normal stress for directions parallel to the free surface, *i.e.* the planar stress that normally corresponds to residual surface stress. This is shown in Figure 6.8 for the same atomic system discussed above. We observe that the stress distribution is virtually the same for both the Hardy and virial expressions. Both display a build-up of finite stress below the surface, representing a material’s surface tension, and a drop-off to zero at the effective surface of the solid.

6.4.4 Remarks

Our analysis has shown that the definition for Cauchy stress in an atomic system developed by Hardy does a better job than the expression based on the virial theorem. In general, fluctuations in the Hardy stress are lower in magnitude and decay faster with increasing averaging volume size. Also, the behavior of the Hardy expression for stress near a free surface is consistent with the mechanical definition of stress.

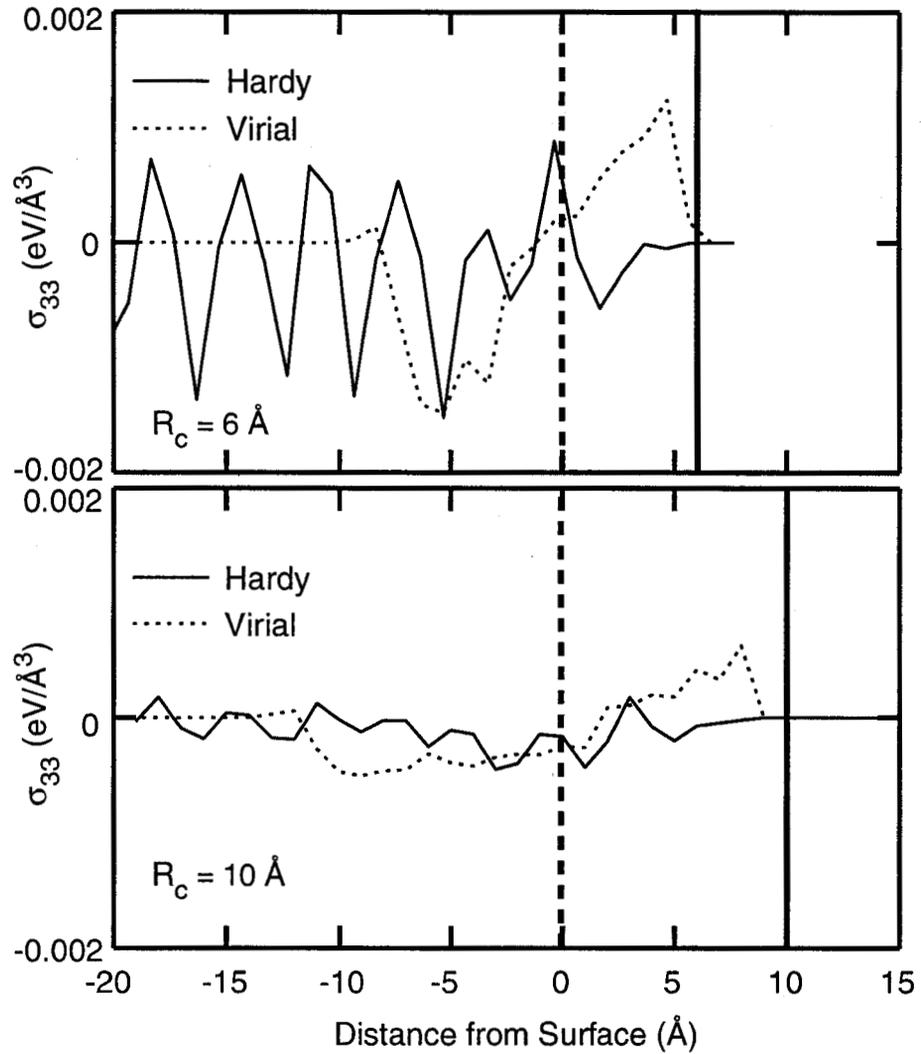


Figure 6.7: Virial and Hardy stress for an atomic system at zero temperature and pressure with a free surface. The heavy, dashed line denotes the position of the top layer of atoms, both at zero, while the heavy, solid line denotes the effective position of the free surface of the crystal.

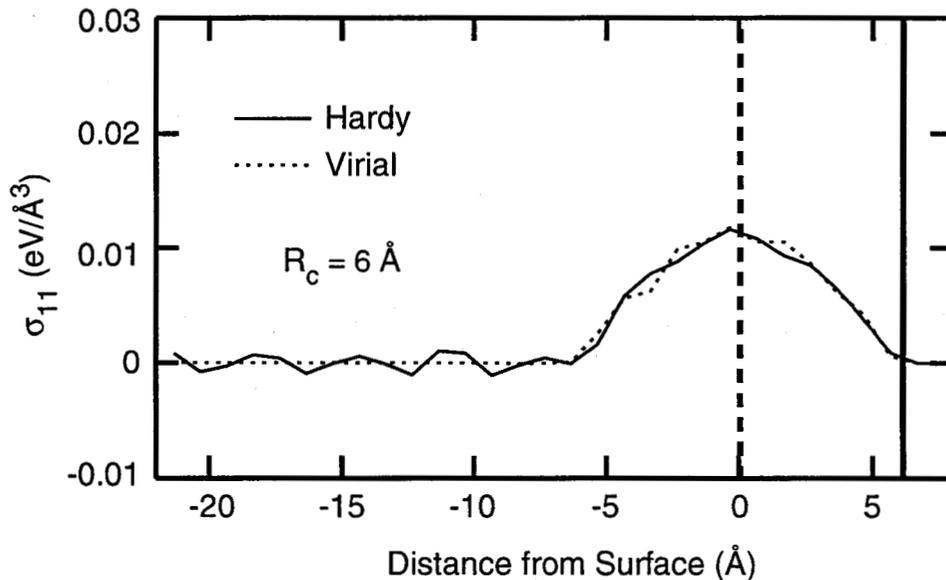


Figure 6.8: The normal stresses for the cubic directions parallel to the free surface for the system shown in Figure 6.7.

6.5 Extending Hardy's formulation to non-central potentials

Section 6.2.2 discussed the four assumptions made by Hardy regarding the form of the interatomic potential energies and interaction forces. In this section, we revisit these assumptions and challenge the ones that require that Hardy's formulation be applied only to "central" potentials, *e.g.* pair potentials and the embedded atom method. We will present revisions that allow Hardy's method to be applied to certain non-central potentials, such as 3-body potentials like the Stillinger-Weber potential for silicon [11]. However, these revisions will also be accompanied by caveats regarding symmetry of the Cauchy stress tensor.

6.5.1 Bonds, Energies and Forces in Atomistic Mechanics

Configurations and Invariance

For a finite system of N particles a set of their positions

$$\kappa = \{\mathbf{x}^\alpha, \alpha = 1..N\} \quad (6.54)$$

with their masses m^α constitutes a 'configuration' in a static setting (momenta \mathbf{p}^α or velocities \mathbf{v}^α are necessary to describe a configuration in a dynamic setting). The energy of the system Φ depends on the configuration

$$\Phi = \Phi(\kappa) = \Phi(\{\mathbf{x}^\alpha\}); \quad (6.55)$$

however, a basic symmetry rule, invariance under superposed rigid body motion or change in coordinate frame, restricts how the energy depends on the configuration. Invariance requires that

$$\Phi^+ := \Phi(\{\mathbf{x}^{\alpha+}\}) = \Phi(\{\mathbf{x}^\alpha\}) =: \Phi \quad (6.56)$$

where

$$\mathbf{x}^{\alpha+} = \mathbf{Q}\mathbf{x}^\alpha + \mathbf{a}, \quad \mathbf{Q} \in Orth^+ \quad (6.57)$$

i.e. that the energy cannot change with rigid rotations and translations of the configuration. This implies that the energy cannot depend directly on the particles' positions.

Bonds and Energy

Every atomistic system of particles has a substructure made up of bonds \mathcal{B} , so that the total energy can be decomposed as:

$$\Phi = \sum_{K \in \mathcal{B}} \phi^K. \quad (6.58)$$

The energy of an individual bond depends only on a subset of the configuration, e.g. two $\{\mathbf{x}^\alpha, \mathbf{x}^\beta\}$ or three $\{\mathbf{x}^\alpha, \mathbf{x}^\beta, \mathbf{x}^\gamma\}$ or four atoms $\{\mathbf{x}^\alpha, \mathbf{x}^\beta, \mathbf{x}^\gamma, \mathbf{x}^\delta\}$. By applying the invariance principle, it is clear that ϕ^K can only depend on invariants like a distance

$$I_d = \|\mathbf{x}^{\alpha\beta}\| \quad \text{where } \mathbf{x}^{\alpha\beta} := \mathbf{x}^\alpha - \mathbf{x}^\beta, \quad (6.59)$$

a cosine of an angle

$$I_a = \frac{1}{\|\mathbf{x}^{\alpha\beta}\| \|\mathbf{x}^{\beta\gamma}\|} \mathbf{x}^{\alpha\beta} \cdot \mathbf{x}^{\beta\gamma}, \quad (6.60)$$

an area

$$I_s = \|\mathbf{x}^{\alpha\beta} \times \mathbf{x}^{\beta\gamma}\|, \quad (6.61)$$

or a volume

$$I_v = [\mathbf{x}^{\beta\alpha}, \mathbf{x}^{\gamma\alpha}, \mathbf{x}^{\delta\alpha}] := (\mathbf{x}^{\beta\alpha} \times \mathbf{x}^{\gamma\alpha}) \cdot \mathbf{x}^{\delta\alpha}. \quad (6.62)$$

In all these invariants the difference in positions removes the dependence on the rigid translation \mathbf{a} and the inner product or cross product removes the dependence on the rigid rotation \mathbf{Q} .

Forces

If forces are defined to be conjugate to changes in particle positions (they could be defined to be conjugate to other kinematic variable, e.g. the invariants I_i), then

$$-\delta\Phi = \mathbf{F}^\alpha \delta\mathbf{x}^\alpha \Rightarrow \mathbf{F}^\alpha = -\partial_{\mathbf{x}^\alpha} \Phi. \quad (6.63)$$

So

$$\mathbf{F}^\alpha = -\partial_{\mathbf{x}^\alpha} \Phi = \sum_{K \in \mathcal{B}} \sum_{i \in \{d, a, s, v, \dots\}} \partial_{I_i} \phi_K \partial_{\mathbf{x}^\alpha} I_i \quad (6.64)$$

6.5. EXTENDING HARDY'S FORMULATION TO NON-CENTRAL POTENTIALS

where the sum over bonds can be restricted to only the bonds that involve particle α without loss in generality. For a pair bond dependent on relative distance a contribution to the force \mathbf{F}^α would be

$$\frac{\partial \phi_K}{\partial I_d} \frac{\partial I_d}{\partial \mathbf{x}^\alpha} = \frac{\partial \phi_K}{\partial I_d} \frac{1}{\|\mathbf{x}^{\alpha\beta}\|} \mathbf{x}^{\alpha\beta}. \quad (6.65)$$

For a triplet bond, the angle dependence would lead to contributions

$$\frac{\partial \phi_K}{\partial I_a} \frac{\partial I_a}{\partial \mathbf{x}^\alpha} = \frac{\partial \phi_K}{\partial I_a} \frac{1}{\|\mathbf{x}^{\alpha\beta}\| \|\mathbf{x}^{\beta\delta}\|} (\mathbf{x}^{\beta\delta} - \frac{\mathbf{x}^{\alpha\beta} \cdot \mathbf{x}^{\beta\delta}}{\|\mathbf{x}^{\alpha\beta}\|^2} \mathbf{x}^{\alpha\beta}) \quad (6.66)$$

for particle α and

$$\frac{\partial \phi_K}{\partial I_a} \frac{\partial I_a}{\partial \mathbf{x}^\beta} = \frac{\partial \phi_K}{\partial I_a} \frac{1}{\|\mathbf{x}^{\alpha\beta}\| \|\mathbf{x}^{\beta\delta}\|} \left(\mathbf{x}^{\alpha\beta} + \mathbf{x}^{\beta\delta} - (\mathbf{x}^{\alpha\beta} \cdot \mathbf{x}^{\beta\delta}) \left(\frac{\mathbf{x}^{\alpha\beta}}{\|\mathbf{x}^{\alpha\beta}\|^2} + \frac{\mathbf{x}^{\beta\delta}}{\|\mathbf{x}^{\beta\delta}\|^2} \right) \right) \quad (6.67)$$

for particle β , the 'center' atom. So the bonds that depend on basic arguments like $\mathbf{x}^{\alpha\beta}$ lead to contributions along those directions. These contributions can be grouped by their vector components, $\mathbf{x}^{\alpha\beta}$, $\mathbf{x}^{\beta\gamma}$, etc., and those associated with, say $\mathbf{x}^{\alpha\beta}$, can be named ' $\mathbf{F}^{\alpha\beta}$ ', but this force is not, in general, a derivative of an energy function. Recall that the force \mathbf{F}^α is a sum over relevant bonds of the partial derivative of the bond energy holding the positions of *all* the other involved atoms fixed and can be interpreted as the force on α due to the system. Except for the simple case of pair bonds where the *ad hoc* assumption that the bond energy is divided between the two atoms in some fixed ratio can a force $\mathbf{F}^{\alpha\beta}$ be derived from a potential involving only \mathbf{x}^α and \mathbf{x}^β , as in

$$\mathbf{F}^{\alpha\beta} := -(\partial_{I_d} \phi^\alpha + \partial_{I_d} \phi^\beta) \frac{1}{\|\mathbf{x}^{\alpha\beta}\|} \mathbf{x}^{\alpha\beta} = -\partial_{I_d} \phi^K \frac{1}{\|\mathbf{x}^{\alpha\beta}\|} \mathbf{x}^{\alpha\beta} = \mathbf{F}^\alpha = -\mathbf{F}^\beta \quad (6.68)$$

where $\phi^\alpha = \phi^\beta = \frac{1}{2} \phi_K(\mathbf{x}^\alpha, \mathbf{x}^\beta)$.

6.5.2 Hardy's Assumptions Revisited

Assumption 1 - Individual Atomic Potential Energy

The first assumption by Hardy states that the total potential energy of the system Φ can be divided into individual atomic potential energies ϕ^α ,

$$\Phi = \sum_{\alpha=1}^N \phi^\alpha. \quad (6.69)$$

As discussed above, the system energy Φ is composed of the energetic contributions due to bonds between atoms. In general, this energy can be expressed by the following expansion

$$\begin{aligned} \Phi(\mathbf{x}^\alpha, \mathbf{x}^\beta, \dots, \mathbf{x}^N) &= \sum_{\alpha} \sum_{\beta > \alpha} v_2(\mathbf{x}^\alpha, \mathbf{x}^\beta) + \sum_{\alpha} \sum_{\beta > \alpha} \sum_{\gamma > \beta} v_3(\mathbf{x}^\alpha, \mathbf{x}^\beta, \mathbf{x}^\gamma) \\ &+ \dots + v_N(\mathbf{x}^\alpha, \mathbf{x}^\beta, \dots, \mathbf{x}^N), \end{aligned} \quad (6.70)$$

where v_k represents the potential energy for a unique k-body interaction. We have omitted the v_1 term of the expansion since that term violates the invariance of Φ already mentioned. Equation 6.70 can always be rewritten as

$$\begin{aligned} \Phi(\mathbf{x}^\alpha, \mathbf{x}^\beta, \dots, \mathbf{x}^N) = & \sum_{\alpha} \left\{ \frac{1}{2} \sum_{\beta \neq \alpha} w_2(\mathbf{x}^{\alpha\beta}) \right\} + \sum_{\alpha} \left\{ \frac{1}{3!} \sum_{\beta \neq \alpha} \sum_{\gamma \neq \beta \neq \alpha} w_3(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\gamma}, \mathbf{x}^{\beta\gamma}) \right\} \\ & + \dots + \sum_{\alpha} \left\{ \frac{1}{N!} \sum_{\beta \neq \alpha} \sum_{\gamma \neq \beta \neq \alpha} \dots \sum_{N \neq \dots} w_N(\mathbf{x}^{\alpha\beta}, \dots, \mathbf{x}^{\alpha N}) \right\}, \end{aligned} \quad (6.71)$$

where w_k is the a reformulated version of v_k in terms of the interatomic vectors. It is important to note that each w_k represents the total interaction energy from the unique combination of the atoms involved. For example, w_3 is the total interaction energy between atoms α , β and γ . The use of the factorial symbol (!) compensates for over-counting the contributions, e.g. $\alpha = 1, \beta = 2, \gamma = 3$ and $\alpha = 1, \beta = 3, \gamma = 2$, but it is essential to realize that w_3 equals the same value for all distinct combinations. The individual atomic potential ϕ^α from equation (6.69) can now be identified as

$$\begin{aligned} \phi^\alpha = & \frac{1}{2} \sum_{\beta \neq \alpha} w_2(\mathbf{x}^{\alpha\beta}) + \frac{1}{3!} \sum_{\beta \neq \alpha} \sum_{\gamma \neq \beta \neq \alpha} w_3(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\gamma}, \mathbf{x}^{\beta\gamma}) + \dots + \\ & \frac{1}{N!} \sum_{\beta \neq \alpha} \sum_{\gamma \neq \beta \neq \alpha} \dots \sum_{N \neq \dots} w_N(\mathbf{x}^{\alpha\beta}, \dots, \mathbf{x}^{\alpha N}). \end{aligned} \quad (6.72)$$

The use of equation (6.69) is somewhat misleading, since the energy itself lies within the *bonds*, and is not localized to the positions of the atoms themselves. However, the use of these expressions is mathematically valid and equally distributes the system energy among all its constituent atoms.

Assumption 2 - Dividing up the force on an atom

Hardy's second assumption states that the total force on any atom, \mathbf{F}^α , can be divided into pair-wise forces between atoms,

$$\mathbf{F}^\alpha \equiv -\frac{\partial \Phi}{\partial \mathbf{x}^\alpha} = \sum_{\beta \neq \alpha}^N \mathbf{F}^{\alpha\beta}. \quad (6.73)$$

The assumption is a perfectly valid one as long as there are more atoms than spatial dimensions. Equation (6.73) merely states that the total force on each atom is broken up into $N - 1$ different contributions, in *some* fashion. However, it does not necessarily dictate how that division is performed, nor does it necessarily provide a physical meaning for the expression $\mathbf{F}^{\alpha\beta}$.

Assumption 3 - Functions of interatomic distances only

This assumption states that all potential energy functions should only be functions of interatomic distances, $\phi^\alpha = \phi^\alpha(x^{\alpha\beta}, x^{\alpha\gamma}, \dots, x^{\beta\gamma})$, so that

$$\mathbf{F}^\alpha = - \sum_{\beta \neq \alpha}^N \sum_{\gamma=1}^N \frac{\partial \phi^\gamma}{\partial x^{\alpha\beta}} \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}. \quad (6.74)$$

This assumption is clearly **not** true for all potentials. However, it is true that all interatomic energies can be expressed as functions of the interatomic vectors, $\phi^\alpha = \phi^\alpha(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\gamma}, \dots, \mathbf{x}^{\beta\gamma})$, and thus,

$$\mathbf{F}^\alpha = - \sum_{\beta \neq \alpha}^N \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} = - \sum_{\beta \neq \alpha}^N \sum_{\gamma=1}^N \frac{\partial \phi^\gamma}{\partial \mathbf{x}^{\alpha\beta}}. \quad (6.75)$$

At this point, it might be tempting to say that

$$\mathbf{F}^{\alpha\beta} \equiv - \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}}; \quad (6.76)$$

however, this definition of $\mathbf{F}^{\alpha\beta}$ will not necessarily satisfy the balance of linear momentum within Hardy's formulation.

Assumption 4 - Defining the quantity $\mathbf{F}^{\alpha\beta}$

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

$$\mathbf{F}^{\alpha\beta} = - \left\{ \frac{\partial \phi^\alpha}{\partial x^{\alpha\beta}} + \frac{\partial \phi^\beta}{\partial x^{\alpha\beta}} \right\} \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}}. \quad (6.77)$$

Clearly, this is a false statement for any arbitrary potential. However, a broad range of potentials exist such that the potential energy for each atom will depend only on interatomic *vectors* between the atom under consideration and all other atoms,

$$\phi^\alpha = \phi^\alpha(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\gamma}, \dots, \mathbf{x}^{\alpha N}). \quad (6.78)$$

An example of this type of potential is 3-body portion of the Stillinger-Weber interatomic potential for silicon [11]. The expression for this 3-body energy is

$$w_3 = \varepsilon \lambda \exp\left(\frac{\gamma}{\frac{x^{\alpha\beta}}{\sigma} - a}\right) \exp\left(\frac{\gamma}{\frac{x^{\alpha\gamma}}{\sigma} - a}\right) \left\{ \frac{\mathbf{x}^{\alpha\beta} \cdot \mathbf{x}^{\alpha\delta}}{x^{\alpha\beta} x^{\alpha\delta}} + \frac{1}{3} \right\}^2, \quad (6.79)$$

where ε , λ , γ , σ and a are fitted material parameters. This energy represents the angular bond that exists between atoms α , β and δ , where α is considered the “center” atom and a non-zero energy results whenever the angle

$$\theta_{\beta\alpha\delta} \equiv \arccos\left(\frac{\mathbf{x}^{\alpha\beta} \cdot \mathbf{x}^{\alpha\delta}}{x^{\alpha\beta}x^{\alpha\delta}}\right)$$

deviates from an angle of 109.47° . Please note that (6.79) can be re-cast into a form that depends only on the interatomic distances between atoms, thus satisfying Hardy’s third assumption. However, this new form would violate the fourth assumption since it would have the energy function ϕ^α dependent on the distance $x^{\beta\delta}$.

6.5.3 Using Hardy’s method for 3-body forces

The form of ϕ^α in (6.78) suggests that the expression for $\mathbf{F}^{\alpha\beta}$ should be

$$\mathbf{F}^{\alpha\beta} \equiv - \left\{ \frac{\partial\phi^\alpha}{\partial\mathbf{x}^{\alpha\beta}} + \frac{\partial\phi^\beta}{\partial\mathbf{x}^{\alpha\beta}} \right\}. \quad (6.80)$$

This expression seems to be the simple combination of evaluating (6.78) within (6.75). However, it is crucial to notice that the functional form of each ϕ^α must be consistent with (6.78), and cannot necessarily be expressed as the original form of Φ . As an example, consider the interaction of only 3 atoms (α , β and δ) and only a single 3-body potential energy term Φ ,

$$\Phi = \Phi(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\delta}). \quad (6.81)$$

Using the relation (6.72), the full energy Φ is partitioned equally among the 3 atoms, $\phi^\alpha = \phi^\beta = \phi^\delta = \frac{1}{3}\Phi$. However, before we start taking partial derivatives of these individual energies for equation (6.80), we must express the functional dependency for each energy correctly. For atom α , the expression is trivial,

$$\phi^\alpha = \frac{1}{3}\Phi(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\delta}), \quad (6.82)$$

but for atoms β and δ , the expressions are,

$$\phi^\beta = \phi^\beta(\mathbf{x}^{\beta\alpha}, \mathbf{x}^{\beta\delta}) = \frac{1}{3}\Phi(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\beta} + \mathbf{x}^{\beta\delta}) \quad (6.83)$$

$$\phi^\delta = \phi^\delta(\mathbf{x}^{\delta\alpha}, \mathbf{x}^{\delta\beta}) = \frac{1}{3}\Phi(\mathbf{x}^{\alpha\delta} + \mathbf{x}^{\delta\beta}, \mathbf{x}^{\alpha\delta}) \quad (6.84)$$

In these relations, we have substituted $\mathbf{x}^{\alpha\beta} + \mathbf{x}^{\beta\delta}$ for $\mathbf{x}^{\alpha\delta}$ in the expression for ϕ^β since, according to equation (6.78), it cannot depend directly on $\mathbf{x}^{\alpha\delta}$. Likewise for the ϕ^δ term, we have substituted $\mathbf{x}^{\alpha\delta} + \mathbf{x}^{\delta\beta}$ for $\mathbf{x}^{\alpha\beta}$. Obviously, clarity requires that any expression that uses Φ in a simple way must refer to its original form shown in (6.81). So, when partial derivatives

6.5. EXTENDING HARDY'S FORMULATION TO NON-CENTRAL POTENTIALS

are taken, they must include terms that may indirectly depend on certain variables. For example,

$$\frac{\partial \phi^\beta}{\partial \mathbf{x}^{\alpha\beta}} = \frac{1}{3} \left(\frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} + \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} \frac{\partial \mathbf{x}^{\alpha\delta}}{\partial \mathbf{x}^{\alpha\beta}} \right) = \frac{1}{3} \left(\frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} + \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} \right). \quad (6.85)$$

Equation (6.85) is easily understood. The first term inside the parentheses results from the derivative of Φ with respect to $\mathbf{x}^{\alpha\beta}$ as it appears explicitly within the normal functional form of Φ , but the second term is present because Φ also depends on $\mathbf{x}^{\alpha\delta}$, which itself depends on $\mathbf{x}^{\alpha\beta}$ through the relation $\mathbf{x}^{\alpha\delta} = \mathbf{x}^{\alpha\beta} + \mathbf{x}^{\beta\delta}$. Since

$$\frac{\partial \phi^\alpha}{\partial \mathbf{x}^{\alpha\beta}} = \frac{1}{3} \left(\frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} \right), \quad (6.86)$$

we can now calculate $\mathbf{F}^{\alpha\beta}$ from equation (6.80),

$$\begin{aligned} \mathbf{F}^{\alpha\beta} &= - \left\{ \frac{\partial \phi^\alpha}{\partial \mathbf{x}^{\alpha\beta}} + \frac{\partial \phi^\beta}{\partial \mathbf{x}^{\alpha\beta}} \right\} \\ &= - \left\{ \frac{1}{3} \left(\frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} \right) + \frac{1}{3} \left(\frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} + \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} \right) \right\} \\ &= - \left\{ \frac{2}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} + \frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} \right\}. \end{aligned} \quad (6.87)$$

Similarly, for this example

$$\mathbf{F}^{\alpha\delta} = - \left\{ \frac{2}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} + \frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} \right\}, \quad (6.88)$$

thus the full force on atom α is

$$\begin{aligned} \mathbf{F}^\alpha &= \mathbf{F}^{\alpha\beta} + \mathbf{F}^{\alpha\delta} \\ &= - \left\{ \frac{2}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} + \frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} \right\} - \left\{ \frac{2}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} + \frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} \right\} \\ &= - \left\{ \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} + \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} \right\} \\ &= - \sum_{\eta=\beta,\delta} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\eta}} = - \frac{\partial \Phi}{\partial \mathbf{x}^\alpha}. \end{aligned} \quad (6.89)$$

It is interesting to note that the expression for $\mathbf{F}^{\alpha\beta}$ in (6.87) involves derivatives with respect to interatomic vectors other than just $\mathbf{x}^{\alpha\beta}$, and that it is not necessarily collinear with $\mathbf{x}^{\alpha\beta}$.

It can be shown that equation (6.80) can be used just as equation (6.77) to satisfy both the balance of linear momentum *and* the balance of energy. This produces an expression for the continuum stress tensor,

$$\boldsymbol{\sigma} = - \left\{ \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \mathbf{F}^{\alpha\beta} B^{\alpha\beta}(\mathbf{x}) + \sum_{\alpha=1}^N m^\alpha \mathbf{u}^\alpha \otimes \mathbf{u}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}) \right\}, \quad (6.90)$$

or,

$$\boldsymbol{\sigma} = \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \left\{ \frac{\partial \phi^\alpha}{\partial \mathbf{x}^{\alpha\beta}} + \frac{\partial \phi^\beta}{\partial \mathbf{x}^{\alpha\beta}} \right\} B^{\alpha\beta}(\mathbf{x}) - \sum_{\alpha=1}^N m^\alpha \mathbf{u}^\alpha \otimes \mathbf{u}^\alpha \psi(\mathbf{x}^\alpha - \mathbf{x}). \quad (6.91)$$

Given this expression for stress in terms of the vector derivatives of non-central interatomic potentials, the question remains as to whether (6.91) is a symmetric tensor. The continuum theory that Hardy's formulation is based upon assumes this to be true, and it certainly was true for central potentials. However, unless it can be proven to be a symmetric tensor, our new definition of stress is no longer consistent with standard local continuum theory, and an enhanced continuum theory of some kind must become the basis for a new definition of stress.

We begin by examining the simple case used above of 3 atoms interacting through a single interaction energy term. For this case, we ignore the kinetic portion of the stress tensor, which is inherently symmetric. Starting with equation (6.90) and using equations (6.87) and (6.88), we obtain

$$\begin{aligned} \boldsymbol{\sigma}(\mathbf{x}, t) &= -\frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \mathbf{F}^{\alpha\beta} B^{\alpha\beta}(\mathbf{x}) \\ &= -\mathbf{x}^{\alpha\beta} \otimes \mathbf{F}^{\alpha\beta} B^{\alpha\beta}(\mathbf{x}) - \mathbf{x}^{\alpha\delta} \otimes \mathbf{F}^{\alpha\delta} B^{\alpha\delta}(\mathbf{x}) - \mathbf{x}^{\beta\delta} \otimes \mathbf{F}^{\beta\delta} B^{\beta\delta}(\mathbf{x}) \\ &= \mathbf{x}^{\alpha\beta} \otimes \left\{ \frac{2}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} + \frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} \right\} B^{\alpha\beta}(\mathbf{x}) + \mathbf{x}^{\alpha\delta} \otimes \left\{ \frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} + \frac{2}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} \right\} B^{\alpha\delta}(\mathbf{x}) \\ &\quad + \mathbf{x}^{\beta\delta} \otimes \left\{ -\frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} + \frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} \right\} B^{\beta\delta}(\mathbf{x}). \end{aligned} \quad (6.92)$$

The last line shown above has used the result

$$\mathbf{F}^{\beta\delta} = \left\{ \frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} - \frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} \right\}, \quad (6.93)$$

which was obtained in a similar manner as equations (6.87) and (6.88). The expression for stress can be slightly simplified to

$$\begin{aligned} \boldsymbol{\sigma}(\mathbf{x}, t) &= \mathbf{x}^{\alpha\beta} \otimes \left\{ \frac{2}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} + \frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} \right\} B^{\alpha\beta}(\mathbf{x}) + \mathbf{x}^{\alpha\delta} \otimes \left\{ \frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} + \frac{2}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} \right\} B^{\alpha\delta}(\mathbf{x}) \\ &\quad + \{ \mathbf{x}^{\alpha\delta} - \mathbf{x}^{\alpha\beta} \} \otimes \left\{ -\frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\beta}} + \frac{1}{3} \frac{\partial \Phi}{\partial \mathbf{x}^{\alpha\delta}} \right\} B^{\beta\delta}(\mathbf{x}), \end{aligned} \quad (6.94)$$

however this cannot be shown to be symmetric because we have not yet identified a localization function and thus, cannot combine the different terms.

6.5. EXTENDING HARDY'S FORMULATION TO NON-CENTRAL POTENTIALS

One result we can obtain is the expression for the average stress, $\bar{\sigma}(t)$, for the entire volume V of the system. Integrating both sides of equation (6.94), we obtain

$$\begin{aligned}\bar{\sigma}(t) &= \frac{1}{V} \left(\mathbf{x}^{\alpha\beta} \otimes \left\{ \frac{2}{3} \frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}} + \frac{1}{3} \frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}} \right\} + \mathbf{x}^{\alpha\delta} \otimes \left\{ \frac{1}{3} \frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}} + \frac{2}{3} \frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}} \right\} \right. \\ &\quad \left. + \{ \mathbf{x}^{\alpha\delta} - \mathbf{x}^{\alpha\beta} \} \otimes \left\{ -\frac{1}{3} \frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}} + \frac{1}{3} \frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}} \right\} \right) \\ &= \frac{1}{V} \left(\mathbf{x}^{\alpha\beta} \otimes \frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}} + \mathbf{x}^{\alpha\delta} \otimes \frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}} \right)\end{aligned}\tag{6.95}$$

This result can be shown to produce a symmetric tensor by using the fact that the potential function Φ must depend on the vectors $\mathbf{x}^{\alpha\beta}$ and $\mathbf{x}^{\alpha\delta}$ through invariants, as discussed in section (6.5.1). For the case of 3-body potentials,

$$\Phi = \Phi(\mathbf{x}^{\alpha\beta}, \mathbf{x}^{\alpha\delta}) = \hat{\Phi}(x^{\alpha\beta}, x^{\alpha\delta}, \cos\theta_{\beta\alpha\delta}).\tag{6.96}$$

This is certainly the case for the Stillinger-Weber potential [11], shown in (6.79). Using (6.96) to evaluate the partial derivatives in (6.95), we obtain

$$\begin{aligned}\frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\beta}} &= \frac{\partial\hat{\Phi}}{\partial x^{\alpha\beta}} \frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} + \frac{\partial\hat{\Phi}}{\partial c_\theta} \left[\frac{\mathbf{x}^{\alpha\delta}}{x^{\alpha\beta} x^{\alpha\delta}} - \frac{c_\theta \mathbf{x}^{\alpha\beta}}{x^{\alpha\beta} x^{\alpha\beta}} \right] \\ \frac{\partial\Phi}{\partial\mathbf{x}^{\alpha\delta}} &= \frac{\partial\hat{\Phi}}{\partial x^{\alpha\delta}} \frac{\mathbf{x}^{\alpha\delta}}{x^{\alpha\delta}} + \frac{\partial\hat{\Phi}}{\partial c_\theta} \left[\frac{\mathbf{x}^{\alpha\beta}}{x^{\alpha\beta} x^{\alpha\delta}} - \frac{c_\theta \mathbf{x}^{\alpha\delta}}{x^{\alpha\delta} x^{\alpha\delta}} \right],\end{aligned}\tag{6.97}$$

where c_θ represents $\cos\theta_{\beta\alpha\delta}$. Substitution of (6.97) into (6.95), along with simplification of terms, results in the expression

$$\begin{aligned}\bar{\sigma}(t) &= \frac{1}{V} \left(\left[\frac{\partial\hat{\Phi}}{\partial x^{\alpha\beta}} - \frac{\partial\hat{\Phi}}{\partial c_\theta} \frac{c_\theta}{x^{\alpha\beta}} \right] \frac{\mathbf{x}^{\alpha\beta} \otimes \mathbf{x}^{\alpha\beta}}{x^{\alpha\beta}} + \left[\frac{\partial\hat{\Phi}}{\partial x^{\alpha\delta}} - \frac{\partial\hat{\Phi}}{\partial c_\theta} \frac{c_\theta}{x^{\alpha\delta}} \right] \frac{\mathbf{x}^{\alpha\delta} \otimes \mathbf{x}^{\alpha\delta}}{x^{\alpha\delta}} \right. \\ &\quad \left. + \frac{\partial\hat{\Phi}}{\partial c_\theta} \frac{\{ \mathbf{x}^{\alpha\beta} \otimes \mathbf{x}^{\alpha\delta} + \mathbf{x}^{\alpha\delta} \otimes \mathbf{x}^{\alpha\beta} \}}{x^{\alpha\beta} x^{\alpha\delta}} \right).\end{aligned}\tag{6.98}$$

Clearly, the average stress for the system is a symmetric quantity, but it is not apparent that the local expression for stress, equation (6.94), is also symmetric. Stress will be symmetric only if the quantity $B(\mathbf{x})$ is a constant for all contributing ($B \neq 0$) pairs of atoms. However, if the localization volume boundary separates two interacting atoms, $B(\mathbf{x})$ will not be the same value as for all other pairs, and stress asymmetry may occur. This situation may imply that the localization volume centered at a point contains a net moment. For such situations, it will be necessary to reformulate Hardy's method using an enhanced continuum theory that contains asymmetric Cauchy stress and couple stress tensors. One such theory is the micropolar elasticity theory by Eringen [7], covered in the next chapter.

6.6 Comments

Hardy's method shows a definitive advantage over other expressions for continuum stress presented in this report. Stress can be determined locally in both time and space, and is properly defined with respect to a standard formulation of continuum mechanics. Hardy's use of finite-valued, limited-range localization functions works well in conjunction with the finite boundaries and the boundary conditions typically used in atomistic simulations. Even with this method, some shortcomings are still present. The large fluctuations observed for simple loading conditions lead one to conclude that physical interpretation of the evaluated expressions requires averaging over a minimal span in both space, *i.e.* a minimum characteristic volume, and time. The positive effect of spatial averaging has already been observed, but the effect of temporal averaging has yet to be evaluated. Also, Hardy's technique can only be applied to particular types of atomic interactions. A more generalized approach needs to be developed.

Chapter 7

Eringen's Micropolar Continuum Formulation

7.1 Motivation

Our goal will be to perform a similar formulation to Hardy's for equating a continuum with an atomistic system, using a micropolar continuum instead of the standard non-polar one. The purpose of this exercise will be to derive expressions for continuum quantities of stress, deformation and temperature that require fewer assumptions about the form of the inter-atomic forces than the assumptions Hardy himself makes [10, 18]. As pointed out in chapter 6, these assumptions constrain the inter-atomic potentials to be only certain types, *e.g.* pair and EAM. Non-central potentials, such as the 3-body Stillinger-Weber, did not qualify under these assumptions. It is our hope that the addition of degrees of freedom to the continuum model will require less constraints on these potentials.

7.2 Kinematics of a micromorphic continuum

As in the chapter 6, we consider a continuum body B to go from some original, reference configuration at time zero, B_0 , to a new configuration at a later time t , B_t . A material point on B_0 is described by the vector \mathbf{X} , and its location on B_t at a later time t is given by the transformation $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$. A micromorphic continuum, as it is called by Eringen [19, 7], is a continuum in which each material point \mathbf{x} actually represents the center of mass of a small volume unit, nevertheless named a *macrovolume*. This macrovolume is composed of a finite number of *microvolumes*, each with its own center of mass:

$$\Delta V = \bigcup_{\alpha=1}^N \Delta V^\alpha,$$

and each microvolume ($\alpha = 1, 2, \dots, N$) is designated by its own center of mass \mathbf{x}^α . Here, we use the 'U' symbol to denote that all the microvolumes make-up the macrovolume, but

that the total amount of macrovolume is not merely the sum of the individual microvolumes. Each microvolume center of mass \mathbf{x}^α can be expressed in terms of the macrovolume's center of mass \mathbf{x} and a relative position vector $\boldsymbol{\xi}^\alpha$,

$$\mathbf{x}^\alpha = \mathbf{x} + \boldsymbol{\xi}^\alpha. \quad (7.1)$$

This relation also holds at time zero, in the reference configuration,

$$\mathbf{X}^\alpha = \mathbf{X} + \boldsymbol{\Xi}^\alpha. \quad (7.2)$$

As before, the transformation of \mathbf{X} to \mathbf{x} is determined by the deformation gradient $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$, or in index notation, $F_{iJ} = \frac{\partial x_i}{\partial X_J}$, where $i, J = 1, 2, 3$. To transform the relative position vector of a microvolume from $\boldsymbol{\Xi}^\alpha$ to $\boldsymbol{\xi}^\alpha$, Eringen assumes a homogeneous transformation,

$$\boldsymbol{\xi}^\alpha = \boldsymbol{\chi}(\mathbf{X}, t) \cdot \boldsymbol{\Xi}^\alpha, \quad (7.3)$$

where $\boldsymbol{\chi}$ is called the microdeformation gradient and, like \mathbf{F} , is a tensor.

The velocities and accelerations of the microvolumes can also be expressed as center of mass terms plus relative motion terms. For example,

$$\mathbf{v}^\alpha = \frac{D\mathbf{x}^\alpha}{Dt} = \frac{\partial \mathbf{x}}{\partial t} + \frac{D\boldsymbol{\xi}^\alpha}{Dt} = \mathbf{v} + \dot{\boldsymbol{\chi}} \cdot \boldsymbol{\Xi}^\alpha = \mathbf{v} + \dot{\boldsymbol{\chi}} \cdot \boldsymbol{\chi}^{-1} \cdot \boldsymbol{\xi}^\alpha.$$

So, the velocity of microvolume α is

$$\mathbf{v}^\alpha = \mathbf{v} + \boldsymbol{\nu} \cdot \boldsymbol{\xi}^\alpha, \quad (7.4)$$

where $\boldsymbol{\nu} \equiv \dot{\boldsymbol{\chi}} \cdot \boldsymbol{\chi}^{-1}$ is known as the microgyration tensor. A similar procedure can be done for the acceleration of a microvolume, resulting in the expression

$$\mathbf{a}^\alpha = \mathbf{a} + \boldsymbol{\alpha} \cdot \boldsymbol{\xi}^\alpha, \quad (7.5)$$

where $\boldsymbol{\alpha} \equiv \dot{\boldsymbol{\nu}} + \boldsymbol{\nu} \cdot \boldsymbol{\nu}$.

7.3 Kinematics of a micropolar continuum

At this time, it becomes desirable to express equations (7.1) - (7.5) in index notation. As shown above for the deformation gradient, we use lower-case roman letters for components in the current configuration and upper-case roman letters for components in the reference configuration. These equations are:

$$\begin{aligned} x_i^\alpha &= x_i + \xi_i^\alpha \\ X_J^\alpha &= X_J + \Xi_J^\alpha \\ \xi_i^\alpha &= \chi_{iJ} \Xi_J^\alpha \\ v_i^\alpha &= v_i + \nu_{ij} \xi_j^\alpha, \quad \nu_{ij} \equiv \dot{\chi}_{iK} (\chi^{-1})_{Kj} \\ a_i^\alpha &= a_i + \alpha_{ij} \xi_j^\alpha, \quad \alpha_{ij} \equiv \dot{\nu}_{ij} + \nu_{iq} \nu_{qj} \end{aligned}$$

Recall, for expressions in which the same index appears twice, summation is implied: $a_k b_k \equiv a_1 b_1 + a_2 b_2 + a_3 b_3$.

A *micropolar* continuum is a micromorphic continuum in which the microdeformation gradient χ_{iJ} represents a rigid body rotation. Hence,

$$(\chi^{-1})_{Ki} = \chi_{iK} \quad , \quad \chi^{-1} = \chi^T \quad (7.6)$$

This allows the microgyration tensor to take a simpler form. Consider:

$$\chi_{iJ} (\chi^{-1})_{Jk} = \chi_{iJ} \chi_{kJ} = \delta_{ik}$$

Taking the time derivatives of both sides,

$$\begin{aligned} \frac{D}{Dt} \{ \chi_{iJ} \chi_{kJ} \} &= \frac{D\delta_{ik}}{Dt} = 0 \\ \dot{\chi}_{iJ} \chi_{kJ} + \chi_{iJ} \dot{\chi}_{kJ} &= 0 \\ \nu_{ik} + \nu_{ki} &= 0 \\ \nu_{ik} &= -\nu_{ki} \end{aligned}$$

This result shows that for a micropolar material, the microgyration tensor is skew-symmetric and can be represented by an equivalent vector,

$$\nu_{ik} = -\epsilon_{ikm} \omega_m \quad , \quad \omega_m = -\frac{1}{2} \epsilon_{mpq} \nu_{pq} \quad (7.7)$$

where ω is called the microgyration vector. The symbol ϵ_{ijk} is known as the permutation operator and has the properties,

$$\begin{aligned} \epsilon_{123} &= \epsilon_{231} = \epsilon_{312} = 1 \\ \epsilon_{132} &= \epsilon_{321} = \epsilon_{213} = -1 \\ \epsilon_{ijk} &= 0 \quad \text{if } i = j \text{ or } j = k \text{ or } k = i \end{aligned}$$

The appearance of equation (7.7) reveals why index notation was used instead of direct vector notation. Equation (7.7) can be used to simplify equations (7.4) and (7.5),

$$\begin{aligned} v_i^\alpha &= v_i + \nu_{ij} \xi_j^\alpha \\ &= v_i - \epsilon_{ijm} \omega_m \xi_j^\alpha \\ &= v_i + \epsilon_{imj} \omega_m \xi_j^\alpha. \end{aligned}$$

Hence,

$$v_i^\alpha = v_i + \epsilon_{imj} \omega_m \xi_j^\alpha \quad , \quad \mathbf{v}^\alpha = \mathbf{v} + \boldsymbol{\omega} \times \boldsymbol{\xi}^\alpha. \quad (7.8)$$

For the acceleration of microvolume α ,

$$\begin{aligned} \mathbf{a}^\alpha &= \mathbf{a} + \frac{D}{Dt} \{ \boldsymbol{\omega} \times \boldsymbol{\xi}^\alpha \} \\ &= \mathbf{a} + \dot{\boldsymbol{\omega}} \times \boldsymbol{\xi}^\alpha + \boldsymbol{\omega} \times \dot{\boldsymbol{\xi}}^\alpha \\ \mathbf{a}^\alpha &= \mathbf{a} + \dot{\boldsymbol{\omega}} \times \boldsymbol{\xi}^\alpha + \boldsymbol{\omega} \times (\boldsymbol{\omega} \times \boldsymbol{\xi}^\alpha) \end{aligned} \quad (7.9)$$

7.4 Mass and inertia

As stated above each macrovolume consists of a finite number of microvolumes. Total mass of the macrovolume, m , is equivalent to the summation of the masses of the microvolumes,

$$m = \sum_{\alpha=1}^N m^{\alpha}$$

This expression is true in either the reference configuration,

$$m = \rho_0 \Delta V = \sum_{\alpha=1}^N \rho_0^{\alpha} \Delta V^{\alpha},$$

or the current configuration,

$$m = \rho \Delta \mathcal{V} = \sum_{\alpha=1}^N \rho^{\alpha} \Delta \mathcal{V}^{\alpha}.$$

The property of mass is often called inertia, or resistance to translational motion when acted upon by a force. Since each macrovolume has rotational degrees of freedom defined by the microgyration vector, they also have rotational inertia or moment of inertia. Eringen calls this property micro-inertia and defines it as

$$\rho_0 \mathbf{I}_{KL} \Delta V = \sum_{\alpha=1}^N \rho_0^{\alpha} \Xi_K^{\alpha} \Xi_L^{\alpha} \Delta V^{\alpha} \quad (7.10)$$

for the reference configuration and

$$\rho \mathbf{i}_{mn} \Delta \mathcal{V} = \sum_{\alpha=1}^N \rho^{\alpha} \xi_m^{\alpha} \xi_n^{\alpha} \Delta \mathcal{V}^{\alpha} \quad (7.11)$$

for the current configuration. The relation between the micro-inertia tensors \mathbf{I}_{KL} and \mathbf{i}_{mn} is $\mathbf{i}_{mn} = \chi_{mK} \mathbf{I}_{KL} \chi_{nL}$. Eringen also defines two additional micro-inertia tensors,

$$\mathbf{J}_{KL} \equiv \mathbf{I}_{QQ} \delta_{KL} - \mathbf{I}_{KL} \quad (7.12)$$

and

$$\mathbf{j}_{kl} \equiv \mathbf{i}_{qq} \delta_{kl} - \mathbf{i}_{kl}. \quad (7.13)$$

For our purposes, it will be necessary to consider the product of mass density and micro-inertia as a separate quantity known as mass-micro-inertia, defined in the current configuration as

$$\kappa_{st} \equiv \rho \mathbf{i}_{st} = \frac{1}{\Delta \mathcal{V}} \sum_{\alpha=1}^N m^{\alpha} \xi_s^{\alpha} \xi_t^{\alpha}. \quad (7.14)$$

As before, a secondary mass-micro-inertia can be defined as

$$\lambda_{st} \equiv \rho j_{st} = \frac{1}{\Delta \mathcal{V}} \sum_{\alpha=1}^N m^{\alpha} (\xi_m^{\alpha} \xi_m^{\alpha} \delta_{st} - \xi_s^{\alpha} \xi_t^{\alpha}) = \kappa_{mm} \delta_{st} - \kappa_{st}. \quad (7.15)$$

The use of the mass-micro-inertia tensors κ and λ will become evident when these inertia tensors are used within the framework of the Hardy formulation for atomistic systems. When the microvolumes are considered to be atoms, it makes more sense to consider the mass of a given atom and its inertia contribution to the center of mass of a group of atoms rather than consider the “density” of the atom.

7.5 Balance laws

For a micropolar continuum, there are five balance laws to consider: mass, micro-inertia, linear momentum, angular momentum and energy. The laws for mass and linear momentum appear the same as before,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_k} (\rho v_k) = 0 \quad (7.16)$$

and

$$\frac{\partial (\rho v_k)}{\partial t} = \frac{\partial}{\partial x_j} (\sigma_{jk} - \rho v_j v_k) + \rho b_k. \quad (7.17)$$

For the balance of linear momentum expression, please note that the Cauchy stress tensor, σ_{jk} , is no longer a symmetric tensor, thus $\sigma_{jk,j} \neq \sigma_{kj,j}$. The Hardy formulation has the convention of labeling the quantity $\rho \mathbf{v}$ as the (linear) momentum density \mathbf{p} . When equating the continuum and atomistic regions, Hardy defines the meanings of ρ and \mathbf{p} and calculates $\mathbf{v} = \mathbf{p}/\rho$.

Eringen derives the balance of micro-inertia using the micro-inertia tensor j_{kl} . His expression is

$$\frac{D j_{kl}}{Dt} + (\epsilon_{kpr} j_{lp} + \epsilon_{lpr} j_{kp}) \omega_r = 0.$$

This expression can be re-written by expanding the material derivative $\frac{D}{Dt} = \frac{\partial}{\partial t} + v_i \frac{\partial}{\partial x_i}$, and by adding the quantity zero in the form of j_{kl} times equation (7.16). The final form of this relation is

$$\frac{\partial \lambda_{kl}}{\partial t} = -\frac{\partial}{\partial x_m} (\lambda_{kl} v_m) - (\epsilon_{kpr} \lambda_{lp} + \epsilon_{lpr} \lambda_{kp}) \omega_r. \quad (7.18)$$

Eringen derives the balance of angular momentum in the following form,

$$\rho \frac{D s_k}{Dt} = \frac{\partial \mu_{lk}}{\partial x_l} + \epsilon_{kmn} \sigma_{mn} + \rho c_k.$$

The quantity s_k is known as the intrinsic spin vector and $s_k \equiv j_{kl} \omega_l$. μ_{lk} is known as the couple stress tensor and is representative of stresses inside a body created by traction

moments applied to the surface of the body, just as the Cauchy stress tensor is related to traction forces applied to the surface. This macrovolume may also be experiencing body couples, c_k , just as it is subjected to body forces, b_k . It can be shown that

$$\rho \frac{Ds_k}{Dt} = \frac{\partial (\lambda_{kl}\omega_l)}{\partial t} + \frac{\partial}{\partial x_m} (\lambda_{kl}\omega_l v_m),$$

and the balance of angular momentum can be re-cast as

$$\frac{\partial (\lambda_{kl}\omega_l)}{\partial t} = \frac{\partial}{\partial x_m} (\mu_{mk} - \lambda_{kl}\omega_l v_m) + \epsilon_{kmn}\sigma_{mn} + \rho c_k. \quad (7.19)$$

To be consistent with the Hardy formulation, we can label the quantity $\boldsymbol{\lambda} \cdot \boldsymbol{\omega}$ as the angular momentum density $\boldsymbol{\ell}$. It will be our intention to define $\boldsymbol{\lambda}$ and $\boldsymbol{\ell}$ in terms of atomic quantities and calculate the continuum field $\boldsymbol{\omega}(\mathbf{x}, t)$ as $\boldsymbol{\omega} = \boldsymbol{\lambda}^{-1} \cdot \boldsymbol{\ell}$.

The balance of energy is written by Eringen as

$$\rho \frac{D(\varepsilon + K)}{Dt} = \frac{\partial}{\partial x_k} (\sigma_{kl}v_l + \mu_{kq}\omega_q - q_k) + \rho (b_j v_j + c_k \omega_k + h).$$

In this expression, h is the internal source of heat per unit mass, \mathbf{q} is the heat flux per unit mass, ε is considered the macrovolume's internal energy per unit mass, and K is the volume's kinetic energy per unit mass and is defined as

$$K \equiv \frac{1}{2}v_k v_k + \frac{1}{2}\omega_j j_{jk}\omega_k.$$

If we redefine quantities to per unit volume, $\hat{e} \equiv \rho(\varepsilon + K) = \hat{u} + \frac{1}{2}\rho v_k v_k + \frac{1}{2}\omega_j \lambda_{jk}\omega_k + \hat{t}$, where \hat{u} is potential energy per unit volume and \hat{t} is thermal energy per unit volume, then the energy balance law can be re-cast as

$$\frac{\partial \hat{e}}{\partial t} = \frac{\partial}{\partial x_k} (\sigma_{kl}v_l + \mu_{kq}\omega_q - q_k - \hat{e}v_k) + \rho (b_k v_k + c_k \omega_k + h). \quad (7.20)$$

We now have our five balance laws along with three defined variables:

$$\text{mass: } \frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x_k} (\rho v_k)$$

$$\text{micro-inertia: } \frac{\partial \lambda_{kl}}{\partial t} = -\frac{\partial}{\partial x_m} (\lambda_{kl} v_m) - (\epsilon_{kpr} \lambda_{lp} + \epsilon_{lpr} \lambda_{kp}) \omega_r$$

$$\text{linear momentum: } \frac{\partial p_k}{\partial t} = \frac{\partial}{\partial x_j} (\sigma_{jk} - \rho v_j v_k) + \rho b_k$$

$$\text{angular momentum: } \frac{\partial \ell_k}{\partial t} = \frac{\partial}{\partial x_m} (\mu_{mk} - \lambda_{kl} \omega_l v_m) + \epsilon_{kmn} \sigma_{mn} + \rho c_k$$

$$\text{energy: } \frac{\partial \hat{e}}{\partial t} = \frac{\partial}{\partial x_k} (\sigma_{kl} v_l + \mu_{kq} \omega_q - q_k - \hat{e} v_k) + \rho (b_k v_k + c_k \omega_k + h)$$

$$\text{linear momentum density: } p_k = \rho v_k$$

$$\text{angular momentum density: } \ell_k = \lambda_{kq} \omega_q$$

$$\text{energy density: } \hat{e} = \hat{u} + \frac{1}{2} \rho v_k v_k + \frac{1}{2} \omega_j \lambda_{jk} \omega_k + \hat{t}$$

7.6 Preface to Hardy formulation

The only assumptions made for the theory reviewed in this write-up have been the assumption of micropolar behavior, *i.e.* the microvolume deformation consists of a rigid body rotation relative to the center of mass of the macrovolume, and that the microvolumes do not have any rotational degrees of freedom about their own centers of mass. For our purposes where the microvolumes represent neutrally-charged atoms, these degrees of freedom do not exist. The deformation behavior of the macrovolume is generally nonlinear, and no constitutive models have yet been used.

We defer the development of a Hardy-like formulation for a micropolar continuum to a future publication. However, before such a formulation can be performed, it is important to note the specific meaning of the independent variable \mathbf{x} . For the macrovolume it represents, it is the center of mass of all the contributing microvolumes. Let us select a spatial position \mathbf{x}' . Each atom has its own localization function $\psi(\mathbf{x}^\alpha - \mathbf{x}')$, which can also be considered a “window” function, *i.e.* within a sub-volume centered around \mathbf{x}' , any atoms for which $\psi \neq 0$ influence continuum properties ‘measured’ at that point. However, there is no guarantee that \mathbf{x}' also corresponds to the center of mass, \mathbf{x} , of the set of atoms “visible” within that sub-volume. Hence, the balance laws shown above cannot be used directly to determine continuum fields at the point \mathbf{x}' . Also, the quantities of $\boldsymbol{\lambda}$ and $\boldsymbol{\ell}$ must be re-calculated for positions that are off the center of mass by using the parallel axis theorem. It is clear that we must proceed carefully when developing expressions using a Hardy-like approach.

This page intentionally left blank.

Bibliography

- [1] R.J.E. Clausius. On a mechanical theorem applicable to heat. *Philosophical Magazine*, 40:122–127, 1870.
- [2] J.C. Maxwell. On reciprocal figures, frames and diagrams of forces. *Transactions of the Royal Society Edinburgh*, XXVI:1–43, 1870.
- [3] J.C. Maxwell. Van der waals on the continuity of the gaseous and liquid states. *Nature*, pages 477–480, 1874.
- [4] K.S. Cheung and S. Yip. Atomic-level stress in an inhomogeneous system. *Journal of Applied Physics*, 70(10):5688–5690, 1991.
- [5] J.F. Lutsko. Stress and elastic constants in anisotropic solids: Molecular dynamics techniques. *Journal of Applied Physics*, 64(3):1152–1154, 1988.
- [6] J. Cormier, J.M. Rickman, and T.J. Delph. Stress calculation in atomistic simulations of perfect and imperfect solids. *Journal of Applied Physics*, 89(1):99–104, 2001.
- [7] A.C. Eringen. *Microcontinuum Field Theories I: Foundations and Solids*. Springer-Verlag, New York, 1999.
- [8] D.H. Tsai. The virial theorem and stress calculation in molecular dynamics. *J. Chem. Phys.*, 70:1375–1382, 1979.
- [9] P. Schofield and J.R. Henderson. Statistical mechanics of inhomogeneous fluids. *Proceedings of the Royal Society of London A*, 379:231–240, 1982.
- [10] R.J. Hardy. Formulas for determining local properties in molecular-dynamics simulations: Shock waves. *Journal of Chemical Physics*, 76(1):622–628, 1982.
- [11] F.H. Stillinger and T.A. Weber. Computer simulation of local order in condensed phases of silicon. *Physical Review B*, 31:5262–5271, 1985.
- [12] R.A. Gingold and J.J. Monaghan. Smoothed particle hydrodynamics: theory and application to non-spherical stars. *Monthly Notices of the Royal Astronomical Society*, 181:375–389, 1977.

BIBLIOGRAPHY

- [13] P. Lancaster and K. Salkauskas. Surfaces generated by moving least squares methods. *Mathematics of Computation*, 37:141–158, 1981.
- [14] T. Belytschko, Y.Y. Lu, and L. Gu. Element-free Galerkin methods. *International Journal for Numerical Methods in Engineering*, 37:229–256, 1994.
- [15] W.K. Liu and Y. Chen. Reproducing kernel particle methods. *International Journal for Numerical Methods in Fluids*, 20:1081–1106, 1995.
- [16] S.M. Foiles, M.I. Baskes, and M.S. Daw. Embedded-atom-method functions for the fcc metals cu, ag, au, ni, pd, pt, and their alloys. *Phys. Rev. B*, 33:7983–7991, 1986.
- [17] R.J. Hardy, S. Root, and D.R. Swanson. Continuum properties from molecular simulations. In *Shock Compression of Condensed Matter*, Proceedings of the American Physical Society Topical Conference, pages 1–4. American Physical Society, 2001.
- [18] R.J. Hardy. Draft of a manuscript. 2002.
- [19] A.C. Eringen. Theory of micropolar elasticity. In H. Lubowitz, editor, *Fracture, an advanced treatise*, volume 2, chapter 7, pages 621–728. Academic Press, London, UK, 1968.
- [20] R.J. Hardy and A.M. Karo. Stress and energy flux in the vicinity of a shock front. In *Shock Compression of Condensed Matter*, Proceedings of the American Physical Society Topical Conference, pages 161–164. American Physical Society, 1989.
- [21] J.W. Mintmire, J.J.C. Barrett, D.H. Robertson, and C.T. White. Atomistic simulations of shock induced pore collapse in model materials. *Chemical Physics Reports*, 17(1-2):37–46, 1998.
- [22] J.W. Mintmire, D.H. Robertson, and C.T. White. Molecular-dynamics simulations of void collapse in shocked model-molecular solids. *Physical Review B*, 49(21):14859–14864, 1994.
- [23] D.H. Robertson, D.W. Brenner, and C.T. White. Split shock waves from molecular dynamics. *Physical Review Letters*, 67(22):3132–3135, 1991.
- [24] M.A. Makeev and A. Madhukar. Simulations of atomic-level stresses in systems of buried Ge/Si islands. *Physical Review Letters*, 86(24):5542–5545, 2001.
- [25] O. Vafek and M.O. Robbins. Molecular dynamics study of the stress singularity at a corner. *Physical Review B*, 60(17):12002–12006, 1999.
- [26] I. Daruka, A.-L. Barabási, S.J. Zhou, T.C. Germann, P.S. Lomdahl, and A.R. Bishop. Molecular-dynamics investigation of the surface stress distribution in a Ge/Si quantum dot superlattice. *Physical Review B*, 60(4):R2150–R2153, 1999.

- [27] O. Kum, W.G. Hoover, and C.G. Hoover. Temperature maxima in stable two-dimensional shock waves. *Physical Review E*, 56(1):462–465, 1997.
- [28] W.G. Hoover. Isomorphism linking smooth particles and embedded atoms. *Physica A*, 260:244–254, 1998.
- [29] W.G. Hoover. Nonequilibrium molecular dynamics. *Annual Review of Physical Chemistry*, 34:103–127, 1983.
- [30] N.J. Ramer, E.J. Mele, and A.M. Rappe. Theoretical examination of stress fields in $\text{pb}(\text{zr}_{0.5}\text{ti}_{0.5})\text{o}_3$. *Ferroelectrics*, 206-207:31–46, 1998.
- [31] Lord Rayleigh. On a theorem analogous to the virial theorem. *Philosophical Magazine, S. 5.*, 50(303):210–213, 1900.
- [32] Lord Rayleigh. On the pressure of gases and the equation of virial. *Philosophical Magazine, S. 6.*, 9(52):494–505, 1905.
- [33] Lord Rayleigh. On the momentum and pressure of gaseous vibrations, and on the connexion with the virial theorem. *Philosophical Magazine, S. 6.*, 10(57):364–374, 1905.
- [34] V. Vitek and T. Egami. Atomic-level stresses in solids and liquids. *Physics Status Solidi (B)*, 144:145–156, 1987.
- [35] R.G. Hoagland, M.S. Daw, S.M. Foiles, and M.I. Baskes. The nature of crack tip fields in atomic scale modelsof aluminum. In *Atomic Scale Calculations of Structure in Materials*, volume 193 of *Materials Research Society Symposium Proceedings*, pages 283–288. Materials Research Society, 1990.
- [36] S.Y. Hu, Y.L. Li, and K. Watanabe. Calculation of internal streses around cu precipitates in the bcc fe matrix by atomic simulation. *Modelling and Simulation in Materials Science and Engineering*, 7:641–655, 1999.
- [37] M.F. Horstemeyer and M.I. Baskes. Atomistic finite deformation simulations: A discussion on length scale effects in relation to mechanical stresses. *Journal of Engineering Materials and Technology / Transactions of the ASME*, 121:114–119, 1999.
- [38] G. Marc and W.G. McMillan. The virial theorem. *Advances in Chemical Physics*, 58:209–361, 1985.
- [39] L.A. Zepeda-Ruiz, D. Maroudas, and W.H. Weinberg. Theoretical study of the energetics, strain fields, and semicoherent interface structures in layer-by-layer semiconductor heteroepitaxy. *Journal of Applied Physics*, 85(7):3677–3695, 1999.
- [40] A. Machov'a Stress calculations on the atomistic level. *Modelling and Simulation in Materials Science and Engineering*, 9:327–337, 2001.

BIBLIOGRAPHY

- [41] J.A. Zimmerman. *Continuum and Atomistic Modeling of Dislocation Nucleation at Crystal Surface Ledges*. PhD thesis, Stanford University, 2000.
- [42] M. Baus and R. Lovett. Stress-strain relations in nonuniform equilibrium fluids. *Physical Review A*, 44(2):1211–1218, 1991.
- [43] O.H. Nielsen and R.M. Martin. Quantum-mechanical theory of stress and force. *Physical Review B*, 32(6):3780–3791, 1985.
- [44] J.H. Irving and J.G. Kirkwood. The statistical mechanical theory of transport processes. iv. the equations of hydrodynamics. *Journal of Chemical Physics*, 18(6):817–829, 1950.
- [45] J.G. Kirkwood and F.P. Buff. The statistical mechanical theory of surface tension. *Journal of Chemical Physics*, 17(3):338–343, 1949.
- [46] R.J. Swenson. Comments on virial theorems for bounded systems. *American Journal of Physics*, 51:940–942, 1983.
- [47] S. Yip, J. Li, M. Tang, and J. Wang. Mechanistic aspects and atomic-level consequences of elastic instabilities in homogeneous crystals. *Materials Science and Engineering A*, A317:236–240, 2001.
- [48] D.A. Faux, G. Jones, and E.P. O’Reilly. Calculation of strain relaxation in strained-layer structures: comparison of atomistic and continuum methods. *Modelling and Simulation in Materials Science and Engineering*, 2:9–20, 1994.
- [49] M.P. Allen and D.J. Tildesley. *Computer Simulation of Liquids*. Clarendon Press, Oxford, 1987.
- [50] R.W. Smith and D.J. Srolovitz. Void formation during film growth: A molecular dynamics simulation study. *J. Appl. Phys.*, 79(3):1448–1457, 1996.
- [51] M. Born and K. Huang. *Dynamical Theories of Crystal Lattices*. Clarendon Press, Oxford, 1956.
- [52] K. Huang. On the atomic theory of elasticity. *Proc. Roy. Soc. London*, A203:178–94, 1950.
- [53] S. Kohlhoff, P. Gumbsch, and H.F. Fischmeister. Crack propagation in BCC crystals studied with a combined finite-element and atomistic model. *Phil. Mag. A*, 64:851–78, 1991.
- [54] J.Q. Broughton, F.F. Abraham, N. Bernstein, and E. Kaxiras. Concurrent coupling of length scales: Methodology and application. *Phys. Rev. B*, 60:2391–2403, 1999.

-
- [55] C.B. Kafadar and A.C. Eringen. Micropolar media - I the classical theory. *Int. J. Engng. Sci.*, 9:271–305, 1971.
- [56] S. Atluri and T. Zhu. A new meshless local Petrov-Galerkin approach in computational mechanics. *Computational Mechanics*, 22:117–127, 1998.
- [57] T. Zhu, J. Zhang, and S. Atluri. A local boundary integral equation (LBIE) method in computational mechanics, and a meshless discretization approach. *Computational Mechanics*, 21:223–235, 1998.
- [58] T. Belytschko, L. Gu, and Y.Y. Lu. Fracture and crack growth by element free Galerkin methods. *Modelling and Simulation in Materials Science and Engineering*, 2:519–534, 1994.
- [59] T. Belytschko, D. Organ, and Y. Krongauz. A coupled finite-element, element-free Galerkin method. *Computational Mechanics*, 17:186–195, 1995.
- [60] T. Belytschko, Y.Y. Lu, L. Gu, and M.R. Tabbara. Element-free Galerkin methods for static and dynamic fracture. *International Journal of Solids and Structures*, 17:186–195, 1995.
- [61] Y.Y. Lu, T. Belytschko, and M.R. Tabbara. Element-free Galerkin methods for wave propagation and dynamic fracture. *Computer Methods in Applied Mechanics and Engineering*, 126:131–153, 1995.
- [62] T. Belytschko, Y. Krongauz, M. Fleming, D. Organ, and W.K. Liu. Smoothing and accelerated computations in the element free Galerkin methods. *Journal of Computational and Applied Mathematics*, 74:111–126, 1996.
- [63] T. Belytschko and M.R. Tabbara. Dynamic fracture using element-free Galerkin methods. *International Journal for Numerical Methods in Engineering*, 39:923–938, 1996.
- [64] T. Belytschko, Y. Krongauz, D. Organ, M. Fleming, and P. Krysl. Meshless methods: an overview and recent developments. *Computer Methods in Applied Mechanics and Engineering*, 139:3–47, 1996.
- [65] S. Beissel and T. Belytschko. Nodal integration of the element-free Galerkin method. *Computer Methods in Applied Mechanics and Engineering*, 139:49–74, 1996.
- [66] D. Organ, T. Fleming, T. Terry, and T. Belytschko. Continuous meshless approximations for nonconvex bodies by diffraction and transparency. *Computational Mechanics*, 18:1–11, 1996.
- [67] P. Krysl and T. Belytschko. Element-free Galerkin method: convergence of the continuous and discontinuous shape functions. *Computer Methods in Applied Mechanics and Engineering*, 148:257–277, 1997.

BIBLIOGRAPHY

- [68] J. Dolbow and T. Belytschko. Numerical integration of the Galerkin weak form in meshfree methods. *Computational Mechanics*, 23:219–230, 1999.
- [69] N. Moes, J. Dolbow, and T. Belytschko. A finite element method for crack growth without remeshing. *International Journal of Numerical Methods in Engineering*, 46:131–150, 1999.
- [70] P. Krysl and T. Belytschko. The element free Galerkin method for dynamic propagation of arbitrary 3-D cracks. *International Journal of Numerical Methods in Engineering*, 44:767–800, 1999.
- [71] J.S. Chen, C. Pan, C.T. Wu, and W.K. Liu. Reproducing kernel particle methods for large deformation analysis of nonlinear structures. *Computer Methods in Applied Mechanics and Engineering*, 139:195–227, 1996.
- [72] J.S. Chen, C.T. Wu, S. Yoon, and Y. You. A stabilized conforming nodal integration for Galerkin meshfree methods. *International Journal of Numerical Methods in Engineering*, 2000. accepted for publication.
- [73] J.S. Chen, C.T. Wu, and S. Yoon. Nonlinear version of stabilized conforming nodal integration for Galerkin meshfree methods. *International Journal of Numerical Methods in Engineering*, 2000. submitted for publication.
- [74] Y. Krongauz and T. Belytschko. EFG approximation with discontinuous derivatives. *International Journal for Numerical Methods in Engineering*, 41:1215–1233, 1998.
- [75] T.J. Liszka, C.A.M. Duarte, and W.W. Tworzydło. hp-meshless cloud method. *Computer Methods in Applied Mechanics and Engineering*, 139:263–288, 1996.
- [76] W.K. Liu and Y. Chen. Wavelet and multiple scale reproducing kernel method. *International Journal for Numerical Methods in Fluids*, 21:901–931, 1995.
- [77] W.K. Liu, S. Jun, S. Li, J. Adee, and T. Belytschko. Reproducing kernel methods for structural dynamics. *International Journal for Numerical Methods in Engineering*, 38:1655–1679, 1995.
- [78] S. Li and W.K. Liu. Moving least square reproducing kernel method (II): Fourier analysis. *Computer Methods in Applied Mechanics and Engineering*, 139:159–194, 1996.
- [79] W.K. Liu, Y. Chen, R.A. Uras, and C.T. Chang. Generalized multiple scale reproducing kernel particle methods. *Computer Methods in Applied Mechanics and Engineering*, 139:91–158, 1996.
- [80] W.K. Liu, Y. Chen, C.T. Chang, and T. Belytschko. Advances in multiple scale kernel particle methods. *Computational Mechanics*, 18:73–111, 1996.

-
- [81] S. Li and W.K. Liu. Moving least square reproducing kernel method (I): Methodology and convergence. *Computer Methods in Applied Mechanics and Engineering*, 143:113–154, 1997.
- [82] S. Li and W.K. Liu. Moving least square reproducing kernel method (III): Wavelet packet and its applications. *Computer Methods in Applied Mechanics and Engineering*, 1997.
- [83] W.K. Liu, W. Hao, Y. Chen, Jun S., and J. Gosz. Multiresolution reproducing kernel particle methods. *Computational Mechanics*, 20:295–309, 1997.
- [84] J.S. Chen, S. Yoon, H. Wang, and W.K. Liu. An improved reproducing kernel method for nearly incompressible finite elasticity. *Computer Methods in Applied Mechanics and Engineering*, 1998. *accepted for publication*.
- [85] S. Li and W.K. Liu. Synchronized reproducing kernel interpolant via multiple wavelet expansion. *Computational Mechanics*, 21:28–47, 1998.
- [86] F.C. Guenther and W.K. Liu. Implementation of boundary conditions for meshless methods. *Computer Methods in Applied Mechanics and Engineering*, 163:205–230, 1998.
- [87] W.K. Liu and S. Jun. Multiple scale reproducing kernel particle methods for large deformation problems. *International Journal for Numerical Methods in Engineering*, 41:1339–1362, 1998.
- [88] S. Jun, W.K. Liu, and T. Belytschko. Explicit reproducing kernel particle methods for large deformation problems. *International Journal for Numerical Methods in Engineering*, 41:137–166, 1998.
- [89] W.K. Liu, R.A. Uras, and Y. Chen. Enrichment of the finite element method with the reproducing kernel particle method. *Journal of Applied Mechanics*, 64:861–870, 1998.
- [90] S. Hao, W.K. Liu, and C.T. Chang. Computer implementation of damage models by finite element and meshfree methods. *Computer Methods in Applied Mechanics and Engineering*, 1998. *accepted for publication*.
- [91] S. Li and W.K. Liu. Reproducing kernel hierarchical partition of unity (I): Formulation and theory. *International Journal for Numerical Methods in Engineering*, 45:251–288, 1999.
- [92] S. Li and W.K. Liu. Reproducing kernel hierarchical partition of unity (II): Applications. *International Journal for Numerical Methods in Engineering*, 45:289–317, 1999.
- [93] G.J. Wagner and W.K. Liu. Application of essential boundary conditions in mesh-free methods: A corrected collocation method. *International Journal for Numerical Methods in Engineering*, 47:1367–1379, 2000.

BIBLIOGRAPHY

- [94] W.K. Liu, S. Hao, T. Belytschko, S. Li, and C.T. Chang. Multiple scale meshfree methods for damage fracture and localization. *Computational Materials Science*, 16:197–205, 1999.
- [95] W.K. Liu and S. Li. Numerical simulations of strain localization in inelastic solids using meshfree methods. *International Journal of Numerical Methods for Engineering*, 1999. *accepted for publication*.
- [96] S. Li, W. Hao, and W.K. Liu. Mesh-free simulations of shear banding in large deformation. *International Journal of Solids and Structures*, 37:7185–7206, 2000.
- [97] W.K. Liu, S. Hao, T. Belytschko, S. Li, and C.T. Chang. Multi-scale methods. *International Journal for Numerical Methods in Engineering*, 47:1343–1361, 2000.
- [98] L.W. Cordes and B. Moran. Treatment of material discontinuity in the element-free Galerkin method. *Computer Methods in Applied Mechanics and Engineering*, 139:75–89, 1996.
- [99] J.M. Melenk and I. Babuška. The partition of unity finite element method: Basic theory and applications. *Computer Methods in Applied Mechanics and Engineering*, 139:289–314, 1996.
- [100] B. Nayroles, G. Touzot, and P. Villon. Generalizing the finite element method: Diffuse approximation and diffuse elements. *Computational Mechanics*, 10:307–318, 1992.
- [101] J.T. Oden, C.A.M. Duarte, and O.C. Zienkiewicz. A new cloud-based hp finite element method. *Computer Methods in Applied Mechanics and Engineering*, 153:117–126, 1998.
- [102] N. Sukumar, B. Moran, and T. Belytschko. The natural element method. *International Journal for Numerical Methods in Engineering*, 43:839–887, 1998.
- [103] M.R. Tabbara and C.M. Stone. A computational method for quasi-static fracture. *Computational Mechanics*, 22:203–210, 1998.

Chapter 9

DISTRIBUTION:

1	MS 0188	D.L. Chavez, LDRD Office, 1030
1	MS 0316	J.B. Aidun, 9235
1		M.J. Stevens, 9235
1		A.P. Thompson, 9235
1	MS 0316	S.J. Plimpton, 9212
1	MS 0824	A.C. Ratzel, 9110
1	MS 0841	T.C. Bickel, 9100
1	MS 0847	H.S. Morgan, 9120
1	MS 0893	R.M. Brannon, 9123
1		E.D. Reedy Jr., 9123
1	MS 1411	H.E. Fang, 1834
1		C.C. Battaile, 1834
1		M.V. Braginsky, 1834
1		S.M. Foiles, 1834
1		E.A. Holm, 1834
5		J.J. Hoyt, 1834
5		E.B. Webb III, 1834
1	MS 1415	J.E. Houston, 1114
1	MS 9001	M.E. John, 8000

CHAPTER 9. DISTRIBUTION

Attn:

J. Vitko, 8100, MS 9004
D.R. Henson, 8200, MS 9007
W.J. McLean, 8300, MS 9054
P.N. Smith, 8500, MS 9002
K.E. Washington, 8900, MS 9003

1	MS 9042	P.A. Spence, 8727
1		P.M. Gullett, 8727
1		Y. Ohashi, 8727
1	MS 9108	S.L. Robinson, 8414
1		G.C. Story, 8414
1	MS 9161	E.P. Chen, 8726
1		C.J. Kimmer, 8726
5		P.A. Klein, 8726
1		D.A. Zeigler, 8726
15		J.A. Zimmerman, 8726
1	MS 9161	J.C. Hamilton, 8721
1		D.J. Siegal, 8721
1	MS 9402	D.F. Cowgill, 8724
1		K.L. Hertz, 8724
1		B.P. Somerday, 8724
1	MS 9405	R.H. Stulen, 8700
		Attn:
		J.M. Hruby, 8702, MS 9401
		K.L. Wilson, 8703, MS 9402
		G.D. Kubiak, 8705, MS 9409
		R.Q. Hwang, 8721, MS 9161
		W.R. Even Jr., 8722, MS 9403
		J.C.F. Wang, 8723, MS 9403
		C.H. Cadden, 8724, MS 9402
		J.R. Garcia, 8725, MS 9042
		C.C. Henderson, 8729, MS 9401
		J.E.M. Goldsmith, 8730, MS 9409
		W.C. Replogle, 8731, MS 9409
1	MS 9405	S. Aubry, 8726

5		D.J. Bammann, 8726
1		A.A. Brown, 8726
1		G.R. Feijoo, 8726
1		J.W. Foulk, 8726
1		Y. Hammi, 8726
1		D.A. Hughes, 8726
5		R.E. Jones, 8726
1		E.B. Marin, 8726
1		R.A. Regueiro, 8726
1		D. Suh, 8726
1	MS 9950	T.D. Nguyen, 8726
1	MS 9950	G.J. Wagner, 8728
3	MS 9018	Central Technical Files, 8945-1
1	MS 0899	Technical Library, 9616
1	MS 9021	Classification Office, 8511/ Technical Library, MS 0899, 9616
1		DOE/OSTI via URL