Towards Constitutive Modeling Based on Atomistics

Jacob Fish and Cyrille Schwob[1]

Departments of Civil, Mechanical and Aerospace Engineering

Rensselaer Polytechnic Institute

Troy, NY 12180

Abstract: Mathematical homogenization theory, which serves as a foundation for bridging multiple spatial and temporal scales for continuum systems, is generalized to provide a unified mathematical framework for bridging not only multiple continuum scales in space and time, but also multiple continuum and discrete scales. We commence our study to one-dimensional chain of atoms as well to the BCC crystals. The solution of the one-dimensional model problem has been found to be in good agreement with the molecular dynamics simulation of the chain of atoms, whereas the classical approach based on the Cauchy-Born hypothesis is shown to produce significant errors.

1.0 Introduction

Significant progress has been made over the past two decades in applying high performance computing to the numerical simulation of complex initial/boundary value problems describing single- or multi- physics phenomena, such as mechanical, thermal, diffusion-reaction, and electro-magnetic processes. The initial-boundary value problem is governed by balance equations, kinematics, and constitutive equations with appropriate initial and boundary conditions for each physical process of interest. The balance and the kinematics equations are well known for many physical processes. On the other hand constitutive models are not completely understood since they represent a gross response of the small-scale phenomena. The goal of this paper is to present a systematic approach for constructing mathematically rigorous atomistically based constitutive models and related numerical simulation tools.

There are several reasons for our approach. First, there is a growing desire to capitalize on insight gained at the atomistic scale in the design of new materials. Second, the miniaturization of electronic and mechanical devices in nanotechnology applications, such as micro-electromechanical systems, results in instances where internal structure of the material is of the same length scale as the dimension of the device. The third, is the over simplicity of some of the existing semi-atomistic models.

In recent years, a great deal of emphasis has been placed on the development of methods capable of embedding atomistic features into continuum analysis. The task of describing failure phenomena on the continuum scale is a daunting one at best. Even with today's powerful computers, the brute force approach of direct atomistic simulation [1], i.e., where the material is simply modeled as a collection of atoms, is neither possible due to

1. Currently at Département de Mecanique, Ecole Polytechnique, 91128 Palaiseau Cedex, France

the vast number of atoms involved, nor desirable.

At the other extreme are methods based on the so-called Quasi-Continuum (QC) approach [3], [4], which states that atomic environment at a continuum point is completely characterized by the deformation gradient. There are two versions of the QC method depending on the interpretation of the deformation gradient. The Global QC variant [4] is based on the Cauchy-Born hypothesis [2] in conjunction with periodic boundary conditions of the atomistic cell. Its main shortcoming, is that in the limit when the continuum FE mesh size approaches interatomic distance the continuum formulation *does not* converge to the ordinary atomistic description due to the underlying assumptions of periodicity and the fact that atomic vibrations are not accounted for. The Local Quasi-Continuum variant [3], on the other hand, selects a small subset of representative atoms to represent the kinematics of the system. The position of the remaining atoms is then obtained by interpolation. This approaches suffers from the fact that the continuum is incorrectly described in the case of complex latices. The combination of the two QC approaches seems to be a natural choice, but then the inconsistency is pushed to the interface between the two descriptions.

A significant shortcoming of the approaches based on the Cauchy-Born hypothesis is that they do not possess an internal length scale, which have been shown to have a dominant affect on local (and indirectly affect gross) material behavior. To overcome the limitations of the local approach a mathematical homogenization theory with multiple temporal and spatial scales recently developed in [5]-[7] is generalized to deal with mixed continuum-discrete systems. The theory represents a mathematically rigorous framework designated to account for diverse spatial and temporal scales. Fast spatial scale is introduced to account for rapid spatial fluctuations of the atomistic scale whereas slow temporal scale is designated to capture the long-term behavior of the continuum solution. The size of the atomistic cell is assumed to be much smaller than the characteristic size of the macro domain. The macroscopic position vector x is assumed to be a continuous function, whereas the discreteness of the atomic positions implies the discreteness of the atomic position vector y. Hamilton energy principal serves as a starting point of the formulation as opposed to the partial differential equations which form the basis for continuum formulations.

To this end we note that there is an important class of coupled discrete-continuum simulation techniques, which is not considered in this work, where small atomistic regions are tied to a continuum description through appropriate boundary conditions [4]. Typically, the idea is to describe “interesting” parts of the simulation atomistically, while other parts of the system are described by a model based on continuum theory. The atomistic description is typically required in dislocation core and other parts of the system with strong nonlinearities.

The contents of this paper are as follows. We start by considering a one-dimensional model with nearest neighbor interactions. Although such a simplification may appear excessive, many essential features can be illustrated, while retaining the advantage of minimal algebraic complexity. The analytical solution of this model is found to be in good agreement with the molecular dynamic simulation of the wave propagating in a chain of atoms, whereas the classical approach based on the Cauchy-Born hypothesis is

shown to produce significant errors. We conclude by considering a three dimensional structure of the BCC crystal.

2.0 One-Dimensional Chain of Atoms

2.1 Problem Statement

Consider wave propagation in a one-dimensional chain of atoms as shown in Figure 1. For simplicity, we assume that each atom acts as though it was connected to its nearest neighbor by a spring. The total energy stored in the crystal is comprised of the kinetic and potential energies. The one-dimensional crystal model with masses m_1 and m_2 is spaced at intervals αl and $(1-\alpha)l$ in equilibrium position. The force applied to every atom depends on the relative displacement of the nearby atoms as well as spring stiffnesses k_1 and k_2.

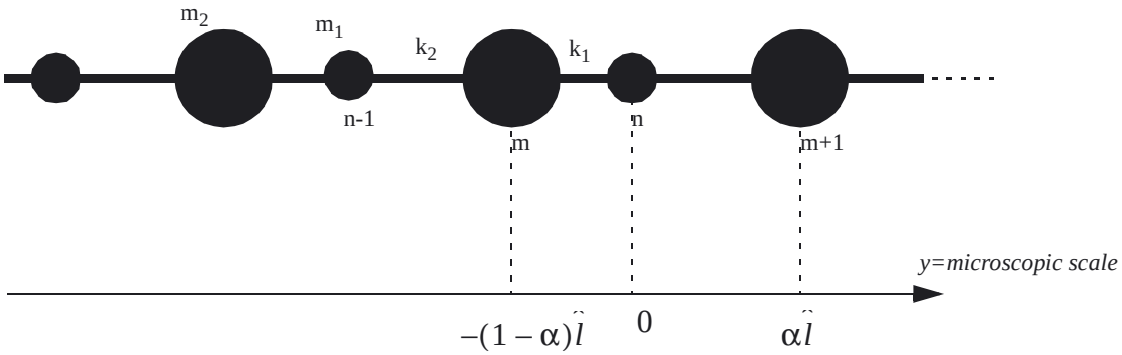

Figure 1: One-dimensional chain of atoms

The length of the atomistic unit cell in the physical domain is l. We denote by L the total length of the chain, and by ε the ratio $\frac{l}{L} \ll 1$. In the particular case of a diatomic chain, we have: $k_1 = k_2$ and $\alpha = 1/2$.

Let u_i be the displacement of atom i and W_y be the internal energy of atoms in the unit cell denoted as: $W_y = \frac{1}{2}[k_1(u_n - u_m)^2 + k_2(u_n - u_{m+1})^2]$. Therefore the total energy W is given by:

$$W = \sum W_Y = \sum_n \frac{1}{2}[k_1(u_n - u_m)^2 + k_2(u_n - u_{m+1})^2]$$

The kinetic energy of the atomistic unit cell is $K_Y = \frac{1}{2}[m_1\dot{u}_n^2 + m_2\dot{u}_m^2]$ and the total kinetic energy is:

$$K = \sum K_Y = \sum_n \frac{1}{2}[m_1\dot{u}_n^2 + m_2\dot{u}_m^2]$$

From the Hamilton principle, $\delta\left(\int_{t_1}^{t_2}(K-W)dt\right) = 0$, we obtain:

$$\int_{t_1}^{t_2} m_1\dot{u}_n\delta\dot{u}_n + m_2\dot{u}_m\delta\dot{u}_m - ((k_1+k_2)u_n - k_1u_m - k_2u_{m+1})\delta u_n$$

$$-((k_1+k_2)u_m - k_1u_n - k_2u_{n-1})\delta u_m dt = 0 \qquad \forall(\delta u_m, \delta u_n)$$

which yields the set of discrete equations:

$$\forall m \qquad \alpha\rho_1\ddot{u}_n + \frac{1}{\hat{l}^2}\frac{(k_1+k_2)lu_n - k_1lu_m - k_2lu_{m+1}}{\varepsilon^2} = 0$$

$$(1-\alpha)\rho_2\ddot{u}_m + \frac{1}{\hat{l}^2}\frac{(k_1+k_2)lu_m - k_1lu_n - k_2lu_{n-1}}{\varepsilon^2} = 0 \tag{1}$$

where $\rho_1 = m_1/\alpha l$, $\rho_2 = m_2/(1-\alpha)l$ are masses per unit length and $\hat{l} = l/\varepsilon = O(\varepsilon^0)$ is the size of the unit cell in the stretched coordinate system.

Remark 1: In order to perform asymptotic expansion of equation (1) it is important to identify the scale of the coefficients. For a homogeneous cylinder of Young's modulus *E*, length *l* and cross-sectional area *S*, the relation between the spring stiffness and Young modulus is given by

$$\frac{k_i l}{S} \sim E \tag{2}$$

If ρ is the density, we have $\frac{\rho_1}{S} \sim \rho$. Therefore $\frac{k_i l}{\rho_i} = O(\varepsilon^0)$, and consequently it is appropriate to introduce an asymptotic expansion for solving equations (1).

2.2 Continuum modeling of atomistic chain

To simultaneously model phenomena at both the continuum and discrete scales, we utilize the double scale asymptotic expansion:

$$u(x,y) = u^0(x,y) + \varepsilon u^1(x,y) + \ldots$$

where *x* is the continuum scale position vector, and $y = x/\varepsilon$ denotes the position of atoms. We assume that *x* is a continuous variable whereas *y* is discrete, and that for a given *y*, $u(x,y)$ is continuous and differentiable with respect to *x*. Assuming that $u(x,y)$ is $\hat{l}$-periodic and denoting $x_n = n \cdot l$ and $x_m = (n-1+\alpha)l$ we have $u_n = u(x_n, 0)$ and $u_m = u(x_m, \alpha l)$.

In addition to the fast spatial variable, we introduce two temporal scale t and τ, where t is the usual time coordinate and τ is a slow time scale defined by: $\tau = \varepsilon^2 t$. Thus, the corresponding multiple scale asymptotic expansion is given as:

$$u(x, y, t, \tau) = u^0(x, y, t, \tau) + \varepsilon u^1(x, y, t, \tau) + \ldots \tag{3}$$

The asymptotic analysis consists of inserting the asymptotic expansion (3) into the equations of motion, identifying the terms with the equal power of ε, and then solving the resulting problems. Following the aforementioned procedure and expressing the temporal derivative in term of the slow time coordinates, $\dot{u} = \frac{du}{dt} = u_{,t} + \varepsilon^2 u_{,\tau}$, we obtain a series of equations in ascending power of ε starting with ε^{-2}.

For each k we assume that $u^k(x, y)$ is $\hat{l}$-periodic in y, i.e., $u^k(x, y + \hat{l}) = u^k(x, y)$. For a given function $v(x, y)$ we define two functions $f_1(v)$ and $f_2(v)$ as:

$$f_1(v) = (k_1 + k_2) lv(x_n; 0) - k_1 lv(x_m; -(1-\alpha)\hat{l}) - k_2 lv(x_{m+1}; \alpha\hat{l})$$

$$f_2(v) = (k_1 + k_2) lv(x_m; -(1-\alpha)\hat{l}) - k_1 lv(x_n; 0) - k_2 lv(x_{n-1}; -\hat{l})$$

If v is $\hat{l}$-periodic in y, using Taylor expansion it can be shown that the following identities are satisfied:

i) $f_1(v) + f_2(v) = O(\varepsilon)$

ii) $f_1(v) = (k_1 + k_2) l[v(x_n, 0) - v(x_n, \alpha\hat{l})]$

$$- \sum_{1 \le s \le S} \frac{\varepsilon^s}{s!} [(\alpha\hat{l})^s k_1 l + (-1)^s ((1-\alpha)\hat{l})^s k_2 l] \frac{\partial^s}{\partial x^s} (v(x_n, \alpha\hat{l})) + O(\varepsilon^{s+1})$$

$$= f_1^0(v) + \varepsilon f_1^1(v) + \varepsilon^2 f_1^2(v) + \varepsilon^3 f_1^3(v) + \varepsilon^4 f_1^4(v) + \ldots$$

iii) $f_2(v) = (k_1 + k_2) l[v(x_m, \alpha\hat{l}) - v(x_m, 0)]$

$$- \sum_{1 \le s \le S} \frac{\varepsilon^s}{s!} [(-1)^s (\alpha\hat{l})^s k_1 l + ((1-\alpha)\hat{l})^s k_2 l] \frac{\partial^s}{\partial x^s} (v(x_m, 0)) + O(\varepsilon^{s+1})$$

$$= f_2^0(v) + \varepsilon f_2^1(v) + \varepsilon^2 f_2^2(v) + \varepsilon^3 f_2^3(v) + \varepsilon^4 f_2^4(v) + \ldots$$

Finally, for a given function *q(x,y)* we introduce the averaging operator over the unit cell domain:

$$\langle q(x, y) \rangle = \alpha q(x, 0) + (1-\alpha) q(x, \alpha\hat{l})$$

2.2.1 O(1) Homogenization

•At $O(\varepsilon^{-2})$ we have: $f_2^0(u^0) = 0$ and $f_1^0(u^0) = 0$, which yields:

$u^0(x_n, 0) = u^0\left(x_n, \frac{\hat{l}}{2}\right)$ and $u^0(x_m, 0) = u^0\left(x_m, \frac{\hat{l}}{2}\right)$, and therefore:

$$u^0(x, y, t, \tau) = u^0(x, t, \tau) \tag{4}$$

- At $O(\varepsilon^{-1})$ we have: $f_1^0(u^1) + f_1^1(u^0) = 0$ and $f_2^0(u^1) + f_2^1(u^0) = 0$.

The above equations together with the normalization condition $\langle u^1 \rangle = 0$ allow us to determine u^1 :

$$u^1(x, y, t, \tau) = H(y) u^0_{,x}(x, t, \tau) \tag{5}$$

where *H(y)* is defined by:

$$H(0) = \frac{1-\alpha}{k_1 + k_2}[\alpha k_2 - (1-\alpha)k_1]\hat{l}$$

$$H(\alpha\hat{l}) = \frac{\alpha}{k_1 + k_2}[(1-\alpha)k_1 - \alpha k_2]\hat{l}$$

- At $O(1)$ we have the following two equations:

$$\alpha\rho_1 u^0_{,tt}(x_n) + \frac{1}{\hat{l}^2}[f_1^0(u^2) + f_1^1(u^1) + f_1^2(u^0)] = 0 \quad ,$$

$$(1-\alpha)\rho_2 u^0_{,tt}(x_m) + \frac{1}{\hat{l}^2}[f_2^0(u^2) + f_2^1(u^1) + f_2^2(u^0)] = 0$$

Adding the above two equations, and taking into account the properties of f_1 and f_2 we get the leading order continuum equation of motion:

$$\rho_0 u^0_{,tt} - E_0 u^0_{,xx} = 0 \tag{6}$$

where:

$$\rho_0 = \alpha\rho_1 + (1-\alpha)\rho_2 \text{ and } E_0 = \frac{k_1 k_2}{k_1 + k_2} l = k_0 l .$$

2.2.2 $O(\varepsilon)$ Homogenization

u^2 follows from the $O(1)$ perturbation equations together with the normalization condition $\langle u^2 \rangle = 0$, which yields:

$$u^2(x, y, t, \tau) = P(y)u^0_{,xx}(x, t, \tau) \tag{7}$$

where *P(y)* is defined by:

$$P(0) = \frac{(1-\alpha)\hat{l}^2}{k_1+k_2}\left[\left(\frac{\alpha^2 k_2 + (1-\alpha)^2 k_1}{2}\right) - \alpha k_0 \frac{\rho_1}{\rho_0} - \frac{\alpha}{k_1+k_2}(\alpha k_2 - (1-\alpha)k_1)^2\right],$$

$$P(\alpha\hat{l}) = -\frac{\alpha\hat{l}^2}{k_1+k_2}\left[\left(\frac{\alpha^2 k_2 + (1-\alpha)^2 k_1}{2}\right) - \alpha k_0 \frac{\rho_1}{\rho_0} - \frac{\alpha}{k_1+k_2}(\alpha k_2 - (1-\alpha)k_1)^2\right].$$

The $O(\varepsilon)$ perturbations equations are:

$$\alpha\rho_1 u^1_{,tt}(x_n, 0) + \frac{1}{\hat{l}^2}[f^0_1(u^3) + f^1_1(u^2) + f^2_1(u^1) + f^3_1(u^0)] = 0,$$

$$(1-\alpha)\rho_2 u^1_{,tt}(x_m, \alpha\hat{l}) + \frac{1}{\hat{l}^2}[f^0_2(u^3) + f^1_2(u^2) + f^2_2(u^1) + f^3_2(u^0)] = 0$$

We can determine u^3 from the above two equations together with the normalization condition for u^3, which gives:

$$u^3(x, y, t, \tau) = M(y)u^0_{,xxx}(x, t, \tau) \tag{8}$$

where *M(y)* is given by:

$$M(0) = \hat{l}^3 \cdot \frac{1-\alpha}{k_1+k_2}\left\{\frac{\alpha^3 k_2 - (1-\alpha)^3 k_1}{6} + \alpha^2 \frac{(\alpha k_2 - (1-\alpha)k_1)^3}{(k_1+k_2)^2} + \alpha\frac{\alpha k_2 - (1-\alpha)k_1}{k_1+k_2}\left[k_0\frac{\rho_1}{\rho_0}(2\alpha-1) - (\alpha^2 k_2 + (1-\alpha)^2 k_1)\right]\right\}$$

$$M(\alpha\hat{l}) = -\hat{l}^3 \frac{\alpha}{k_1+k_2}\left\{\frac{\alpha^3 k_2 - (1-\alpha)^3 k_1}{6} + \alpha^2 \frac{(\alpha k_2 - (1-\alpha)k_1)^3}{(k_1+k_2)^2} + \alpha\frac{\alpha k_2 - (1-\alpha)k_1}{k_1+k_2}\left[k_0\frac{\rho_1}{\rho_0}(2\alpha-1) - (\alpha^2 k_2 + (1-\alpha)^2 k_1)\right]\right\}$$

2.2.3 $O(\varepsilon^2)$ Homogenization

The $O(\varepsilon^2)$ perturbations equations are:

$$\alpha\rho_1(u^2_{,tt} + 2u^0_{,t\tau})(x_n, 0) + \frac{1}{\hat{l}^2}[f^4_1(u^0) + f^3_1(u^1) + f^2_1(u^2) + f^1_1(u^3) + f^0_1(u^4)] = 0$$

$$(1-\alpha)\rho_2(u^2_{,tt}+2u^0_{,t\tau})(x_m,\alpha\hat{l})+\frac{1}{\hat{l}^2}[f^4_2(u^0)+f^3_2(u^1)+f^2_2(u^2)+f^1_2(u^3)+f^0_2(u^4)]\;=\;0$$

Adding the above two equations and making use of the leading order continuum equation of motion (6), yields the higher order continuum equation of motion:

$$\frac{E'_d}{\varepsilon^2}u^0_{,xxxx}-2\rho_0u^0_{,t\tau}\;=\;0 \tag{9}$$

where:

$$E'_d\;=\;l^3\Bigg\{\frac{P_4}{12}-\frac{P_1P_3}{3(k_1+k_2)}+\left[\frac{P_2}{2}-\alpha k_0\frac{\rho_1}{\rho_0}-\frac{\alpha P_1^2}{k_1+k_2}\right]\times\left[\frac{(1-2\alpha)P_2}{2(k_1+k_2)}+k_0\frac{2\alpha(1-\alpha)(\rho_0-\rho_1)}{\rho_0(k_1+k_2)}\right]$$

$$-\alpha\frac{{P_1}^2}{(k_1+k_2)^2}\left[k_0\frac{\rho_1}{\rho_0}(2\alpha-1)-P_2+\alpha\cdot\frac{P_1^2}{k_1+k_2}\right]\Bigg\}$$

where P_k is defined by: $P_k\;=\;\alpha^k k_2+(-1)^k(1-\alpha)^k k_1$.

2.2.4 Nonlocal continuum model

The dependence on slow time can be eliminated by combining the two continuum equations of motion with multiple temporal scales:

$$\rho_0u^0_{,tt}-E_0u^0_{,xx}\;=\;0,$$

$$\frac{E'_d}{\varepsilon^2}u^0_{,xxxx}-2\rho_0u^0_{,t\tau}\;=\;0$$

which yields the nonlocal continuum model

$$\rho_0\ddot{u}^0-E_0u^0_{,xx}\;=\;E'_du^0_{,xxxx} \tag{10}$$

where $\ddot{u}_0$ denotes the total temporal derivative.

In the case of a diatomic chain ($k_1\;=\;k_2$ and $\alpha\;=\;1/2$) we have:

$$E'_d\;=\;l^2\frac{kl}{32}\left[\left(\frac{\rho_1-\rho_2}{2\rho_0}\right)^2+\frac{1}{3}\right]$$

It is instructive to compare the above nonlocal continuum model, to the one obtained from the homogenization of continuum unit cell (see [5]-[7]):

$$\rho_0\ddot{u}^0-E_0u^0_{,xx}\;=\;E_du^0_{,xxxx}$$

where

$$E_d = \frac{kl^3}{24}\left[\left(\frac{\rho_1 - \rho_2}{2\rho_0}\right)^2\right]$$

The difference between the two is:

$$E_d - E'_d = \frac{kl^3}{96}\left[\left(\frac{\rho_1 - \rho_2}{2\rho_0}\right)^2 - 1\right]$$

Assuming $\rho_2 \le \rho_1$, we can denote $\rho_2 = \alpha\rho_1$, where $\alpha \in [0, 1]$. Therefore

$$\left(\frac{\rho_1 - \rho_2}{2\rho_0}\right)^2 = \left(\frac{1-\alpha}{1+\alpha}\right)^2 = f(\alpha)$$

One finds easily that $f(\ ]0, 1]) = [0, 1[$, which implies $E_d \le E'_d$ with equality holding if and only if $\rho_2 = 0$.

Most importantly it can be seen that for the homogeneous atomic chain E_d vanishes whereas E'_d does not, revealing a well known fact that discrete medium is always dispersive as opposed to the homogeneous continuum medium.

2.3 Numerical results

To assess the accuracy of the proposed formulation, we compare the analytical solution of the continuum model with multiple temporal scales (6), (9) to the reference solution obtained numerically by solving equations (1). We consider the following initial (ICs) and boundary (BCs) conditions:

(ICs): $u_0(x, 0, 0) = f(x) \qquad u_{0;t}(x, 0, 0) = 0$

(BCs): $u_0(0, t, \tau) = 0 \qquad u_{0,x}(L, t, \tau) = 0$

The following initial disturbance in displacements is assumed:

$$f(x) = f_0 a_0 [x - (x_0 - \delta)]^2 [x - (x_0 + \delta)]^2 \{1 - H(x - (x_0 + \delta))\}\{1 - H(x_0 - \delta - x)\}$$

where $a_0 = 1/\delta^4$ and $H(x)$ is the Heaviside step function; f_0, x_0 and δ are the magnitude, the location of the maximum value, and the half-width of the initial pulse.

The analytical solution of equations (6) and (9), satisfying the above (ICs) and (BCs) is given by (see [5]-[7]):

$$u_0(x, t) = \sum_{n \ge 1} B_n \sin\frac{\lambda_n x}{c} \cos[(\lambda_n - \omega_n)t]$$

where: $c = \sqrt{\frac{E_0}{\rho_0}}$, $\lambda_n = (2n-1)\frac{\pi c}{L}$, $\omega_n = \frac{E'_d}{2c\rho_0}\left(\frac{\lambda_n}{c}\right)^3$ and:

$$B_n = \frac{256L^2 f_0}{\delta^4[(2n-1)\pi]^5}\left\{[12L^2 - ((2n-1)\delta\pi)^2]\sin\frac{(2n-1)\pi x_0}{2L}\sin\frac{(2n-1)\pi\delta}{2L}\right.$$
$$\left. - 6(2n-1)\delta\pi L\sin\frac{(2n-1)\pi x_0}{2L}\cos\frac{(2n-1)\pi\delta}{2L}\right\}$$

Numerical experiments are conducted for the following two problems:

Problem 1: The atomistic properties considered are: $\rho_1 = \rho_2 = 4.62\times10^{-17} kgm^{-1}$ and $k_1 = k_2 = 10 Nm^{-1}$. The dimension of the unit cell is set to $l = 2.15\ angström$. We consider a chain of 100 atoms. The continuum properties are calculated as $k_0 = 5 Nm^{-1}$, $\rho_0 = 4.62\times10^{-17} kgm^{-1}$ and $E'_d = 1.04\times10^{-30} Nm^2$.

Problem 2: The atomistic properties considered are $\rho_1 = \rho_2 = 4.62\times10^{-17} kgm^{-1}$, $2k_1 = k_2 = 20 Nm^{-1}$. The dimension of the unit cell is set to $l = 2.15\ angström$, and we consider a chain of 100 atoms. The continuum properties are calculated as $k_0 = 6.67 Nm^{-1}$, $\rho_0 = 4.62\times10^{-17} kgm^{-1}$ and $E'_d = 1.85\times10^{-30} Nm^2$.

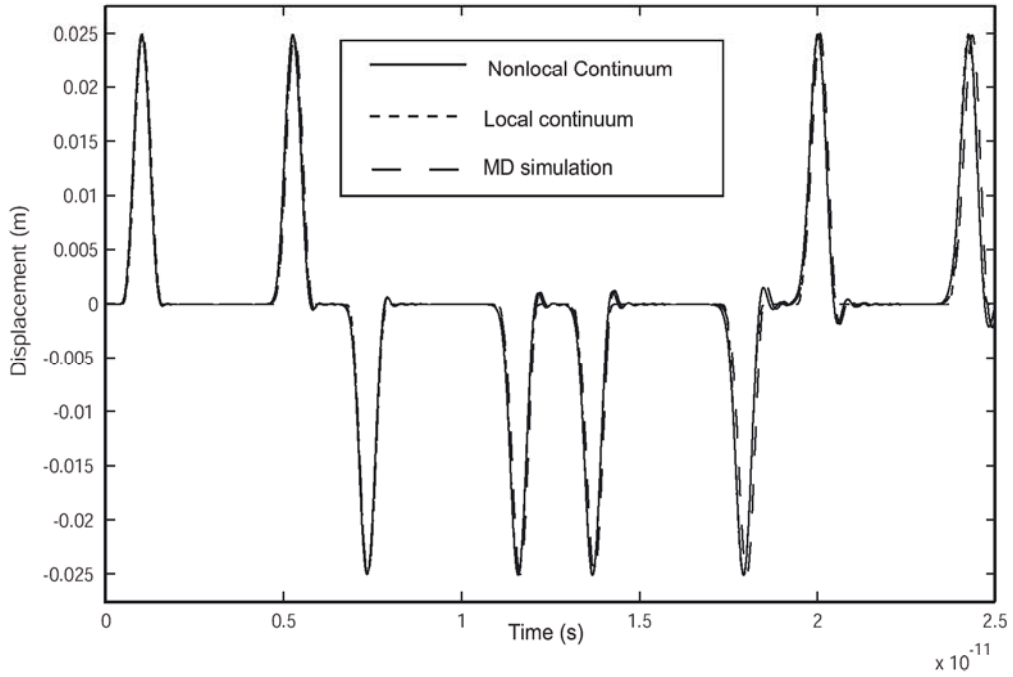

Figure 2: Problem 1, $\delta/l = 10$

Figures 2 and 3 (Problem 1) show the time-varying displacement at $x/L = 2/3$ for the cases of $\delta/l = 10$ and $\delta/l = 4$, respectively. In each of the two figures we compare the analytical dispersive continuum solution u_0, the classical local continuum solution

based on the Cauchy-Born hypothesis and the reference solution obtained by numerical simulation. Figures 4 and 5 give the corresponding solution for Problem 2.

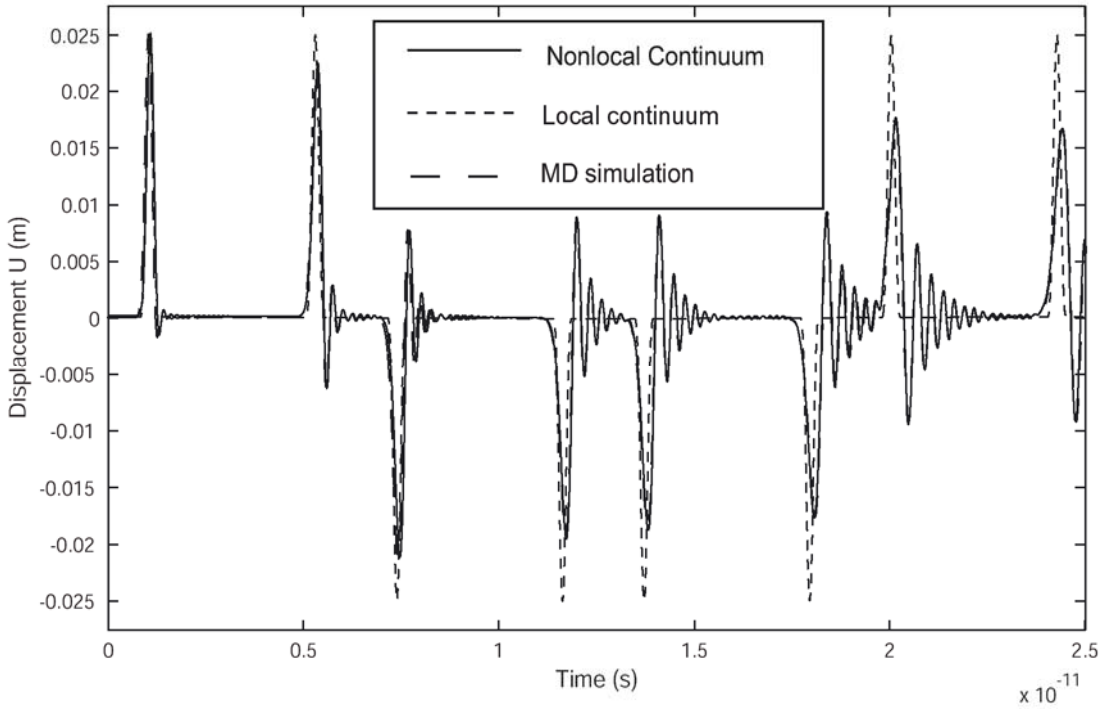

Figure 3: Problem 1, $\delta/l = 4$

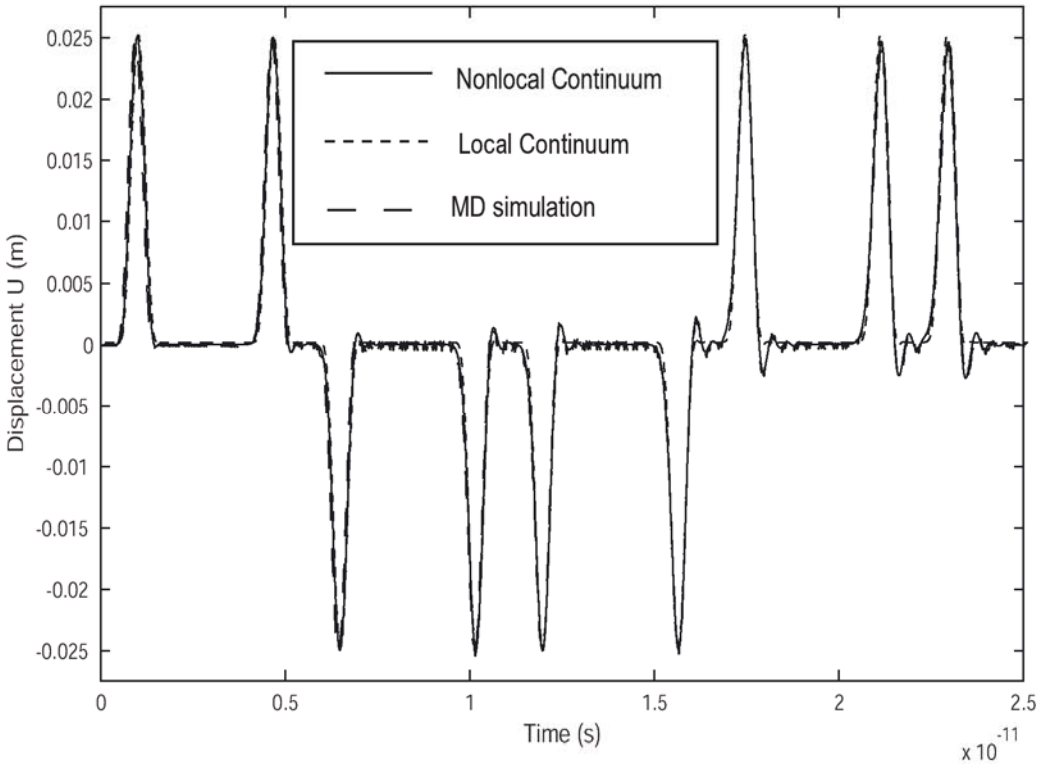

Figure 4: Problem 2, $\delta/l = 10$

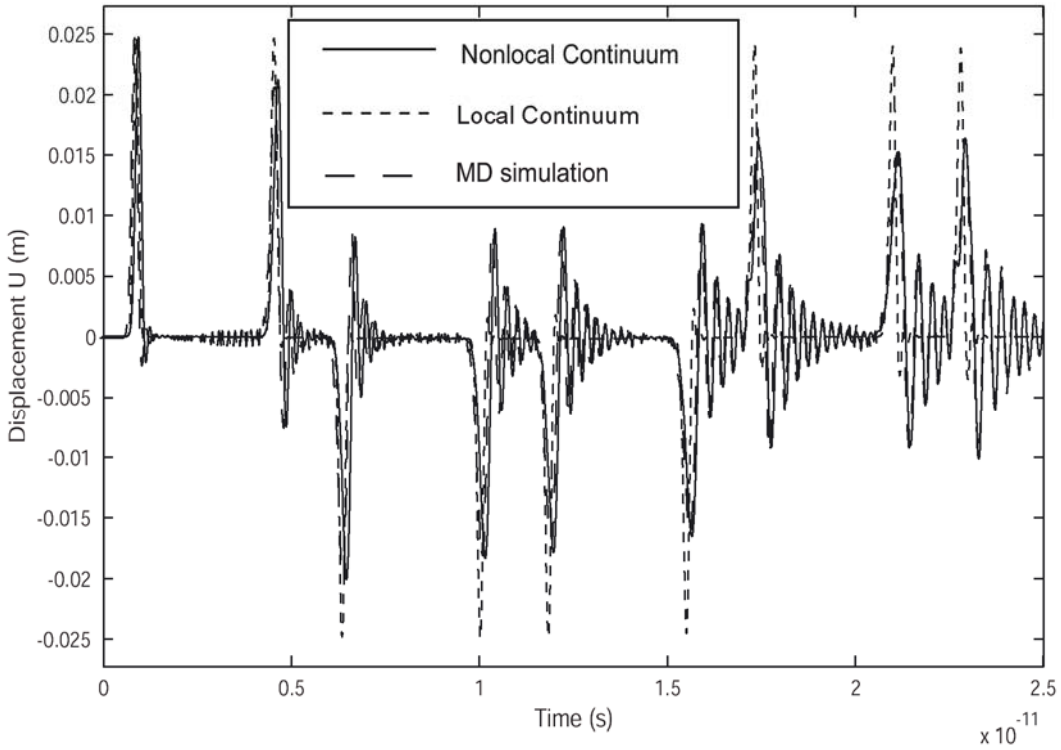

Figure 5: Problem 2, $\delta / l = 4$

3.0 The BCC Crystal

3.1 Problem Statement

We consider a Body Centered Cubic (BCC) crystal of two atoms: one of type 1 (mass m_1) and one of type two (mass m_2). We assume that the atom of type two acts as if it was connected to its nearest eight neighbors by a spring of stiffness k_2, whereas the atom of type one is connected to its nearest eight neighbors by a spring of stiffness k_2 and to its six second neighbors by a spring of stiffness k_1 (see Figure 6). The total energy consists of the kinetic and potential energies of all atoms in the system. Due to periodicity the energetics of the atomistic unit cell can be expressed in terms of the two representative atoms positioned at points *A* and *B* as shown in Figure 6. To specify the location of an atom in a cell, we place a local stretched coordinate system with an origin at point *A*. The positions of the two representative atoms in the stretched local coordinate system is specified by two vectors $\boldsymbol{y}_j$:

$$ {}^t\boldsymbol{y}_1 = (0, 0, 0) \quad \text{and} \quad {}^t\boldsymbol{y}_2 = \frac{\hat{l}}{2}(1, 1, 1). $$

Thus the equilibrium position of the jth atom ($j \in \{1, 2\}$) in the (m, n, p)th cell where (m, n, p) are integers, is given by:

$$ \boldsymbol{x}_{mnpj} = (m\boldsymbol{e}_1 + n\boldsymbol{e}_2 + p\boldsymbol{e}_3)l + \varepsilon \boldsymbol{y}_j $$

The cartesian components of $\boldsymbol{x}_{mnpj}$ are denoted as $x^{\alpha}_{mnpj}, \alpha = 1, 2, 3$. The displacement of the representative atom *(mnp,j)* is denoted by the vector $\boldsymbol{u}_{mnpj}$.

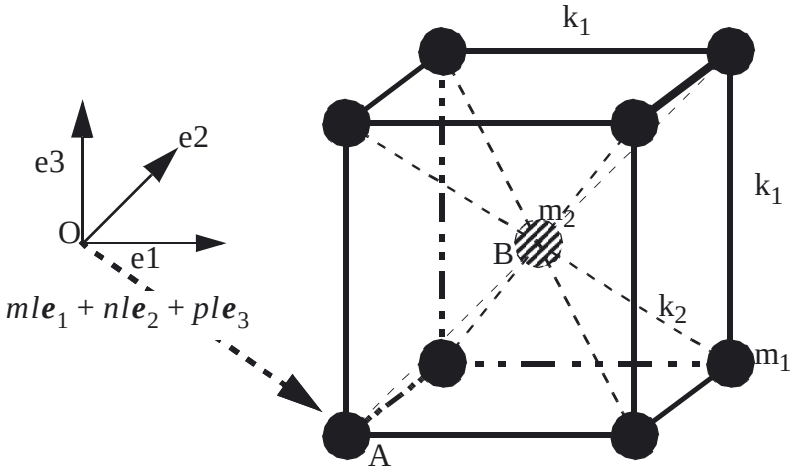

Figure 6: The unit cell of BCC crystal

For any two atoms $a = (m, n, p, j)$ and $b = (m', n', p', j')$, we denote by r_{ab} and $k_{ab} \in \{0, k_1, k_2\}$ the distance and the stiffness of the spring between the two atoms, respectively. The potential energy of the crystal can be then expressed as:

$$2\Phi = \frac{1}{2} \sum_{(a,\, b)} k_{ab} (\delta r_{ab})^2$$

3.1.1 Equations of motion

The equations of motion for any atom $a = (m, n, p, j)$ can be written as:

$$\forall \alpha \in \{1, 2, 3\}, \quad m_j \ddot{u}^{\alpha}_a + \sum_b \sum_{\beta} \left(\frac{\partial^2 \Phi}{\partial x^{\alpha}_a \partial x^{\beta}_b} \right) u^{\beta}_b = 0$$

Further defining

$$\Phi^2 = -\frac{k_1}{l} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}; \; \Phi^3 = -\frac{k_1}{l} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}; \; \Phi^4 = -\frac{k_1}{l} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}; \; \Phi^5 = -\frac{k_2}{3l} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix};$$

$$\Phi^6 = -\frac{k_2}{3l} \begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{bmatrix}; \; \Phi^7 = -\frac{k_2}{3l} \begin{bmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix}; \; \Phi^8 = -\frac{k_2}{3l} \begin{bmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix}$$

and exploiting identities $\left(\frac{\partial^2 \Phi}{\partial x_a^\alpha \partial x_b^\beta}\right) = k_{ab}\left[\frac{\partial}{\partial x_a^\alpha}(\delta r_{ab})\right]\left[\frac{\partial}{\partial x_b^\beta}(\delta r_{ab})\right]$ and

$\frac{\partial}{\partial x_a^\alpha}(\delta r_{ab}) = \frac{x_a^\alpha - x_b^\alpha}{r_{ab}}$ yields the following equations of motion for $\forall(m, n, p)$:

$$\frac{\rho_2}{2}\ddot{\boldsymbol{u}}_{mnp2} + \Phi^5[\boldsymbol{u}_{mnp1} + \boldsymbol{u}_{(m+1)(n+1)(p+1)1}] + \Phi^6[\boldsymbol{u}_{(m+1)np1} + \boldsymbol{u}_{m(n+1)(p+1)1}]$$

$$+ \Phi^7[\boldsymbol{u}_{(m+1)(n+1)p1} + \boldsymbol{u}_{mn(p+1)1}] + \Phi^8[\boldsymbol{u}_{m(n+1)p1} + \boldsymbol{u}_{(m+1)n(p+1)1}]$$

$$= \frac{2}{\varepsilon^2 \hat{l}^2}\left(\sum_{5 \le s \le 8} \Phi^s\right)\boldsymbol{u}_{mnp2}$$

$$\frac{\rho_1}{2}\ddot{\boldsymbol{u}}_{mnp1} + \frac{1}{\varepsilon^2 \hat{l}^2}\{\Phi^2[\boldsymbol{u}_{mn(p+1)1} + \boldsymbol{u}_{mn(p-1)1}] + \Phi^3[\boldsymbol{u}_{(m-1)np1} + \boldsymbol{u}_{(m+1)np1}]$$

$$+ \Phi^4[\boldsymbol{u}_{m(n-1)p1} + \boldsymbol{u}_{m(n+1)p1}] + \Phi^5[\boldsymbol{u}_{mnp2} + \boldsymbol{u}_{(m-1)(n-1)(p-1)2}]$$

$$+ \Phi^6[\boldsymbol{u}_{(m-1)np2} + \boldsymbol{u}_{m(n-1)(p-1)2}] + \Phi^7[\boldsymbol{u}_{(m-1)(n-1)p2} + \boldsymbol{u}_{mn(p-1)2}]$$

$$+ \Phi^8[\boldsymbol{u}_{m(n-1)p2} + \boldsymbol{u}_{(m-1)n(p-1)2}]\} = \frac{2}{\varepsilon^2 \hat{l}^2}\left(\sum_{2 \le s \le 8} \Phi^s\right)\boldsymbol{u}_{mnp1}$$

where $\rho_1 = 2m_1/l^3$ and $\rho_2 = 2m_2/l^3$.

Remark 2: In three-dimensional case the corresponding relation to equation (2) is:

$$\frac{k_i}{l\rho_i} = O(1)$$

where the cross-sectional area in 1D has been substituted by a square of the distance between the two nearest atoms. Moreover, exploiting the definition of Φ^i we get

$$\frac{\|\Phi^j\|}{\rho_i} = O(1)$$

and therefore it is appropriate to introduce an asymptotic expansion for solving the above equations of motion.

3.2 Nonlocal Continuum

As in 1D case we substitute the following multiscale asymptotic expansion:

$$\boldsymbol{u}(\boldsymbol{x}, \boldsymbol{y}, t, \tau) = \boldsymbol{u}^0(\boldsymbol{x}, \boldsymbol{y}, t, \tau) + \varepsilon \boldsymbol{u}^1(\boldsymbol{x}, \boldsymbol{y}, t, \tau) + \ldots$$

into the equations of motion, which yields series of equations in ascending power of ε starting with ε^{-2}. We again assume that x is a continuous variable, whereas y is discrete, and therefore, for a given value of y $\boldsymbol{u}(x, y)$ is continuous and differentiable with respect to x. Thus the displacements of atoms can be expressed as:

$$\boldsymbol{u}_{mnpj} = \boldsymbol{u}(\boldsymbol{x} = \boldsymbol{x}_{mnpj}, \boldsymbol{y} = \boldsymbol{y}_j)$$

We further assume that $\boldsymbol{u}^k(x, y)$ is Y-periodic in the y-variable where $Y = [0, \hat{l}]^3$.

In subsequent derivations we utilize the following Taylor expansion:

$$\boldsymbol{u}_{(m+i)(n+j)(p+k)(r)} = \sum_{s \le S} \frac{(\varepsilon \hat{l})^s}{s!} \frac{d^s}{dx^s} \boldsymbol{u}(\boldsymbol{x}_{mnpl}, \boldsymbol{y}_r) \bullet^t \left(i + \frac{r-l}{2}, j + \frac{r-l}{2}, k + \frac{r-l}{2} \right)^s + O(\varepsilon^{S+1})$$

where for a given vector $\boldsymbol{v}$ we denote:

$$d^s \boldsymbol{v}(\boldsymbol{x}_{mnpl}, \boldsymbol{y}_r) \bullet \boldsymbol{v}^s = \frac{d^s}{dx^s} \boldsymbol{u}(\boldsymbol{x}_{mnpl}, \boldsymbol{y}_r) \bullet \boldsymbol{v}^s = \frac{d^s}{dx^s} \boldsymbol{u}(\boldsymbol{x}_{mnpl}, \boldsymbol{y}_r) \underbrace{(\boldsymbol{v}, \boldsymbol{v}, \ldots, \boldsymbol{v})}_{s-times}$$

For a given function $\boldsymbol{v}(x,y)$, we introduce:

$$f_1(\boldsymbol{v}) = -2 \left(\sum_{2 \le s \le 8} \Phi^s \right) \boldsymbol{v}(\boldsymbol{x}_{mnp1}, \boldsymbol{y}_1) + \Phi^2 [\boldsymbol{v}(\boldsymbol{x}_{mn(p+1)1}, \boldsymbol{y}_1) + \boldsymbol{v}(\boldsymbol{x}_{mn(p-1)1}, \boldsymbol{y}_1)]$$

$$+ \Phi^4 [\boldsymbol{v}(\boldsymbol{x}_{m(n+1)p1}, \boldsymbol{y}_1) + \boldsymbol{v}(\boldsymbol{x}_{m(n-1)p1}, \boldsymbol{y}_1)] + \Phi^3 [\boldsymbol{v}(\boldsymbol{x}_{(m+1)np1}, \boldsymbol{y}_1) + \boldsymbol{v}(\boldsymbol{x}_{(m-1)np1}, \boldsymbol{y}_1)]$$

$$+ \Phi^5 [\boldsymbol{v}(\boldsymbol{x}_{mnp2}, \boldsymbol{y}_2) + \boldsymbol{v}(\boldsymbol{x}_{(m-1)(n-1)(p-1)2}, \boldsymbol{y}_2)] + \Phi^6 [\boldsymbol{v}(\boldsymbol{x}_{(m-1)np2}, \boldsymbol{y}_2) + \boldsymbol{v}(\boldsymbol{x}_{m(n-1)(p-1)2}, \boldsymbol{y}_2)]$$

$$+ \Phi^7 [\boldsymbol{v}(\boldsymbol{x}_{(m-1)(n-1)p2}, \boldsymbol{y}_2) + \boldsymbol{v}(\boldsymbol{x}_{mn(p-1)2}, \boldsymbol{y}_2)] + \Phi^8 [\boldsymbol{v}(\boldsymbol{x}_{m(n-1)p2}, \boldsymbol{y}_2) + \boldsymbol{v}(\boldsymbol{x}_{(m-1)n(p-1)2}, \boldsymbol{y}_2)]$$

and:

$$f_2(\boldsymbol{v}) = -2\left(\sum_{5 \le s \le 8} \Phi^s\right)\boldsymbol{v}(\boldsymbol{x}_{mnp2}, \boldsymbol{y}_2) + \Phi^5[\boldsymbol{v}(\boldsymbol{x}_{mnp1}, \boldsymbol{y}_1) + \boldsymbol{v}(\boldsymbol{x}_{(m+1)(n+1)(p+1)1}, \boldsymbol{y}_1)]$$

$$+ \Phi^6[\boldsymbol{v}(\boldsymbol{x}_{(m+1)np,1}, \boldsymbol{y}_1) + \boldsymbol{v}(\boldsymbol{x}_{m(n+1)(p+1)1}, \boldsymbol{y}_1)] + \Phi^7[\boldsymbol{v}(\boldsymbol{x}_{(m+1)(n+1)p1}, \boldsymbol{y}_1) + \boldsymbol{v}(\boldsymbol{x}_{mn(p+1)1}, \boldsymbol{y}_1)]$$

$$+ \Phi^8[\boldsymbol{v}(\boldsymbol{x}_{m(n+1)p1}, \boldsymbol{y}_1) + \boldsymbol{v}(\boldsymbol{x}_{(m+1)n(p+1)1}, \boldsymbol{y}_1)]$$

If $\boldsymbol{v}$ is Y-periodic, then using the Taylor expansions it can be easily shown that the following identities hold (for simplicity we denote $\boldsymbol{x}_1 = \boldsymbol{x}_{mnp1}$ and $\boldsymbol{x}_2 = \boldsymbol{x}_{mnp2}$):

i) $f_1(\boldsymbol{v}) + f_2(\boldsymbol{v}) = O(\varepsilon)$

ii) $$f_1(\boldsymbol{v}) = -2\left(\sum_{5 \le s \le 8} \Phi^s\right)[\boldsymbol{v}(\boldsymbol{x}_1, \boldsymbol{y}_1) - \boldsymbol{v}(\boldsymbol{x}_1, \boldsymbol{y}_2)] + 2\sum_{1 \le s \le S} \frac{(\varepsilon\hat{l})^{2s}}{(2s)!}\Big\{ \Phi^2 d^{2s}\boldsymbol{v}(\boldsymbol{x}_1, \boldsymbol{y}_1) \bullet \boldsymbol{e}_3^{2s}$$

$$+ \Phi^3 d^{2s}\boldsymbol{v}(\boldsymbol{x}_1, \boldsymbol{y}_1) \bullet \boldsymbol{e}_1^{2s} + \Phi^4 d^{2s}\boldsymbol{v}(\boldsymbol{x}_1, \boldsymbol{y}_1) \bullet \boldsymbol{e}_2^{2s} + \Phi^5 d^{2s}\boldsymbol{v}(\boldsymbol{x}_1, \boldsymbol{y}_2) \bullet \left(\frac{\boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3}{2}\right)^{2s}$$

$$+ \Phi^6 d^{2s}\boldsymbol{v}(\boldsymbol{x}_1, \boldsymbol{y}_2) \bullet \left(\frac{-\boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3}{2}\right)^{2s} + \Phi^7 d^{2s}\boldsymbol{v}(\boldsymbol{x}_1, \boldsymbol{y}_2) \bullet \left(\frac{\boldsymbol{e}_1 + \boldsymbol{e}_2 - \boldsymbol{e}_3}{2}\right)^{2s}$$

$$+ \Phi^8 d^{2s}\boldsymbol{v}(\boldsymbol{x}_1, \boldsymbol{y}_2) \bullet \left(\frac{\boldsymbol{e}_1 - \boldsymbol{e}_2 + \boldsymbol{e}_3}{2}\right)^{2s}\Big\} + O(\varepsilon^{2(S+1)})$$

$$= f_1^0(\boldsymbol{v}) + \varepsilon^2 f_1^2(\boldsymbol{v}) + \varepsilon^4 f_1^4(\boldsymbol{v}) + \ldots$$

iii)

$$f_2(\boldsymbol{v}) = -2\left(\sum_{5 \le s \le 8} \Phi^s\right)[\boldsymbol{v}(\boldsymbol{x}_2, \boldsymbol{y}_2) - \boldsymbol{v}(\boldsymbol{x}_2, \boldsymbol{y}_1)]$$

$$+ 2\sum_{1 \le s \le S} \frac{(\varepsilon\hat{l})^{2s}}{(2s)!}\Big\{ \Phi^5 d^{2s}\boldsymbol{v}(\boldsymbol{x}_2, \boldsymbol{y}_1) \bullet \left(\frac{\boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3}{2}\right)^{2s} + \Phi^6 d^{2s}\boldsymbol{v}(\boldsymbol{x}_2, \boldsymbol{y}_1) \bullet \left(\frac{-\boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3}{2}\right)^{2s}$$

$$+ \Phi^7 d^{2s}\boldsymbol{v}(\boldsymbol{x}_2, \boldsymbol{y}_1) \bullet \left(\frac{\boldsymbol{e}_1 + \boldsymbol{e}_2 - \boldsymbol{e}_3}{2}\right)^{2s} + \Phi^8 d^{2s}\boldsymbol{v}(\boldsymbol{x}_1, \boldsymbol{y}_2) \bullet \left(\frac{\boldsymbol{e}_1 - \boldsymbol{e}_2 + \boldsymbol{e}_3}{2}\right)^{2s}\Big\} + O(\varepsilon^{2(S+1)})$$

$$= f_2^0(\boldsymbol{v}) + \varepsilon^2 f_2^2(\boldsymbol{v}) + \varepsilon^4 f_2^4(\boldsymbol{v}) + \ldots$$

3.2.1 O(1) Homogenization

- At $O(\varepsilon^{-2})$ we have: $f_1^0(\boldsymbol{u}^0) = 0$ and $f_2^0(\boldsymbol{u}^0) = 0$, which yields:

$$\boldsymbol{u}^0(\boldsymbol{x}_1, \boldsymbol{y}_1) = \boldsymbol{u}^0(\boldsymbol{x}_1, \boldsymbol{y}_2) \quad \text{and} \quad \boldsymbol{u}^0(\boldsymbol{x}_2, \boldsymbol{y}_1) = \boldsymbol{u}^0(\boldsymbol{x}_2, \boldsymbol{y}_2) ,$$

or:

$$\boldsymbol{u}^0(\boldsymbol{x}, \boldsymbol{y}, t, \tau) = \boldsymbol{u}^0(\boldsymbol{x}, t, \tau) \tag{11}$$

- At $O(\varepsilon^{-1})$ we have: $f_1^0(\boldsymbol{u}^1) = 0$ and $f_2^0(\boldsymbol{u}^1) = 0$, which yields:

$$\boldsymbol{u}^1(\boldsymbol{x}_1, \boldsymbol{y}_1) = \boldsymbol{u}^1(\boldsymbol{x}_1, \boldsymbol{y}_2) \quad \text{and} \quad \boldsymbol{u}^1(\boldsymbol{x}_2, \boldsymbol{y}_1) = \boldsymbol{u}^1(\boldsymbol{x}_2, \boldsymbol{y}_2) ,$$

which together with the normalization condition for $\boldsymbol{u}^1$ gives:

$$\boldsymbol{u}^1(\boldsymbol{x}, \boldsymbol{y}, t, \tau) = 0 \tag{12}$$

- At $O(1)$ we have the two equations:

$$\frac{1}{2}\rho_1 \boldsymbol{u}^0_{,tt}(\boldsymbol{x}_1) + \frac{1}{\tilde{\tilde{l}}^2}[f_1^0(\boldsymbol{u}^2) + f_1^2(u^0)] = 0 ,$$

$$\frac{1}{2}\rho_2 \boldsymbol{u}^0_{,tt}(x_2) + \frac{1}{\tilde{\tilde{l}}^2}[f_2^0(\boldsymbol{u}^2) + f_2^2(\boldsymbol{u}^0)] = 0 \tag{13}$$

Adding the above two equations, and taking into account the properties of f_1 and f_2 yields the leading order continuum equation of motion:

$$\rho_0 \boldsymbol{u}^0_{,tt} + \Phi^2 d^2\boldsymbol{u}^0 \bullet \begin{pmatrix}0\\0\\1\end{pmatrix}^2 + \Phi^3 d^2\boldsymbol{u}^0 \bullet \begin{pmatrix}1\\0\\0\end{pmatrix}^2 + \Phi^4 d^2\boldsymbol{u}^0 \bullet \begin{pmatrix}0\\1\\0\end{pmatrix}^2 + \frac{1}{2}\Phi^5 d^2\boldsymbol{u}^0 \bullet \begin{pmatrix}1\\1\\1\end{pmatrix}^2$$
$$+ \frac{1}{2}\Phi^6 d^2\boldsymbol{u}^0 \bullet \begin{pmatrix}-1\\1\\1\end{pmatrix}^2 + \frac{1}{2}\Phi^7 d^2\boldsymbol{u}^0 \bullet \begin{pmatrix}1\\1\\-1\end{pmatrix}^2 + \frac{1}{2}\Phi^8 d^2\boldsymbol{u}^0 \bullet \begin{pmatrix}1\\-1\\1\end{pmatrix}^2 = 0$$

which can be rewritten as:

$$\forall i \in \{1, 2, 3\}, \qquad \rho_0 u^0_{i,\,tt} = \left[\left(\delta_{\underline{ij}}\left(\frac{k_1}{l} - \frac{4k_2}{3l}\right) + \frac{2k_2}{3l}\right)u^0_{j,\,j}\right]_{,i} + \frac{4k_2}{3l}\left(\frac{u^0_{i,\,j} + u^0_{j,\,i}}{2}\right)_{,j} \tag{14}$$

where summation convention over repeated subscripts is adopted, except for underscored subscripts, and $\rho_0 = (\rho_1 + \rho_2)/2$. In tensorial notation the above formulae can be expressed as:

$$\forall i \in \{1, 2, 3\}, \qquad \rho_0 u^0_{i,\,tt} = D^0_{ijmn}\varepsilon^0_{mn,\,j} \tag{15}$$

where ε^0 is symmetric gradient of $\boldsymbol{u}^0$, and $\boldsymbol{D}^0$ is a fourth-rank tensor defined by:

$$D^0_{ijmn} = \delta_{ij}\delta_{mn}\left(\frac{2k_2}{3l} + \delta_{im}\left(\frac{k_1}{l} - \frac{4k_2}{3l}\right)\right) + \delta_{im}\delta_{jn}\frac{4k_2}{3l}$$

Equation (14) is validated in the Appendix.

3.2.2 O(ε) Homogenization

We can determine $\boldsymbol{u}^2$ from equations (13) together with the normalization condition for $\boldsymbol{u}^2$, which yields:

$$u^2_i(\boldsymbol{x}, \boldsymbol{y}, t, \tau) = P_{ijmn}(\boldsymbol{y})\varepsilon^0_{mn,j}(\boldsymbol{x}, t, \tau) \tag{16}$$

where $\boldsymbol{P}(\boldsymbol{y})$ is a Y-periodic fourth-rank tensor defined by:

$$P_{ijmn}(\boldsymbol{y}_2) = \frac{\hat{l}^2}{16}\left\{\delta_{ij}\delta_{mn}\left[\left(1 - \frac{\rho_2}{\rho_0}\right) - \delta_{im}\left(3\frac{\rho_2}{\rho_0}\frac{k_1}{k_2} + 2\left(1 - \frac{\rho_2}{\rho_0}\right)\right)\right] + 2\delta_{im}\delta_{jn}\left(1 - \frac{\rho_2}{\rho_0}\right)\right\}$$

$$P_{ijmn}(\boldsymbol{y}_1) = -P_{ijmn}(y_2)$$

The resulting $O(\varepsilon)$ perturbations equations are given as:

$$\frac{1}{2}\rho_1\boldsymbol{u}^1_{,tt}(\boldsymbol{x}_1, \boldsymbol{y}_1) + \frac{1}{\hat{l}^2}[f^0_1(\boldsymbol{u}^3) + f^2_1(\boldsymbol{u}^1)] = 0 \ ,$$

$$\frac{1}{2}\rho_2\boldsymbol{u}^1_{,tt}(\boldsymbol{x}_2, \boldsymbol{y}_2) + \frac{1}{\hat{l}^2}[f^0_2(\boldsymbol{u}^3) + f^2_2(\boldsymbol{u}^1)] = 0$$

We can determine $\boldsymbol{u}^3$ from the above two equations and the normalization condition for $\boldsymbol{u}^3$. Since $\boldsymbol{u}^1 = 0$ we get $\boldsymbol{u}^3(\boldsymbol{x}, \boldsymbol{y}, t, \tau) = 0$.

3.2.3 O(ε^2) Homogenization - simple trigonal Bravais crystal

The simple Bravais crystal is characterized by: $\rho_1 = \rho_2 = \rho_0$ and $k_1 = 0$. In this case, we have $\boldsymbol{u}^2(\boldsymbol{x}, \boldsymbol{y}) = 0$, and therefore the $O(\varepsilon^2)$ perturbations equations reduce to:

$$\rho_1\boldsymbol{u}^0_{,t\tau}(\boldsymbol{x}_1) + \frac{1}{\hat{l}^2}[f^4_1(\boldsymbol{u}^0) + f^0_1(\boldsymbol{u}^4)] = 0$$

$$\rho_2\boldsymbol{u}^0_{,t\tau}(\boldsymbol{x}_2) + \frac{1}{\hat{l}^2}[f^4_2(\boldsymbol{u}^0) + f^0_2(\boldsymbol{u}^4)] = 0$$

Adding the above two equations yields:

$$2\rho_0 \boldsymbol{u}^0_{,t\tau} + \frac{\hat{l}^2}{12}\left[\Phi^2 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}0\\0\\1\end{pmatrix}^4 + \Phi^3 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}1\\0\\0\end{pmatrix}^4 + \Phi^4 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}0\\1\\0\end{pmatrix}^4 \right.$$
$$\left. + \frac{1}{8}\left(\Phi^5 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}1\\1\\1\end{pmatrix}^4 + \Phi^6 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}-1\\1\\1\end{pmatrix}^4 + \Phi^7 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}1\\1\\-1\end{pmatrix}^4 + \Phi^8 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}1\\-1\\1\end{pmatrix}^4\right)\right] = 0$$

which may be rewritten as:

$$\forall i \in \{1, 2, 3\}, \qquad 2\rho_0 u^0_{i,\,t\tau} - E_{ijprmn}\varepsilon^0_{mn,\,j} = 0$$

where $\boldsymbol{E}$ is a sixth-rank tensor defined by:

$$E_{ijprmn} = \frac{\hat{l}^2}{12}\left\{\delta_{\underline{pr}}\delta_{\underline{pi}}\delta_{\underline{mn}}\delta_{\underline{ij}}\left[\frac{k_2}{6} + \delta_{\underline{im}}\left(k_1 - \frac{k_2}{3}\right)\right] - \delta_{\underline{pr}}\delta_{\underline{im}}\delta_{\underline{pn}}\delta_{\underline{jp}}\frac{2k_2}{3}\right.$$
$$+ \delta_{\underline{ip}}\delta_{\underline{im}}\delta_{\underline{ij}}\delta_{\underline{nr}}k_2 + (1-\delta_{\underline{ir}})(1-\delta_{\underline{ip}})\delta_{\underline{im}}\delta_{\underline{pn}}\delta_{\underline{jr}}k_2$$
$$\left. + (1-\delta_{\underline{ir}})\delta_{\underline{ip}}\delta_{\underline{mn}}\delta_{\underline{jr}}\left[\frac{k_2}{2} + (1-\delta_{\underline{im}})(1-\delta_{\underline{jm}})k_2\right]\right\}$$

3.2.4 O(ε^2) Homogenization - The general case

In the general case, the $O(\varepsilon^2)$ perturbations equations are:

$$\frac{\rho_1}{2}\boldsymbol{u}^2_{,tt}(\boldsymbol{x}_1, \boldsymbol{y}_1) + \rho_1 \boldsymbol{u}^0_{,t\tau}(\boldsymbol{x}_1) + \frac{1}{\hat{l}^2}[f_1^4(\boldsymbol{u}^0) + f_1^2(\boldsymbol{u}^2) + f_1^0(\boldsymbol{u}^4)] = 0$$

$$\frac{\rho_2}{2}\boldsymbol{u}^2_{,tt}(\boldsymbol{x}_2, \boldsymbol{y}_2) + \rho_2 \boldsymbol{u}^0_{,t\tau}(\boldsymbol{x}_2) + \frac{1}{\hat{l}^2}[f_2^4(\boldsymbol{u}^0) + f_2^2(\boldsymbol{u}^2) + f_2^0(\boldsymbol{u}^4)] = 0 \ .$$

Adding the above two equation, we get:

$$\frac{\rho_1}{2}\boldsymbol{u}^2_{,tt}(\boldsymbol{x}, \boldsymbol{y}_1) + \frac{\rho_2}{2}\boldsymbol{u}^2_{,tt}(\boldsymbol{x}, \boldsymbol{y}_2) + 2\rho_0 \boldsymbol{u}^0_{,t\tau} + \frac{\hat{l}^2}{12}\left[\Phi^2 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}0\\0\\1\end{pmatrix}^4 + \Phi^3 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}1\\0\\0\end{pmatrix}^4 \right.$$
$$\left. + \Phi^4 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}0\\1\\0\end{pmatrix}^4 + \frac{1}{8}\Phi^5 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}1\\1\\1\end{pmatrix}^4 + \Phi^6 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}-1\\1\\1\end{pmatrix}^4 + \Phi^7 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}1\\1\\-1\end{pmatrix}^4 + \Phi^8 d^4\boldsymbol{u}^0 \bullet \begin{pmatrix}1\\-1\\1\end{pmatrix}^4\right]$$
$$+ \left[\Phi^2 d^2\boldsymbol{u}^2 \bullet \begin{pmatrix}0\\1\\0\end{pmatrix}^2 + \Phi^3 d^2\boldsymbol{u}^2 \bullet \begin{pmatrix}0\\1\\0\end{pmatrix}^2 + \Phi^4 d^2\boldsymbol{u}^2 \bullet \begin{pmatrix}0\\1\\0\end{pmatrix}^2\right] = 0$$

One sees easily that:

$$\left[\Phi^2 d^2\boldsymbol{u}^2 \bullet \begin{pmatrix}0\\0\\1\end{pmatrix}^2 + \Phi^3 d^2\boldsymbol{u}^2 \bullet \begin{pmatrix}1\\0\\0\end{pmatrix}^2 + \Phi^4 d^2\boldsymbol{u}^2 \bullet \begin{pmatrix}0\\1\\0\end{pmatrix}^2\right]_i = \frac{k_1}{l}(P_{ijmn}\varepsilon^0_{mn,j})_{,\underline{ii}} \ .$$

Then, using the result of the previous section for the Bravais crystal, and making use of the leading order continuum equation of motion, we find:

$$\forall i \in \{1, 2, 3\}, \quad 2\rho_0 u^0_{i,t\tau} - \frac{1}{\varepsilon^2} E^0_{ijprmn}\varepsilon^0_{mn,rpj} = 0 \tag{17}$$

where $\boldsymbol{E}^0$ is a sixth-rank tensor defined by:

$$E^0_{ijprmn} = \varepsilon^2\left\{E_{ijprmn} - \frac{(\rho_2 - \rho_1)}{2\rho_0} D^0_{\alpha mnr}(P_{ij\alpha p}(y_2) + P_{ijp\alpha}(y_2)) + \frac{k_1}{l}\delta_{\underline{pr}}\delta_{\underline{ir}}P_{ijmn}(y_1)\right\}$$

The two continuum equations of motion are given by:

$$\forall i \in \{1, 2, 3\}, \quad \rho_0 u^0_{i,tt} = D^0_{ijmn}\varepsilon^0_{mn,j},$$

$$\forall i \in \{1, 2, 3\}, \quad 2\rho_0 u^0_{i,t\tau} - \frac{1}{\varepsilon^2} E^0_{ijprmn}\varepsilon^0_{mn,rpj} = 0$$

The dependence on the slow time scale can be eliminated by combining the two continuum equations, which yields

$$\forall i \in \{1, 2, 3\}, \quad \rho_0 \ddot{u}^0_i - D^0_{ijmn}\varepsilon^0_{mn,j} - E^0_{ijprmn}\varepsilon^0_{mn,rpj} = 0$$

4.0 Conclusions

The proposed framework for constitutive modeling based directly on atomistics is generic, but currently, is at the embryonic stage of implementation, limited to idealized scenarios, such as perfect latices, quadratic potentials and nearest neighbor interaction conditions. Further research is essential to promote the proposed methodology from the status of “interesting and having potential” to a practical analysis and design tool. The methodology’s essential features, that need to be generalized to realistic situations, are summarized below: (i) consideration of real solids with defects, (ii) accounting for temperature effects, and (iii) using realistic potentials (provided that they can be derived from the "first principles" based on the Density Functional Theory).

5.0 References

1 V. Vitek, "Atomistic modeling: an overview" Encyclopedia of Advanced Materials," ed. D. Bloor, Pergamon, Oxford, pp.153-161, (1994).

2 F. Milstein, “Mechanics of Solids” eds. H.G. Hopkins and M.J.Sewel, Pergamon Press, Oxford, (1982).

3 E. B. Tadmor, R. Phillips and M. Ortiz, "Quasicontinuum analysis of defects in solids," *Phil. Mag. A*, Vol. 73, pp. 1529-1563, (1996)

4 J. Q. Broughton, F. F. Abraham, N. Berstein and E. Kaxiras, Concurrent coupling of length scales: Methodology and application," *Phys. Review B*, Vol.60, pp. 2391-2403.

5 J. Fish and W. Chen , *Uniformly valid multiple spatial-temporal scale modelling for wave propagation in heterogeneous media,* Mechanics of composite materials and structures, vol.8, 2000

6 J. Fish, W.Chen and G. Nagai, "Nonlocal dispersive model for wave propagation in heterogeneous media. Part 1: One-Dimensional Case," *International Journal for Numerical Methods in Engineering*, Vol. 54, pp. 331-346, (2002).

7 J. Fish, W.Chen and G. Nagai, "Nonlocal dispersive model for wave propagation in heterogeneous media. Part 2: Multi-Dimensional Case," *International Journal for Numerical Methods in Engineering*, Vol. 54, pp. 347-363, (2002).

6.0 Appendix

In this section, we derive elastic material properties for the BCC crystal. We denote by σ and ε the stress and strain vectors, respectively:

$$\sigma = (\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{23}, \sigma_{13}, \sigma_{12}) \text{ and } \varepsilon = (\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, \varepsilon_{23}, \varepsilon_{13}, \varepsilon_{12})$$

Assuming small displacements of the atoms in the crystal the constitutive relation can be approximated by a linear relation: $\sigma = \boldsymbol{C}\varepsilon$ where $\boldsymbol{C}$ is a 6×6 matrix.

The symmetry of the cubic crystal implies that the number of elastic constants can be reduced to *3*, denoted as (a, b, c). The structure of the constitutive matrix $\boldsymbol{C}$ is given by:

$$\boldsymbol{C} = \begin{pmatrix} a & b & b & 0 & 0 & 0 \\ b & a & b & 0 & 0 & 0 \\ b & b & a & 0 & 0 & 0 \\ 0 & 0 & 0 & c & 0 & 0 \\ 0 & 0 & 0 & 0 & c & 0 \\ 0 & 0 & 0 & 0 & 0 & c \end{pmatrix}$$

In order to determine the three constants, we consider the following three independent loading cases:

i) *Hydrostatic pressure:* $\sigma_{11} = \sigma_{22} = \sigma_{33} = -p$ *and others* $\sigma_{ij} = 0$.

The resultant strain can be from the constitutive equation, which gives:

$$\varepsilon_{11} = \varepsilon_{22} = \varepsilon_{33} = -\frac{p}{a + 2b}, \text{ others } \varepsilon_{ij} = 0.$$

For a given overall strain field, we can calculate the deformation of the springs. The resulting forces in the springs should be equilibrated, i.e., $-pl^2 = k_1\delta + 2k_2\delta$ where $\frac{\delta}{l} = \varepsilon_{ii}$, which produces the first relation between the constants: $a + 2b = \frac{k_1 + 2k_2}{l}$

ii) *Shear stress:* $\sigma_{11} = -\sigma_{22} = \tau$ *others* $\sigma_{ij} = 0$.

The resulting strains are: $\varepsilon_{11} = -\varepsilon_{22} = \frac{\tau}{a-b}$, others $\varepsilon_{ij} = 0$. We also have: $\tau l^2 = k_1\delta$ where $\frac{\delta}{l} = \varepsilon_{11}$, which the second relation between the constants: $a - b = \frac{k_1}{l}$.

iii) *Shear stress:* $\sigma_{23} = \tau$, *others* $\sigma_{ij} = 0$

The strains are given by: $\varepsilon_{23} = \frac{\tau}{c}$, and other strain components vanish $\varepsilon_{ij} = 0$.

Equilibrium yields: $\tau l^2 = \frac{4k_2 l}{3}\varepsilon_{23}$ and the last relation between the constants: $c = \frac{4k_2}{3l}$.

Finally, we have: $a = \frac{k_1}{l} + \frac{2k_2}{3l}$, $b = \frac{2k_2}{3l}$, and $c = \frac{4k_2}{3l}$.

The resulting local equation of motion, $\rho\ddot{u}_i = \sigma_{ij,j}$, are given as:

$$\forall i \in \{1, 2, 3\}, \qquad \rho_0 u^i_{,tt} = \left[\left(\delta_{ij}\left(\frac{k_1}{l} - \frac{4k_2}{3l}\right) + \frac{2k_2}{3l}\right)u_{j,j}\right]_{,i} + \frac{4k_2}{3l}\left(\frac{u_{i,j} + u_{j,i}}{2}\right)_{,j}$$

which is identical to equation (14).