



A temperature equation for coupled atomistic/continuum simulations

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Abstract

We present a simple method for calculating a continuum temperature field directly from a molecular dynamics (MD) simulation. Using the idea of a projection matrix previously developed for use in the bridging scale, we derive a continuum temperature equation which only requires information that is readily available from MD simulations, namely the MD velocity, atomic masses and Boltzmann constant. As a result, the equation is valid for usage in any coupled finite element (FE)/MD simulation. In order to solve the temperature equation in the continuum where an MD solution is generally unavailable, a method is utilized in which the MD velocities are found at arbitrary coarse scale points by means of an evolution function. The evolution function is derived in closed form for a 1D lattice, and effectively describes the temporal and spatial evolution of the atomic lattice dynamics. It provides an accurate atomistic description of the kinetic energy dissipation in simulations, and its behavior depends solely on the atomic lattice geometry and the form of the MD potential. After validating the accuracy of the evolution function to calculate the MD variables in the coarse scale, two 1D examples are shown, and the temperature equation is shown to give good agreement to MD simulations.

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1. Introduction

Multiple scale simulations methods are a new class of methods designed to concurrently link simulation methods which operate at disparate length and time scales. The notion of concurrent linking implies that the individual simulations dynamically transmit relevant information regarding deformation, heat or temperature to the other simulations.

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Many multiple scale methods have been recently proposed. The universal link between them is that they attempt to concurrently couple an atomistic simulation, typically molecular dynamics (MD), with a continuum simulation, typically finite elements (FE). Furthermore, it is generally assumed that the atomistic region exists in only a small part of the problem domain, while the continuum region surrounds the atomistic region. Because of this decomposition of atomistic and continuum regions, multiple scale methods are most applicable to problems in which a local phenomena demands the atomic resolution provided by MD, while the bulk behavior of the material can be well approximated using a homogeneous, or continuum representation. Examples of such problems include fracture, surface friction and strain localization. A review of existing methods and their applications can be found in [1,2].

One potential issue arising in multiple scale simulations is that in many problems of interest, a large amount of fine scale (molecular level) energy is generated in the region to be simulated using MD. In order for the MD simulation to proceed accurately, it is crucial that this fine scale energy be passed out of the fine scale region directly to the surrounding coarse scale (continuum) region. If this transfer of energy between coarse and fine scales does not occur, the fine scale internal energy will be reflected back to the fine scale region, and the MD simulation will be artificially contaminated by spurious heat generation.

Using principles introduced in the bridging scale work by Wagner and Liu [3], we derive a continuum temperature equation directly from the microscopic definition of temperature. We then demonstrate the accuracy of the equation in calculating the continuum temperature for problems in which the continuum and atomistic systems overlap each other entirely, and show that when the FE nodal spacing is the same as the atomic spacing, the temperature equation yields the same temperature as is calculated directly from MD. In order to make the temperature equation a global equation, i.e. valid in the surrounding continuum where the atomic description is absent, we propose a method to derive an extended MD solution in the continuum, or coarse scale. This method is based on the usage of the lattice evolution function to describe the dissipation of kinetic energy in the system at the atomistic level. The extended MD solution is found utilizing an evolution function, which is derived analytically for a 1D lattice. Using the coarse scale MD solution, we solve the temperature equation globally via example problems, and evaluate the performance of the combined approximation. Finally, we conclude with remarks on future research directions.

2. Overview of bridging scale

The bridging scale method was introduced by Wagner and Liu [3] to couple FE and MD for dynamic simulations. The equations of interest that will be relevant here were derived in [3] as well as in a review article [1], but the crucial equations will be re-derived here. The fundamental idea is to decompose the total displacement field $\mathbf{u}(\mathbf{x})$ into coarse and fine scales

$$\mathbf{u}(\mathbf{x}) = \bar{\mathbf{u}}(\mathbf{x}) + \mathbf{u}'(\mathbf{x}). \quad (1)$$

The total solution \mathbf{u} can be derived from *any* molecular level simulation which gives the displacement of each atom. For our purposes, we shall assume that the molecular level simulation of choice will be molecular dynamics (MD), for which the displacement is denoted \mathbf{q} . The coarse scale is defined to be

$$\bar{\mathbf{u}}(\mathbf{X}_\alpha) = \sum_I N_I^\alpha \mathbf{d}_I \quad (2)$$

and is calculated via the finite element method. Here, $N_I^\alpha = N_I(\mathbf{X}_\alpha)$ is the shape function of node I evaluated at atom α , and \mathbf{d}_I is the displacement associated with node I .

The fine scale will be defined to be the projection of the coarse scale subtracted from the total solution \mathbf{u}_α . In other words, the fine scale represents that part of the total solution that the coarse scale cannot represent. We will select this projection operator to minimize the mass-weighted square of the fine scale, which can be written as

$$\text{Error} = \sum_{\alpha} m_{\alpha} \left(\mathbf{q}_{\alpha} - \sum_I N_I^{\alpha} \mathbf{w}_I \right)^2, \quad (3)$$

where m_{α} is the atomic mass of an atom α and \mathbf{w}_I are temporary coarse scale degrees of freedom. It should be emphasized that (3) is only one of many possible ways to define an error metric. In order to solve for \mathbf{w} , the error is minimized yielding the following result:

$$\mathbf{w} = \mathbf{M}^{-1} \mathbf{N}^T \mathbf{M}_A \mathbf{q}, \quad (4)$$

where the coarse scale mass matrix \mathbf{M} is defined as

$$\mathbf{M} = \mathbf{N}^T \mathbf{M}_A \mathbf{N} \quad (5)$$

and \mathbf{M}_A is a diagonal matrix with the atomic masses on the diagonal. The fine scale \mathbf{u}' can thus be written as

$$\mathbf{u}' = \mathbf{q} - \mathbf{N} \mathbf{w} \quad (6)$$

or

$$\mathbf{u}' = \mathbf{q} - \mathbf{P} \mathbf{q}, \quad (7)$$

where the projection matrix \mathbf{P} is defined to be

$$\mathbf{P} = \mathbf{N} \mathbf{M}^{-1} \mathbf{N}^T \mathbf{M}_A. \quad (8)$$

We note that \mathbf{P} satisfies the definition of a projection matrix, i.e. $\mathbf{P} \mathbf{P} = \mathbf{P}$. In comparing (6) and (7), we see that if \mathbf{q} and \mathbf{u} satisfy the same equation of motion, the coarse scale solution is simply the projection of the MD solution

$$\mathbf{N} \mathbf{d} = \mathbf{P} \mathbf{q}. \quad (9)$$

The total displacement \mathbf{u} can finally be written as the sum of the coarse and fine scales as

$$\mathbf{u} = \mathbf{N} \mathbf{d} + \mathbf{q} - \mathbf{P} \mathbf{q}. \quad (10)$$

Using the total displacement \mathbf{u} , the multi-scale Lagrangian can be written as the difference of the kinetic and potential energies as

$$\mathcal{L}(\mathbf{u}, \dot{\mathbf{u}}) = \mathcal{K}(\dot{\mathbf{u}}) - V(\mathbf{u}). \quad (11)$$

The coupled multi-scale equations of motion can be derived from the Lagrangian as

$$\mathbf{M}_A \ddot{\mathbf{q}} = \mathbf{f} \quad (12)$$

and

$$\mathbf{M} \ddot{\mathbf{d}} = \mathbf{N}^T \mathbf{f}. \quad (13)$$

Eqs. (12) and (13) are simply the MD and finite element equations of motion, with the coupling of the two equations occurring through the MD force \mathbf{f} . Further details can be found in [1,3].

2.1. Properties of the projection matrix

In this section, we discuss the relevant properties of the bridging scale projection matrix \mathbf{P} . As we will show via example, the projection matrix when applied to any random data has the effect of giving a least squares fit of the data, with the quality of the fit dictated by the polynomial order of the shape functions \mathbf{N} .

For our first example, we consider a coupled 1D continuum/atomistic system in which one finite element overlaps 21 regularly spaced atoms between $x = 0$ and $x = 1$. We prescribe a linear displacement field \mathbf{q} on

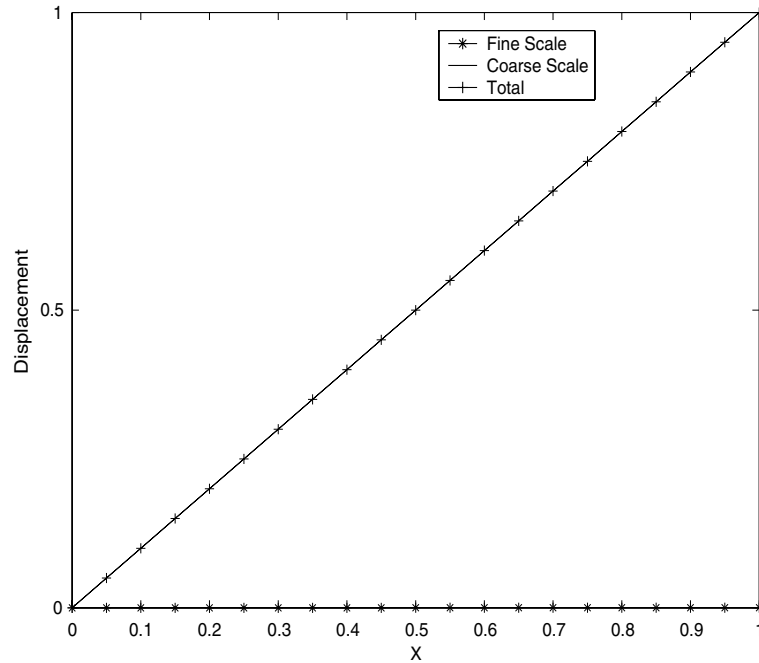


Fig. 1. Effect of multi-scale projection matrix \mathbf{P} if MD displacement field is linear. Linear finite element basis used.

the atomistic system, and apply the projection matrix \mathbf{P} to \mathbf{q} to obtain the coarse scale (continuum) displacement field as dictated by (9). For the FE shape functions \mathbf{N} , linear polynomials are used. According to the statement made above, the coarse scale displacement field should exactly match the MD displacement field because the FE shape functions are the same order as the MD displacement field. As shown in Fig. 1, this is indeed the case, i.e. the FE shape function basis contains a linear description, so the projected solution matches exactly.

However, if the FE basis does not contain the MD displacement field, then the projected FE solution will not capture the entire MD solution. This is seen in our second example. In this case, the MD displacement field \mathbf{q} was defined to be quadratic, while the FE shape functions \mathbf{N} which comprise \mathbf{P} were kept as linear. As shown in Fig. 2, the FE (coarse scale) solution does not match the MD quadratic displacement field for this case. Instead, the projected FE displacement field minimizes the least squares error between the linear FE and quadratic MD displacement fields.

3. Continuum temperature equation

In this section, we derive a continuum temperature equation directly from the microscopic definition of temperature. The idea is motivated by work done by Wagner [4]. In order to do so, we first summarize the MD notions of temperature. According to the equipartition formula [5], the MD *system* temperature T is directly related to the MD system kinetic energy K by assuming that each degree of freedom has an average kinetic energy of $k_B T/2$, i.e.

$$K = \frac{N_{sd}}{2} N k_B T, \quad (14)$$

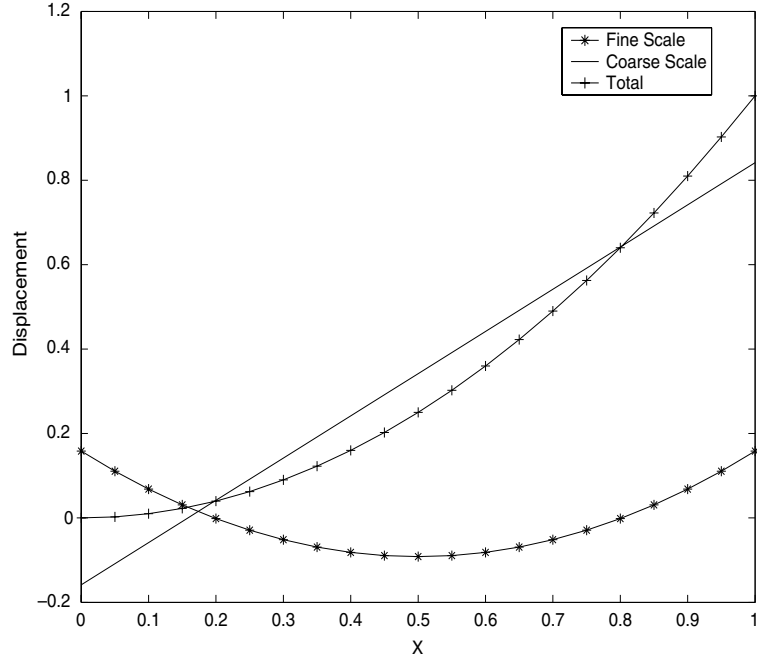


Fig. 2. Effect of multi-scale projection matrix \mathbf{P} if MD displacement field is quadratic. Linear finite element basis used.

where N_{sd} is the number of spatial dimensions in the problem, N is the number of atoms in the system, and k_{B} is the Boltzmann constant. Therefore, the temperature associated with an atom α undergoing 1D motion is given by

$$T_{\alpha} = \frac{m_{\alpha}}{k_{\text{B}}} \dot{q}_{\alpha}^2, \quad (15)$$

where m_{α} is the mass of atom α and \dot{q}_{α} is the velocity of atom α . In order to derive the coarse scale temperature equation, we will use the bridging scale projection matrix \mathbf{P} to project the temperature of each atom. Applying \mathbf{P} to the right-hand side of (15) and denoting \mathbf{T} to be a vector of the individual atomic temperatures, we obtain

$$\mathbf{T} = \mathbf{P} \left(\frac{1}{k_{\text{B}}} \mathbf{M}_{\text{A}} \mathbf{g} \right), \quad (16)$$

where \mathbf{M}_{A} is a diagonal matrix of the atomic masses and the components of \mathbf{g} and $\dot{\mathbf{q}}$ are related by $\dot{q}_i^2 = g_i$. We next approximate the atomistic temperature using FE shape functions as $\mathbf{T} = \mathbf{N}\boldsymbol{\theta}$, where $\boldsymbol{\theta}$ are the nodal temperatures. Expanding the projection operator according to (8) and pre-multiplying both sides by $\mathbf{N}^{\text{T}}\mathbf{M}_{\text{A}}$ gives

$$\mathbf{N}^{\text{T}}\mathbf{M}_{\text{A}}\mathbf{N}\boldsymbol{\theta} = \frac{1}{k_{\text{B}}}\mathbf{N}^{\text{T}}\mathbf{M}_{\text{A}}\mathbf{N}\mathbf{M}^{-1}\mathbf{N}^{\text{T}}\mathbf{M}_{\text{A}}(\mathbf{M}_{\text{A}}\mathbf{g}). \quad (17)$$

Using (5), the final form of the temperature equation can be written as

$$M_{IJ}\theta_J = \frac{1}{k_{\text{B}}}\sum_{\alpha} N_I(X_{\alpha})m_{\alpha}^2\dot{q}_{\alpha}^2, \quad (18)$$

where the summation is performed for all atoms α , and the subscripts I and J indicate FE nodal values. Eq. (18) is the major result of this section, and states that a continuum temperature field can be directly acquired from an underlying MD simulation, with the only MD values needed being the atomic masses, atomic velocities and Boltzmann constant. The only necessary continuum variables are the FE shape functions. The key point was to apply the bridging scale projection matrix \mathbf{P} to the atomic temperature field. The resulting continuum temperature is a least squares fit of the underlying atomistic temperature field.

3.1. Numerical validation of temperature equation

In this section, we examine the performance of (18) on two simple 1D problems. These examples, and all future examples in this work are based upon two 1D examples. The first example is taken from the paper by Wagner and Liu [3]. In this problem, atoms cover the x -axis between $x = -1.5$ and $x = 1.5$. A Gaussian-type wave is prescribed as the initial displacement, and is centered around $x = 0$. We shall refer to this problem as the “Gaussian wave” problem. The initial MD configuration for this problem is shown in Fig. 4.

The second benchmark we will use consists of a chain of atoms between $x = 0$ and $x = 1$. In this benchmark, only the left most atom at $x = 0$ is given an initial displacement. The displacement then propagates into the chain of atoms. We shall refer to this problem as the “unit pulse” problem. The initial MD configuration of this problem is depicted in Fig. 3. In these problems, the domain is covered with both atoms and finite elements, i.e. the finite element representation exists everywhere the MD representation exists.

For the MD simulations, a quadratic potential energy function ϕ which is a function of the *relative* displacements Δx between atoms is used

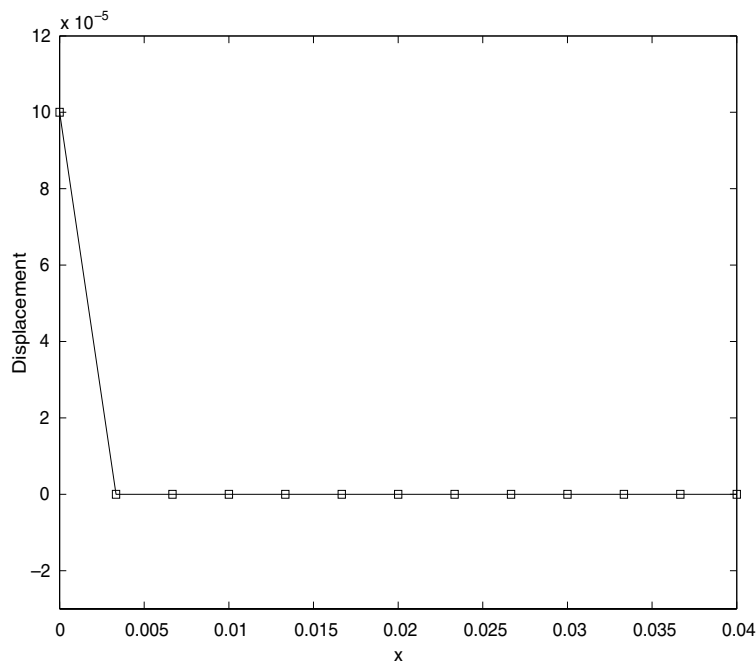


Fig. 3. Initial MD configuration for unit pulse problem.

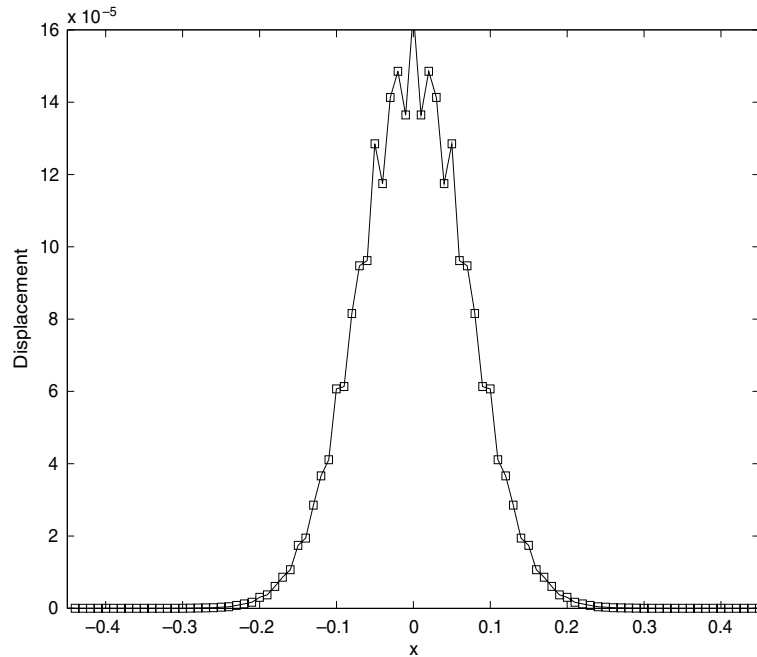


Fig. 4. Initial MD configuration for Gaussian wave problem.

$$\phi = \frac{1}{2}k\Delta\mathbf{x}^2, \quad (19)$$

where k is the spring constant. Minimizing this potential leads to a linear spring force relation between the atoms

$$\mathbf{f} = -k\Delta\mathbf{x}. \quad (20)$$

The MD equations of motion are integrated forward in time using a velocity verlet algorithm. Details on this algorithm can be found in [5]. In the following examples, the atomic masses and the spring constant are both assumed to be unity.

For the first verification example, we show two cases in which the number of FE nodes equals the number of atoms in the system. The goal is to show that when the FE mesh is refined down to the atomic spacing, the temperature as would be calculated for each individual atom is the same as that calculated using the temperature equation (18). The Gaussian wave problem was run using 301 atoms and 301 FE nodes, while the unit pulse problem was run with 101 atoms and 101 FE nodes. The results of both problems are shown in Figs. 5 and 6

$$T_{\text{elem}} = \sum_{\alpha=1}^{n_{\text{atom}}} \frac{m_{\alpha} v_{\alpha}^2}{Nk_{\text{B}}}. \quad (21)$$

The temperature of the FE nodes is within machine precision to that calculated for each atom using (21), proving that the temperature equation (18) yields a convergent solution when the FE nodal spacing equals the atomic spacing. For this example and all future examples, the MD temperature is assumed to be a constant within each finite element, and is computed by averaging over all the atoms within the element according to (21). The FE temperature is also calculated as a constant within each element by averaging the nodal values obtained from (18). A better way to compare the continuum and atomistic temperature fields

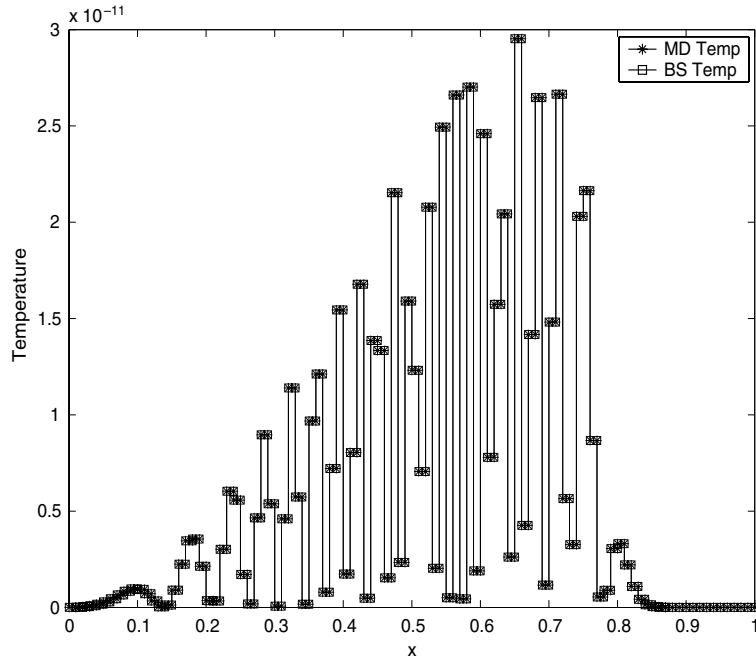


Fig. 5. Temperature comparison between finite element nodes and individual atoms for unit pulse problem with same number of nodes as atoms.

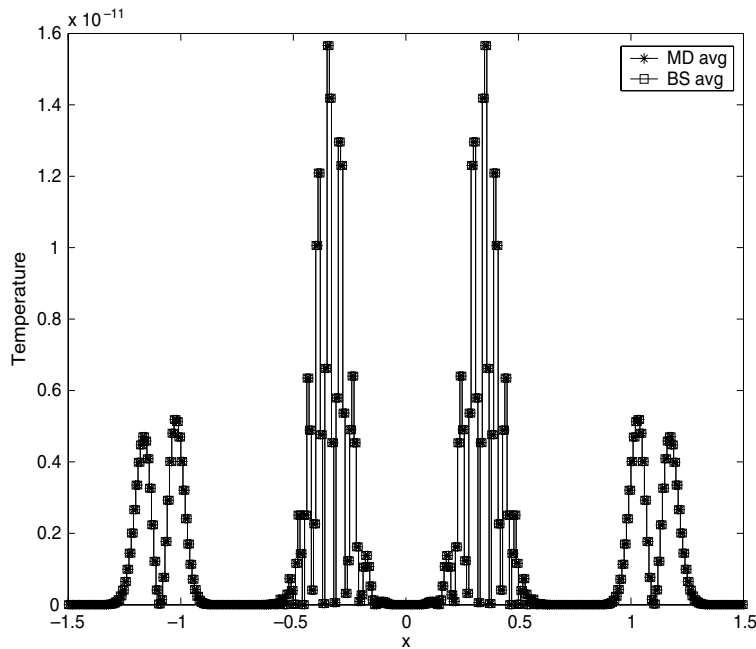


Fig. 6. Temperature comparison between finite element nodes and individual atoms for Gaussian wave problem with same number of nodes as atoms.

would be to calculate a continuous continuum temperature field using meshfree shape functions such as the Reproducing Kernel Particle Method (RKPM) [6], but this approach demands a separate inquiry. For future examples, because the usage of such a refined FE mesh is generally impractical, we continue our numerical studies using coarser meshes.

The initial pulse problem was simulated using 30 finite elements and 301 atoms, which gives 11 atoms per element. The comparison for the continuum temperature and MD temperature is shown in Fig. 7. Here, it is shown that the measured continuum temperature is very close to the average MD temperature for each finite element. One may notice the very small temperature (order 10^{-12}) calculated for this example. The reason for this is that the frequency ω is unity for this example, as the mass and spring constants are both unity as well. Furthermore, the MD velocities are quite small as well (order 10^{-5}). Using different constants and a more realistic problem will give a larger measured temperature.

One possible issue with the temperature equation is that the results are better if the MD velocity field is somewhat regular, or smooth. This manifests itself in Fig. 8 at the tip of the propagating wave. The velocity field behind the front has a regular, decreasing pattern. Furthermore, the MD velocities in this region all have a similar absolute value. At the front, however, the velocity field changes from being somewhat small in magnitude to being fairly large in magnitude rather abruptly. The inability to capture this gradient in velocity is shown by the inaccuracies in temperature near the wave front.

The Gaussian wave benchmark was also run in order to explore the performance of the temperature equation. The results can be seen in Figs. 9 and 10. For this case, 301 atoms and 30 finite elements were used, giving 11 atoms in each finite element. This figure again shows the phenomena described above. In the region from $x = 0$ to $x = 0.5$, the MD velocity is clustered, but the absolute values of the velocities are similar. Therefore, the calculated coarse scale temperature using (18) yields fairly good results in this section. However, in the spatial region from $x = 0.8$ to $x = 1.3$, a velocity gradient appears, as the profile

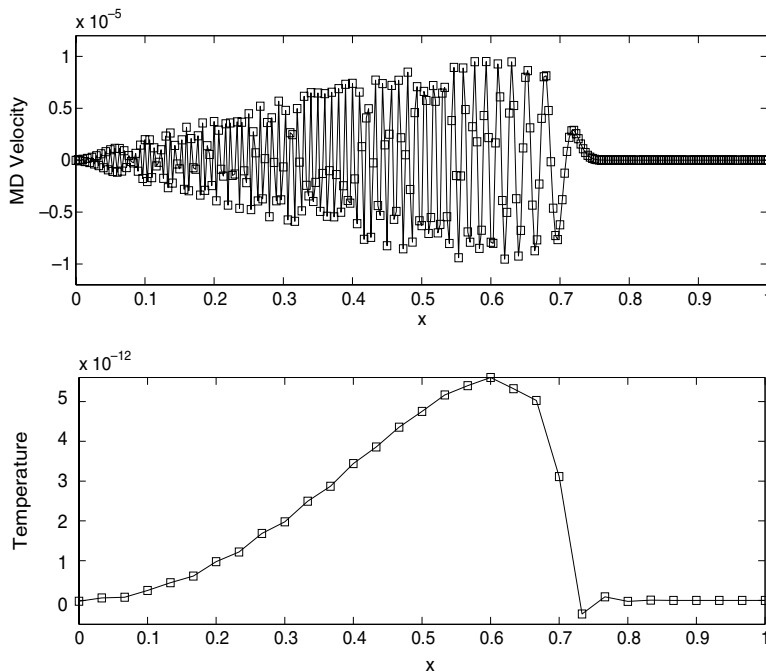


Fig. 7. MD velocity profile and calculated nodal temperature for unit pulse problem.

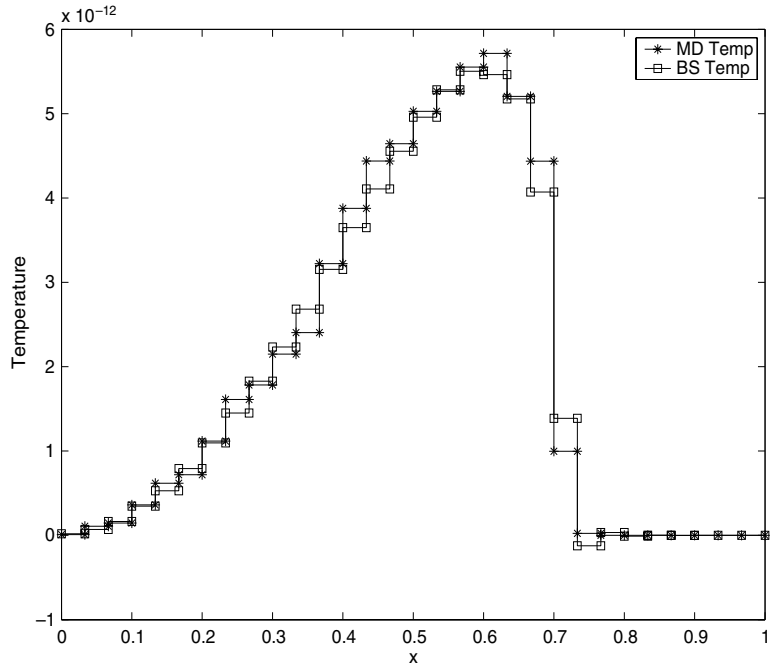


Fig. 8. Temperature calculated using (18) for the coarse scale as compared to the calculated MD temperature from (21) for unit pulse problem.

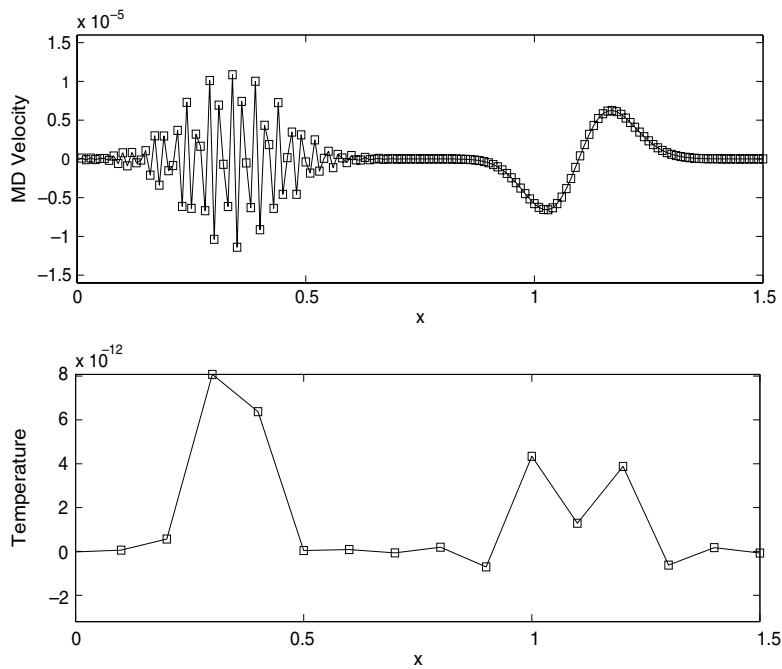


Fig. 9. MD velocity profile and calculated nodal temperature for Gaussian wave problem.

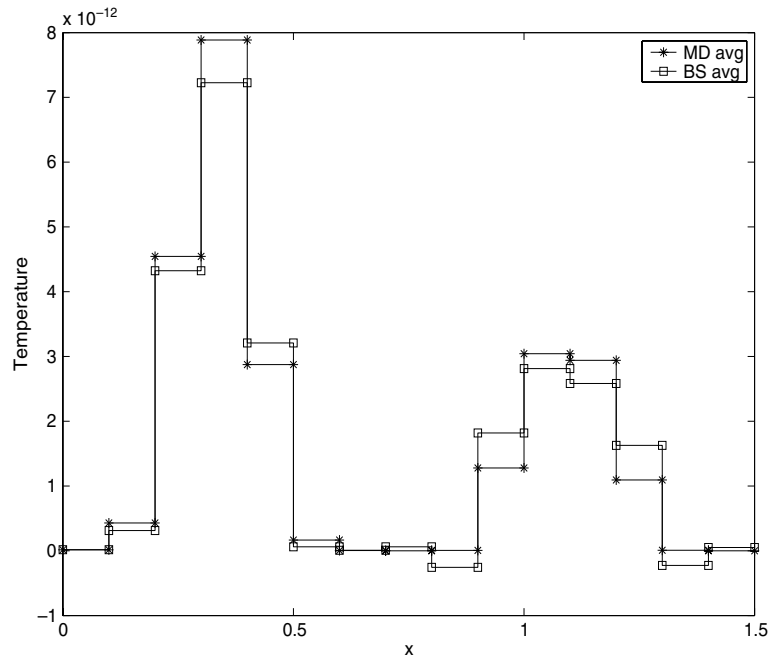


Fig. 10. Temperature calculated using (18) for the coarse scale as compared to the calculated MD temperature from (21) for Gaussian wave problem.

assumes first a negative pulse form and then a positive pulse form. Because this velocity gradient covers multiple elements, it introduces a slight amount of error. More accurate results are obtained if the gradient is confined to one element only.

3.2. Need for coarse scale MD

The numerical examples of the previous section were all performed with the continuum completely overlapping the MD region. However, in most realistic multiple-scale problems, the MD region will only constitute a small portion of the problem domain, while the continuum will cover the bulk of the domain. Therefore, in order to solve (18) in the continuum region, it is necessary to extend the MD solution into the coarse scale region. We shall accomplish this by a method in which the MD solution in the coarse scale can be found as a generalized function of the boundary atom displacements.

4. Coarse scale MD representation

In this section, the methodology for extending the MD solution into the coarse scale so that the temperature equation (18) can be solved globally is derived. The general approach to solving this problem was addressed in [7,8]. The goal of the approach is to replace the actual MD solution in a certain part of the lattice with a boundary condition on one or more parts of the lattice that properly accounts for the effects of the removed lattice. Pictorially, as seen in Fig. 11, the removed part of the lattice would be all atoms numbered $n > 0$. The boundary condition accounting for the motion of the removed atoms would be applied as a force on atom 0 by means of a time history kernel. The difference between the evolution

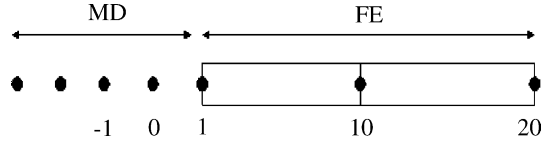


Fig. 11. Pictorial depiction of linearized MD solution, which allows the solution of atoms $n > 0$ based on the displacement of atom 0.

function in this work and the time history kernel derived in [3,7,8] is that in this work, the motion of *any* atom $n > 0$ is found as a function of the motion of atom 0, whereas in the previous works, only the motion of atom 1 in terms of atom 0 was considered.

We now derive the extended MD solution in the coarse scale by first writing the linear equation of motion for an arbitrary atom n

$$\ddot{u}_n - \omega^2(u_{n-1}(t) - 2u_n(t) + u_{n+1}(t)) = m^{-1}f_n(t), \tag{22}$$

where $\omega = \sqrt{\frac{k}{m}}$, k is an elastic spring constant, m is the mass of each atom and f_n is an external force applied to atom n . Writing the equation of motion in this manner implies that the atoms are interacting via the quadratic (harmonic) potential described previously in (19). Applying both a Laplace transform and a discrete Fourier transform to (22) while assuming that the initial velocity and displacements are zero gives

$$s^2\hat{U}(p,s) - \omega^2(e^{-ip}\hat{U}(p,s) - 2\hat{U}(p,s) + e^{ip}\hat{U}(p,s)) = m^{-1}\hat{F}(p,s), \tag{23}$$

where p indicates dependence on Fourier transformed space and s indicates dependence on Laplace transformed space. In deriving (23), we have utilized a property of Fourier transforms called the shifting theorem, which states that

$$\mathcal{F}\{x_{n+a}\} = e^{iap}\hat{x}(p), \tag{24}$$

where a is an integer. Using (24), we define

$$\hat{G}(p,s) = (s^2 - \omega^2(e^{-ip} - 2 + e^{ip}))^{-1}. \tag{25}$$

We shall assume that the coarse scale motion (atoms $n > 0$) is caused by a virtual external load on atom $n = 0$, which implies that $\hat{F}(p,s) = \hat{F}(s)$. The elimination of the dependence of \hat{F} on p arises due to the fact that we are considering a 1D example. Using this assumption along with (25) gives the transform solution of (23)

$$\hat{U}(p,s) = \hat{G}(p,s)F(s). \tag{26}$$

Taking the inverse Fourier transform of (26) gives

$$U_n(s) = G_n(s)F(s). \tag{27}$$

In order to obtain the displacement for an arbitrary atom $n > 0$, we solve (27) for $F(s)$ setting $n = 0$ giving

$$F(s) = G_0^{-1}(s)U_0(s). \tag{28}$$

Substituting (28) into (27) gives the general expression for the displacement of an arbitrary atom $n > 0$ in terms of the displacement of boundary atom 0 to be

$$U_n(s) = G_n(s)G_0^{-1}(s)U_0(s), \tag{29}$$

where we define the Laplace transform of the evolution function $w_n(t)$ to be

$$W_n(s) = G_n(s)G_0(s)^{-1}. \tag{30}$$

Applying an inverse Laplace transform on (29), we obtain

$$u_n(t) = \int_0^t w_n(t - \tau)u_0(\tau) d\tau, \quad (31)$$

which holds for all $n > 0$. Therefore, the important task is to evaluate $W_n(s)$ in (30). In order to do so, we take the inverse Fourier transform of (25) to obtain

$$G_n(s) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{ipm}}{s^2 - \omega^2(e^{ip} - 2 + e^{-ip})} dp. \quad (32)$$

Evaluating the integral for $G_n(s)$ in (32) gives

$$G_n(s) = \frac{(\sqrt{s^2 + 4\omega^2} - s)^{2n}}{(2\omega)^{2n}s\sqrt{s^2 + 4\omega^2}}. \quad (33)$$

Thus, the desired result for $W_n(s)$ reads

$$W_n(s) = \frac{(\sqrt{s^2 + 4\omega^2} - s)^{2n}}{(2\omega)^{2n}}. \quad (34)$$

The inverse Laplace transform of (34) can be evaluated from a standard table of Laplace transforms, and gives the evolution function $w_n(t)$ to be

$$w_n(t) = 2n \frac{J_{2n}(2\omega t)}{t}, \quad (35)$$

where J_{2n} is a Bessel function of order $2n$. Since we are more concerned about finding the time derivatives of the MD displacement such that the temperature equation may be evaluated in the coarse scale, we differentiate (31) in time to give

$$\dot{u}_n(t) = w_n(0)u_0(t) + \int_0^t \dot{w}_n(t - \tau)u_0(\tau) d\tau = \int_0^t \dot{w}_n(t - \tau)u_0(\tau) d\tau \quad (36)$$

so that the atomic velocities at any arbitrary coarse scale point outside the MD region can be calculated. A closed form expression for $\dot{w}_n(t)$ is available by direct differentiation of (35), which gives

$$\dot{w}_n(t) = -\frac{2n}{t^2} J_{2n}(2\omega t) + \frac{2n\omega}{t} (J_{2n-1}(2\omega t) - J_{2n+1}(2\omega t)). \quad (37)$$

Eqs. (37) and (35) are the major results of this section. They state that the MD displacements, velocities and accelerations (which can be calculated by differentiating (37) with respect to time) can be found at any point outside the MD domain. Furthermore, the only required values are a time history of the boundary atom displacement and the value of the velocity or displacement evolution function, which have both been derived in closed form. The final important implication is that because the MD velocities can now be calculated in the coarse scale, the continuum temperature equation (18) can be solved globally, in both the MD and coarse scale regions. The method for doing so will be described in a later section.

Within the MD time loop, the only operation needed to calculate the coarse scale MD velocity $\dot{u}_n(t)$ is a simple matrix-vector multiplication. The size of the matrix $\dot{w}_n(t)$ depends upon the number of coarse scale points the MD solution is desired at along with the number of time history points that are stored. Fortunately, $\dot{w}_n(t)$ can be evaluated before the MD time loop begins, because it is known in advance how many MD timesteps will be used for the simulation. This is advantageous because the expensive computations occur only once; the stored values are then used throughout the MD time loop. Furthermore, if the displacements/velocities are only required at integration points in the coarse scale, then the size of the matrix $\dot{w}_n(t)$ will be decreased dramatically. This point motivates the work done in the next section.

4.1. Validation of extended MD solution

In order to validate the coarse scale MD solution derived in the previous section, we again use our two model problems, the “Gaussian wave” and “unit pulse” problems. For both problems, we calculate the entire MD solution. We then calculate the extended MD solution according to (35) and compare it to the full MD solution of the system.

The results from the Gaussian wave problem and the unit pulse problem are shown in Figs. 12 and 13, respectively. The Gaussian wave was run with 301 atoms, while the unit pulse was run with 101 atoms. For the Gaussian wave problem, the velocities for the atoms between $x = 0.31$ and $x = 1.5$ were found as a function of the displacement of the atom at $x = 0.3$. For the initial pulse problem, the velocities of all atoms between $x = 0.21$ and $x = 1$ were found as a function of the displacement of the atom at $x = 0.2$. As can be seen, the agreement between the direct MD solution and the extended MD solution is excellent. We emphasize the accuracy of the extended MD solution in calculating the velocities because that is the quantity of interest in evaluating the coarse scale temperature equation. The extended MD solution can also be shown to be similarly accurate for displacements and accelerations.

4.2. Coarse scale temperature equation using extended MD solution

As was discussed above, our motivation to obtain an MD solution in the coarse scale was such that the continuum temperature equation (18) could be solved globally. With an accurate MD solution now available at arbitrary points in the coarse scale via the methodology discussed in the previous section, we can approximate the temperature equation correspondingly.

To solve the temperature equation in the coarse scale, we can replace the summation in (18) by an integration *in the coarse scale only* as

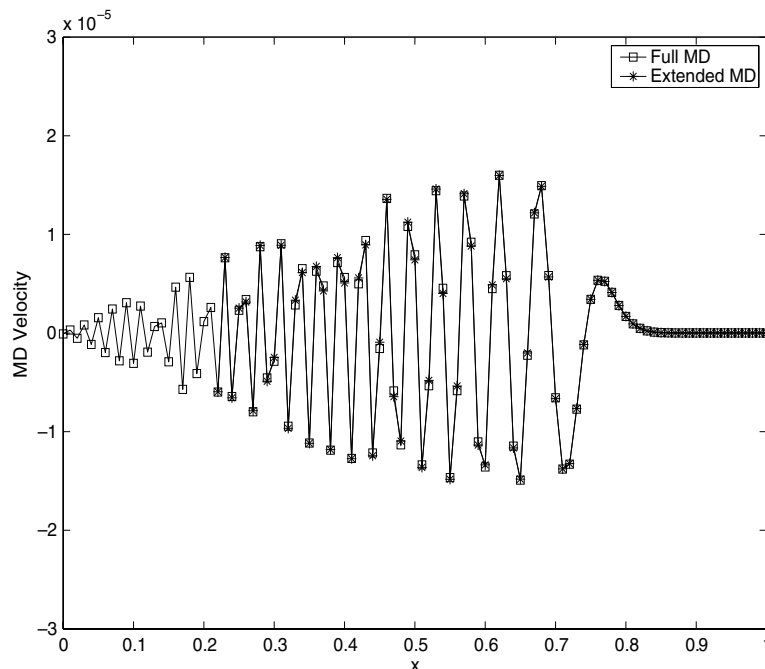


Fig. 12. Direct MD/extended MD velocity comparison for unit pulse problem.

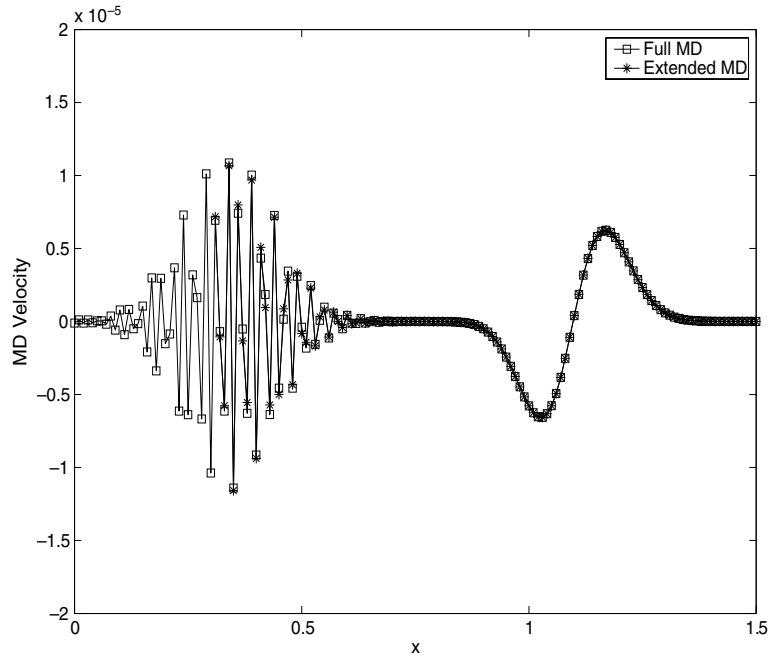


Fig. 13. Direct MD/extended MD velocity comparison for Gaussian wave problem.

$$M_{IJ}\theta_J = \frac{1}{k_B} \int_V N_I(\mathbf{X})m(\mathbf{X})^2 \dot{q}(\mathbf{X})\dot{q}(\mathbf{X}) dX. \tag{38}$$

In practice, this would be accomplished numerically by summing over a discrete set of quadrature points at locations X_n

$$M_{IJ}\theta_J = \frac{1}{k_B} \sum_n N_I(X_n)m(X_n)^2 \dot{q}(X_n)^2 b_n, \tag{39}$$

where b_n is the quadrature weight associated with point X_n . The extended MD solution is used to generate the MD velocities $\dot{q}(X_n)$ at the coarse scale quadrature points. We intentionally use the notation n with reference to the point X_n to emphasize the fact that these points correspond to the arbitrary coarse scale points n described in (36). In deriving (39), we have implicitly assumed that all the atoms in the system have the same mass; this assumption can easily be fixed to represent atoms of different masses.

5. Numerical examples using extended MD solution and coarse scale temperature equation

To verify (39), we again solve the Gaussian wave problem. For the domain between $x = -1.5$ and $x = 0.5$, full atomistic resolution was used, and Eq. (18) was solved. In the region from $x = 0.5$ to $x = 1.5$, the coarse scale approximation (39) was solved using the extended MD solution at the coarse scale quadrature points according to (37). 15 finite elements were used with 301 atoms, giving 21 atoms per finite element. For the coarse scale approximation using (39), two quadrature points per element were used.

A comparison between the direct MD/FE solution and the MD/extended MD/FE solution is given in Figs. 14 and 15, and also Figs. 16 and 17. The results show that the combined MD/extended MD solution

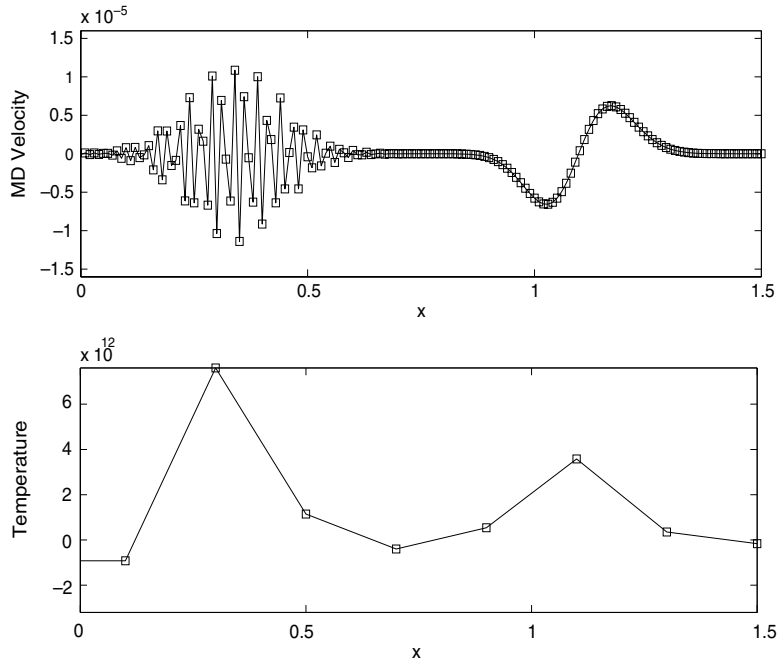


Fig. 14. Direct MD velocity profile along with calculated coarse scale temperature from solving (18) everywhere for Gaussian wave problem.

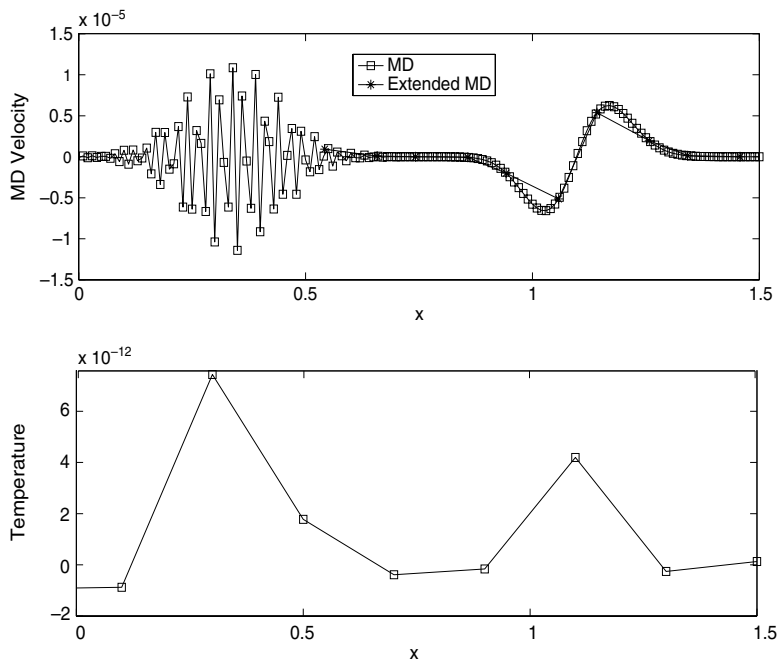


Fig. 15. MD + extended MD velocity profile along with coarse scale temperature comparison using combination of (18) and (39) for Gaussian wave problem.

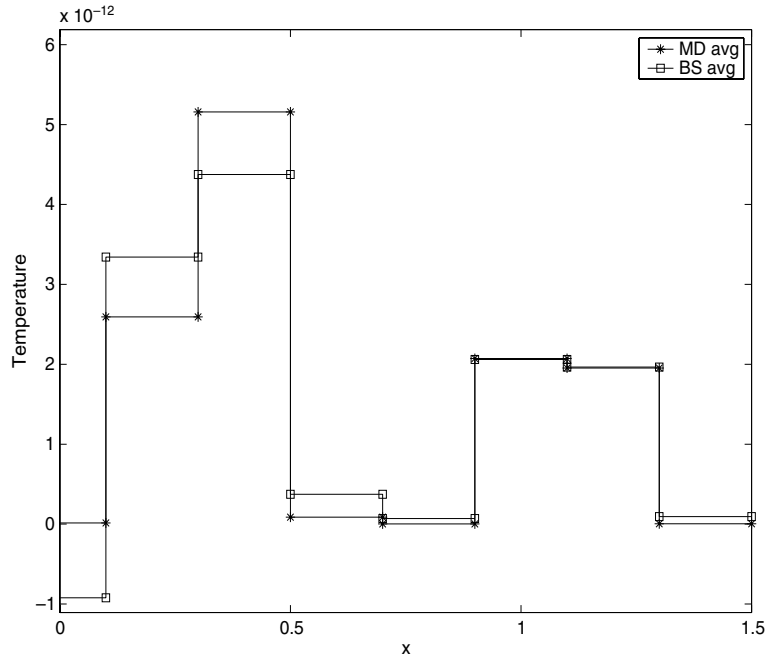


Fig. 16. Temperature calculated comparing direct MD and solving (18) everywhere for Gaussian wave problem.

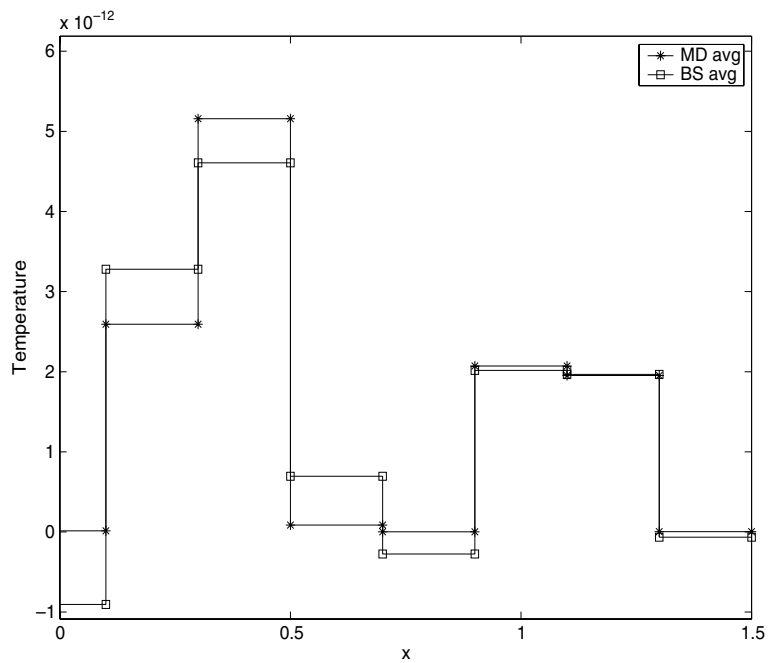


Fig. 17. Temperature calculated using combination of (18) and (39) for Gaussian wave problem.

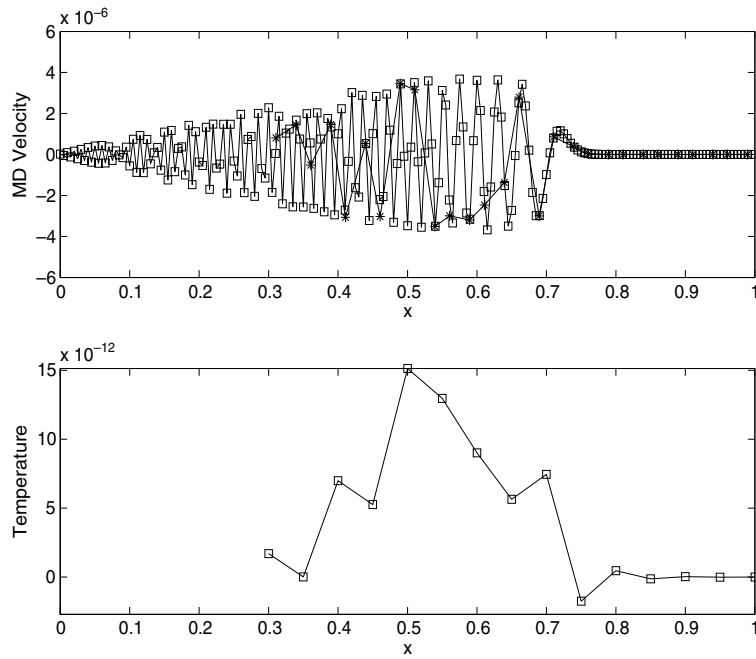


Fig. 18. Extended MD velocity profile along with calculated coarse scale temperature for unit pulse problem.

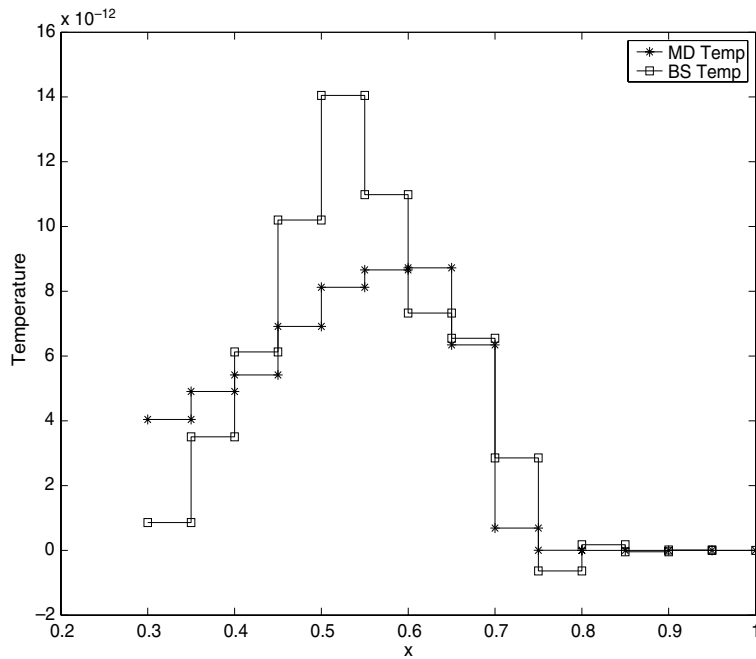


Fig. 19. MD and bridging scale temperature comparison using coarse scale temperature approximation (39) for unit pulse problem.

does not differ greatly to the direct MD/FE solution, validating the coarse scale approximation (39) for certain types of problems.

Caution should be used in applying the coarse scale temperature equation (39). If the MD velocity is rough, and exhibits large spatial gradients, then (39) will not capture the gradients accurately because too few sampling points are used. An analogy can be drawn to deficiencies in finite element analysis of strain localization. Because the stress field changes rapidly across a shearband, finite elements cannot capture this rapidly changing field unless many elements are used, or the elements are embedded with special fields to capture the stress gradients. The errors that can be introduced by insufficient spatial resolution is shown via the unit pulse problem in Figs. 18 and 19.

6. Conclusion

There have been two major thrusts in this work. The first was to derive a continuum temperature equation for use in coupled continuum/atomistic simulations. The temperature equation is derived by using the bridging scale projection operator to project the microscopic temperature field to the continuum. From that point, only standard simulation variables such as the atomic masses, atomic velocities, Boltzmann constant and finite element shape functions are necessary to solve the equation. The equation was shown to give identical results to the actual MD temperature if the FE nodal spacing was the same as the atomic spacing. In the remaining numerical examples, the equation was shown to give an accurate comparison to the actual MD temperature when the elements were much larger than the atomic spacing in two 1D example problems.

While the temperature equation gives an excellent comparison to MD if the atomistic/continuum regions overlap each other completely, the necessity to solve the temperature equation globally motivated the second major thrust of this work, the extended (coarse scale) MD solution described in Section 4. In this approach, the MD variables of interest could be calculated in the coarse scale as a function of the MD boundary atom displacement by means of an evolution function, which serves as an extended version of the time history kernel defined in [3,7,8]. Furthermore, the evolution functions were determined analytically for a 1D lattice, and fully describe the temporal and spatial evolution of the atomic lattice. It was shown in example problems that the MD displacements calculated using this approach were nearly identical to those calculated using a direct MD simulation. This approach can be extended to multiple dimensions, where the evolution function can be found using numerical methods for Fourier and Laplace transform inversion, e.g. [9].

The final numerical examples presented herein used the coarse scale MD velocities to solve the temperature equation. These velocities were evaluated at coarse scale integration points, such that the number of atoms sampled could be reduced from the full system size. It was demonstrated that when the velocity field is sufficiently smooth, this approximation can be used to give accurate measurements for the temperature field.

The future success of this approach will likely hinge on the ability to couple the temperature equation derived herein with the standard continuum energy equation. As was shown, the temperature equation offers a simple and accurate measurement of the underlying microscopic temperature. The continuum energy equation could be solved in the coupled MD/FE region, but would require the determination of additional material constants. Though one can obtain such constants directly from an MD simulation [10], this would constitute a brute-force approach. Therefore, further research needs to be done such that the temperature equation presented here is solved in the coupled MD/FE region, the continuum energy equation is solved in the coarse scale, and the two equations are coupled in some manner. Currently, we believe the most viable approach is to calculate a heat flux from the temperature equation to use as a boundary condition for the continuum energy equation. If it is desired to solve the temperature equation

(18) for the entire system, the temperature calculated in the coarse scale could be used as an input to coarse scale constitutive relations, such that a thermomechanical coupling in the continuum is achieved.

We close by noting that while the MD example problems in this work were restricted to the use of a linear spring force relation, the temperature equation retains its validity when nonharmonic potentials are used to describe the interatomic forces.

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