Numerical Studies of a Coarse-grained Approximation for Dynamics of an Atomic Chain

Ping Lin * and Petr Plecháč †

Abstract

In many applications materials are modeled by a large number of particles (or atoms) where each particle interacts with all others. Near or nearest-neighbor interaction is considered to be a good simplification of the full interaction in the engineering community. However, the resulting system is still too large to be solved using the existing computer power. In this paper we shall use the finite element and/or quasicontinuum idea to both position and velocity variables in order to reduce the number of degrees of freedom. The original and approximate particle systems are related to the discretization of the virtual internal bond model (continuum model). We focus more on the discrete system since the continuum description may not be physically complete as the stress-strain relation is not monotone and thus not necessarily well-posed. We provide numerical justification on how well the coarse-grained solution is close to the-fine grid solution in a temporal average sense.

Descriptive title: Numerical studies of coarse-grained dynamics.
Keywords. Lattice dynamics, particle system, Lennard-Jones potential, finite element method, quasi-continuum approximation.
AMS(MOS) subject classifications. 65C20, 65K10, 65M15, 65M60, 73S10, 73V20.

1 Introduction

The atomic modeling has become an active research area since many practical problems involve microscopic features, such as dislocation and fracture dynamics of materials (see, e.g., [10, 11, 34, 6, 28, 26]). To study these problems we are compelled to consider effects at the scale of lattice. Directly solving the whole system at the atomistic scale (e.g. in the lattice equilibrium or the molecular dynamics) provides a powerful and accurate tool for the analysis of microscopic features. However, because the number of particles (or atoms) in a specimen is huge, it is often impossible to solve the full particle system using the existing computer power. Even if the computational power continues to grow with the present rate it will not be possible to conduct full ab-initio simulations on a specimen of the size relevant for engineering applications. The limiting factors of large number of particles and even larger number of interactions prompted development of methods and methodologies that design coarse-grained models computationally. Several approaches have been proposed and intensively explored in recent years both in materials simulations and theoretical studies, most notably the quasicontinuum method, [34, 23, 17], the coarse-grained molecular dynamics, [29, 27], the heterogeneous multi-scale method, [7, 8], the

*Department of Mathematics, The National University of Singapore, Singapore 117543 (e-mail: matlinp@math.nus.edu.sg).
†Department of Mathematics, University of Tennessee, Knoxville, TN 37996-1300, USA (e-mail: plechac@math.utk.edu).
bridging scale method, [35]. Related approaches have been proposed for simulations involving stochastic systems ([5, 16, 15]) but in this paper we focus on deterministic, molecular dynamics simulations only.

The problem is often simplified by only considering the interaction of one particle with its nearby particles (or even its nearest neighbors). It is believed that the simplified model is a good approximation to the original problem. Nevertheless, even for the simplified problem the system is still huge and impossible to be solved directly. The quasicontinuum approximation gains noticeable attention in engineering literatures (cf. [18, 2, 34]). The principal idea is that in the region where no defect occurs the material is modeled at the macroscopic scale and the theory of continuum elasticity may apply. The approach enables a systematic treatment of lattice defects should these defects arise and exhibits a continuous transition from the lattice to the continuum realms at intermediate length scales. The larger scales are incorporated with the finite element method and they are expected to provide an approximation of the full lattice-scale model. This approximation method has been recently shown to be successful in simulation of materials properties in engineering literature. Also its numerical analysis has been attempted in [20, 3, 8, 21, 9, 12, 24, 25]. There are generalizations of the method to dynamical cases ([10, 22, 29, 27]) but careful numerical or mathematical studies are still in its infancy. In this paper we would like to provide a numerical study of a one-dimensional material. More rigorous analysis will be presented elsewhere later.

We consider a simple 1D model of a crystalline material where \( N \) atoms are distributed on a straight line. Let \( u_i, \ i = 0, 1, \ldots , N \), denote the position in the deformed configuration of the \( i \)-th atom and \( W_{ij}(u_{ij}) \) denote the interaction potential between atoms \( i \) and \( j \), where \( u_{ij} = |u_i - u_j| \). We assume that the energy functions \( W_{ij} \) between any two atoms are all the same and denote it as \( W \). In the simplest models the potential used is the so called Lennard-Jones potential

\[
W(r, r_0) = \frac{A}{4} \left[ -2 \left( \frac{r_0}{r} \right)^6 + \left( \frac{r_0}{r} \right)^{12} \right],
\]

where \( r_0 \) represents the point where the potential function \( W \) attains its minimum. Figure 1 sketches the graph of the energy function. This type of a potential captures several features (non-convex region, singularity) that are computationally relevant and therefore we adopt it in our studies as a simple first approximation.

The 1D particle system is depicted in Figure 2 below. Denoting \( \dot{u}_i \equiv du/dt \) the velocity of
the i-th particle we obtain the total (classical) energy of the chain

\[ H = \sum_{i=0}^{N} \frac{1}{2} \dot{u}_i^2 + \frac{1}{2} \sum_{i=0}^{N} \sum_{j=0,j\neq i}^{N} W(|u_i - u_j|, r_0), \]  

(2)

where the mass of each atom is scaled to one (or absorbed into the definition of the potential function \( W \)). In [4] a few examples of the coefficient \( A \) for the Lennard-Jones potential are given and they are of order \( r_0 \), which is approximately the mass of an atom. Thus after the scaling the coefficient of \( W \) is approximately of the order one. Furthermore, we assume that each atom only interacts with its nearest neighbors. Since the potential function decays fast, see [4], the nearest-neighbor-interaction system is generally expected to be a good approximation to the system that accounts for interactions between all atoms (see [20] for a proof of a special case). In the case of the nearest-neighbor interaction the non-deformed (reference) location of the i-th atom is \( X_i = ir_0 \) if setting \( X_0 = 0 \). We also assume that the atomic chain satisfies certain boundary conditions, e.g.,

\[ u_0 = 0, \quad u_N = a. \]  

(3)

The total energy for this simplified system is

\[ H = \frac{1}{2} \sum_{i=0}^{N} \dot{u}_i^2 + \sum_{i=1}^{N} W(u_i - u_{i-1}, r_0). \]  

(4)

The molecular dynamics model is then obtained from the Hamilton equations

\[ \ddot{u}_i = \frac{1}{r_0} \left[ \sigma \left( \frac{u_{i+1} - u_i}{r_0} \right) - \sigma \left( \frac{u_i - u_{i-1}}{r_0} \right) \right], \quad i = 1, \ldots, N - 1, \]  

(5)

where the function \( \sigma(F) = \frac{dW(F,1)}{dF} \). We define \( x_N = Nr_0 \) to be the non-deformed length of the one-dimensional material and we assume that \( x_N \) is a finite number.

The model consists of a large number of particles. Various methods have been developed to reduce the number of degrees of freedom in this description. We focus on one specific approach that has a direct connection to quasicontinuum approximation. In [10] (see also [22, 19]) a continuous model is developed based on hyperelasticity theory where the particle interaction potential is involved in computing the total energy of the system. The model is then called

**Figure 2:** The one dimensional atomic chain.
virtual internal bond model (VIB). A coarse grid may be used to solve the continuous equation and thus to reduce the size of the system. In 1D (see also [10, 22] for a description of multidimensional cases), the bond stretch \( r = F(x)r_b \), where \( r_b \) is the bond length (i.e. zero force distance, for example, \( r_b = r_0 \) in the case of the Lennard-Jones potential), \( F = \frac{\partial \phi(x,t)}{\partial x} \) and \( \phi(x,t) \) is the mapping which defines the deformation of the material point \( x \in [0, x_N] \) at the time \( t > 0 \). The continuum energy per unit length is considered (see [10, 11]) as a sum over all possible bond length \( r_b \) which can be written as

\[
\Theta = \int_0^\infty D(r_b)W(r, r_b) \, dr_b = \int_0^\infty D(r_b)W(F, 1) \, dr_b,
\]

where \( D(r_b) \) is the bond (a pair of atoms with zero force distance \( r_b \)) density per unit non-deformed length of the material and depends only on \( r_b \) in 1D. Thus, \( \Theta \) is a function of \( F \) and

\[
\Theta(F) = \alpha W(F, 1),
\]

where \( \alpha = \int_0^\infty D(r_b)dr_b \). For the simple atomic chain we consider in this paper all atoms are assumed to be identical, i.e., \( r_b \) can only be \( r_0 \) and thus the bond density can be written as \( D(r_b) = \delta(r_b - r_0) \). So we can have \( \alpha = 1 \) from the definition of the \( \delta \) function. Hence, Hamilton’s principle or Newton’s second law gives the virtual internal bond (VIB) model

\[
\frac{\partial^2 \phi}{\partial t^2} = \frac{\partial}{\partial x} \left[ \sigma \left( \frac{\partial \phi}{\partial x} \right) \right],
\]

satisfying the same boundary conditions

\[
\phi(0, t) = 0, \quad \phi(x_N, t) = a
\]

and initial conditions

\[
\phi(x, 0) = \phi_0(x), \quad \phi_t(x, 0) = v_0(x),
\]

where we have assumed that the density of the non-deformed material is one in order to match the equation (5). Obviously, the molecular dynamics model (5) can be seen as a central difference scheme of (7) in the lattice scale or bond length \( r_0 \) (that is, \( u_i \) in (5) is the deformed position of the atom \( x_i = ir_0 \)). The principle difficulty in this approach is caused by the fact that the continuum description leads to a nonlinear partial differential equation, which, in general, will not be well-posed since the stress-strain relation, i.e., the function \( \sigma(.) \) is not monotone. Thus the resulting partial differential equation is a nonlinear wave equation of a mixed type (cf. [22]). A physically meaningful admissibility criterion for constructing the shock solution is difficult to derive. Nonetheless, at the beginning of Section 3, just for the purpose of reference, we shall depict its solution for a couple of Riemann problems in a short time under a viscosity admissibility criterion.

Other coarse-grained molecular dynamics techniques are developed based on the average energy of the canonical ensemble on a constrained phase space near the thermal equilibrium (see, e.g., [29, 16]) and/or finite temperature quasicontinuum method, e.g., [23]. In such methods the coarse-grained Hamiltonian would be usually in a similar format as (4). Therefore the study of the coarse grid model of (5) may be helpful for understanding the consistency between different sized coarse-grained models.
2 Coarse-grained approximation based on the quasicontinuum idea

As an example we consider a uniform mesh to the one-dimensional material bar as depicted in Figure 2. Let \( U_I(t), I = 0, 1, \ldots, J \), be the deformed position of the finite element node \( X_I = x_{I\ell} \) and \( \ell \) be the number of atoms in every element. Consequently the length of every element is \( h = \ell r_0, X_I = I \ell r_0 = Ih \) and \( N = J \ell \).

Restricting to the simplest case and by using the piecewise linear finite element space or uniform deformation assumption in each element we can write the deformed position and velocity of the \( i \)-th atom in element \([X_{I-1}, X_I]\) as

\[
U_i = \frac{x_i - X_{I-1}}{h} U_I(t) + \frac{X_I - x_i}{h} U_{I-1}(t),
\]

\[
\dot{U}_i = \frac{x_i - X_{I-1}}{h} \dot{U}_I(t) + \frac{X_I - x_i}{h} \dot{U}_{I-1}(t).
\]

If we use the quasicontinuum approximation for the potential energy of the Hamiltonian (4), replace \( u_i \) by \( U_i \), \( \dot{u}_i \) by \( \dot{U}_i \), and use \( \frac{U_i - U_{i-1}}{r_0} = \frac{U_I - U_{I-1}}{h} = \frac{U_I - U_{I-1}}{r_0} \) we obtain a coarse-grained approximate Hamiltonian (noting that we can write \( i = (I-1)\ell + k, k = 0, \ldots, \ell - 1 \):

\[
\tilde{H} = \frac{1}{2} \sum_{I=1}^{J} \sum_{k=0}^{\ell-1} \left[ U_i^2 + 2W\left(\frac{U_I - U_{I-1}}{h}, 1\right) \right]
\]

\[
= \frac{1}{2} \sum_{I=1}^{J} \left[ \sum_{k=0}^{\ell-1} \left( \frac{k}{\ell} \right)^2 \ddot{U}_I^2 + \sum_{k=0}^{\ell-1} \left( \frac{\ell - k}{\ell} \right)^2 \ddot{U}_{I-1}^2 + 2 \sum_{k=0}^{\ell-1} \frac{k(\ell - k)}{\ell^2} \ddot{U}_I \ddot{U}_{I-1} + 2\ell W\left(\frac{U_I - U_{I-1}}{h}, 1\right) \right]
\]

\[
= \frac{1}{2} \sum_{I=1}^{J} \left[ \frac{(\ell - 1)(2\ell - 1)}{6\ell} \ddot{U}_I^2 + \frac{(\ell + 1)(2\ell + 1)}{6\ell} \ddot{U}_{I-1}^2 + \frac{(\ell + 1)(\ell - 1)}{3\ell} \dddot{U}_I \dddot{U}_{I-1}
\]

\[
+ 2\ell W\left(\frac{U_I - U_{I-1}}{h}, 1\right) \right].
\]

Then using Hamilton’s principle with respect to the coarse-grained unknowns we have the coarse-grained equation

\[
M_{II} \dddot{U}_I + M_{II-1} \dddot{U}_{I-1} + M_{II+1} \dddot{U}_{I+1} = \frac{1}{h} \left[ \sigma\left(\frac{U_{I+1} - U_I}{h}\right) - \sigma\left(\frac{U_I - U_{I-1}}{h}\right) \right].
\]

(13)

where the mass matrix \( M_{IJ} \) is

\[
M_{II} = \left( \frac{(\ell - 1)(2\ell - 1)}{6\ell^2} + \frac{(\ell + 1)(2\ell + 1)}{6\ell^2} \right), \quad M_{II-1} = \frac{(\ell + 1)(\ell - 1)}{6\ell^2}, \quad M_{II+1} = \frac{(\ell + 1)(\ell - 1)}{6\ell^2}.
\]

(14)

For the purpose of comparison we apply the piecewise linear finite element method to the continuous VIB model (7) in the spatial variable. We define the finite element partition as before with the uniform element size \( h \) and approximate \( \phi \) in the \( I \)-th element by

\[
\Phi(X,t) = \frac{X - X_{I-1}}{h} \Phi_I(t) + \frac{X - X_I}{h} \Phi_{I-1}(t).
\]

(15)

By straightforward calculation we then have the coarse-grained scheme

\[
\frac{2}{3} \Phi_I + \frac{1}{6} \Phi_{I+1} + \frac{1}{6} \Phi_{I-1} = \frac{1}{h} \left[ \sigma\left(\frac{\Phi_{I+1} - \Phi_I}{h}\right) - \sigma\left(\frac{\Phi_I - \Phi_{I-1}}{h}\right) \right].
\]

(16)
Note that the sum of coefficients in the left-hand side of (16) and the sum of coefficients in the left-hand side of (13) are both equal to one. Although (16) and (13) are a little bit different they both define a consistent scheme of (7).

We remark that the finite element or coarse-grained solution $U_i$ defined in (10) may be a good approximation of the fine scale solution $u_i$. But its time derivative or velocity $\dot{U}_i$ defined in (11) may not be a good approximation of $\dot{u}_i$ since the solution of the central difference scheme of the hyperbolic equation is highly oscillatory and its frequency depends on the size of the discrete system. Nevertheless, we expect that in a certain average sense $\dot{U}_i$ is indeed a good approximation of $\dot{u}_i$. The goal of this paper is to study the approximation properties numerically to obtain basis for a more rigorous theoretical results.

3 Numerical studies

We consider a one-dimensional material bar $x \in [0,1]$ with a possible defect in the middle of the interval. If the deformation gradient $F = \frac{\partial \phi}{\partial x}$ or its discrete version $F = \frac{u_i - u_{i-1}}{r_0}$ is equal to one then the pair of atoms locate at a stable position with the zero interacting force. We consider the material having a defect if $F$ is not equal to one at some point or region. We thus consider examples where initially the strain

$$F = \begin{cases} 
F_l = 1, & x \in [0, 0.5 - \delta) \\
F_m = 1 + \eta, & x \in [0.5 - \delta, 0.5 + \delta] \\
F_r = 1, & x \in (0.5 + \delta, 1]
\end{cases}$$

and the initial velocity $\dot{u}$ is zero. We note that for the Lennard-Jones potential the equation (7) would be hyperbolic if $F_m = 1 + \eta < \sqrt{13/7} \approx 1.10868$ (the potential is convex) and elliptic if $F_m \geq \sqrt{13/7}$ (the potential is non-convex). In the elliptic case the time evolution would be unstable (see [22]). The length of the bar, i.e., the boundary value $a$ or the initial deformation, is obtained from $F$ by direct integration.

For the continuous problem (7) this initial setting gives two Riemann problems for the left-middle region and the middle-right region. Their shock and rarefaction solutions can be constructed accurately for a short time if an admissibility criterion is defined. For example, we can consider the Riemann problem in the left-middle region. We can add a viscosity term $\mu \ddot{u}_{xx}$ to the right hand side of (7), re-write the equation as a first order system in terms of $\dot{u}$ and $F$ and construct its traveling wave solution ($\dot{u}(\frac{s - \omega}{\mu}), F(\frac{s - \omega}{\mu})$) (the shock solution is then seen as a limit of the traveling wave solution for $\mu \to 0$), where $s$ is the shock speed satisfying the Rankine-Hugoniot condition. The existence of this traveling wave solution requires either $s = 0$ or

$$\frac{\sigma(\omega) - \sigma(F_l)}{\omega - F_l} \leq \frac{\sigma(F) - \sigma(F_l)}{F - F_l} \quad \text{if } s < 0,$$

$$\frac{\sigma(\omega) - \sigma(F_l)}{\omega - F_l} \geq \frac{\sigma(F) - \sigma(F_l)}{F - F_l} \quad \text{if } s > 0.$$

for all $\omega$ between $F_l$ and $F$. The above condition is called the generalized viscosity criterion (see, e.g., [14, 30] and [19] for more details). Following [33] the corresponding shock and rarefaction solutions can then be constructed in a short time before hitting the boundary of the domain. The exact form of the solution, albeit involved, was presented in detail in [22].
Figure 3: Time evolution of the exact solution of the continuum model (7) with $\eta = 0.1$.

Since the solution of the discrete system (5) and its coarse grained one (13) become highly oscillatory\(^1\) and the frequency depends on the number of particles (cf. [19]). It is clear that the coarse-grained approximation cannot be a good approximation to the fine grid solution in the pointwise sense. Nonetheless, if integrating out the oscillation through a damping term or an average we may possibly obtain a good approximation in certain sense. In this section we present numerical results with a viscosity damping and a temporal average.

### 3.1 A viscosity damping

As we mentioned earlier, adding a viscosity term to the continuum equation (7) we can obtained an admissibility criterion and construct the shock and rarefaction solution of its Riemann problems. From the theory of numerical conservation laws adding the same numerical viscosity term (taking a properly scaled viscosity coefficient) will remove the oscillation caused by the central difference scheme near the shock and provide a good approximation to the shock solution. We take the numerical viscosity term as

$$\frac{\mu}{r^2_0} \left( \dot{u}_{i-1} - 2\dot{u}_i + \dot{u}_{i+1} \right) \quad \text{or} \quad \frac{\mu}{h^2} \left( \dot{U}_{I-1} - 2\dot{U}_I + \dot{U}_{I+1} \right)$$

for (5) or (13), respectively, and the resulting discrete system may be seen as a central difference scheme for the viscous system. We depict the solution (the strain $\phi_x$, the velocity $\phi_t$ and their discrete analogs) of (7) and (5) for $t \in [0, 0.05]$ (with $J = 256$, $\ell = 1$, $\delta = 0.1$ and $\eta = 0.1$) in Figures 3 and 4. Clearly the discrete solution is a very good approximation to the solution of the continuum model. We can then conclude that the coarse-grained solution will be a good approximation to the fine-grid solution when the viscosity term is added since they are both consistent numerical schemes for the viscous system of the continuum model.

Next we take $\eta = 0.2$. Then $F_m = 1 + \eta$ is in the non-convex region of the Lennard-Jones potential and the corresponding continuum model (7) is elliptic in the region and then the time evolution is unstable (cf. [19]). Nevertheless, the discrete solution still exhibits good approximation properties to the solution of the continuum model as long as $F$ does not stay in the elliptic region for too long times. The solutions (strain and velocity) of (7) and (5) are

---

\(^1\) Numerically the molecular dynamics model (5) represents a central difference scheme for the continuous model (7). It is well known that in this case the numerical solution would oscillate near the shock and the oscillation will then develop and spread out to the entire domain.
Figure 4: Time evolution of the discrete solution of (5) with $\eta = 0.1$ and the numerical viscosity $\mu = 0.005$.

Figure 5: Time evolution of the exact solution of the continuum model (7) with $\eta = 0.2$.

depicted in Figures 5 and 6. Here we take $\mu = 0.01$ (it appears that taking $\mu = 0.005$ is not enough to remove the oscillations when $\eta = 0.2$).

Other damping (or so-called dissipative) terms other than the viscosity can be considered as well. Numerical experiments based on other types of dissipative terms can be found in [1, 31, 32]. However, the shock solution of conservation laws of mixed type depends on the admissibility criterion (derived according to the additional dissipative term) due to the non-uniqueness of its equilibrium solution. It is still not very clear whether the viscosity or other choices of dissipation are physically correct ones in this application. At this point we note that the original physical problem is discrete and therefore we need to know whether the solution of the coarse-grained system is a good approximation to the solution of the fine-grid (or atomic-scale) discrete system in certain sense. Although rigorous existence or a convergence result linking the discrete system with a continuum limit would greatly simplify the study of the approximation properties, it appears to be advantageous to separate this question from the computational model at this stage until better analytical results are available for the study of continuum limits. The numerical study we present in the next section therefore aims at identifying a suitable way to evaluate approximating properties of the coarse-grained computations with respect to the original fine-grid model.
3.2 Temporal averaging

In this section we would like to study whether the coarse-grained model can yield a good approximation to the fine-grid solution when integrating out oscillations in the solution by temporal averaging. We shall consider the average in time and see if the sequence $\frac{1}{T} \int_0^T U_h(t) dt$ (where $U_h = (U_1, \ldots, U_J)$) approaches $\frac{1}{T} \int_0^T u(t) dt$ (where $u = (u_1, \ldots, u_N)$) when reducing the number of particles $\ell$ in each subinterval (or equivalently reducing $h$) for given values of $T$. The heuristics that motivates this idea is an assumption of ergodicity for large molecular dynamics systems. Such assumption is implicitly hidden in most applications of molecular dynamics simulations used for sampling statistical equilibrium of such systems. We emphasize that this analogy serves only as motivation for our numerical studies as the evolution of the model problem at hand can be far from the equilibrium if defects are present or shocks form.

From the discussion in the previous section follows that the non-trivial case occurs when the discrete strain is in the non-convex region of the potential $W$. We explore numerically cases that involve a defect controlled by the parameter $\eta$ in the initial condition. The computational results for $\eta = 0.1$ (the corresponding $F$ in the hyperbolic region), $\eta = 0.2$ and $\eta = 0.4$ (the corresponding $F$ in the elliptic region) are depicted below. We will consider two cases. The first one is such that the defect in the middle of the material and involves only one pair of atoms. The other is such that the middle defect region forms an interval $[0.4, 0.6]$.

Case I. The defect involves only one pair of atoms in the middle.

Figure 7 depicts the time evolution of the position, velocity, strain and stress of particles under two different mesh sizes and $\eta = 0.1$. Figures 8-9 depicts the temporally averaged solution (strain and velocity) for $T = 0.05$ and $T = 0.1$, respectively. We observe that when reducing the mesh size (or $\ell$), the maximum of the velocity solution decreases and the minimum of the viscosity solution increases. Meanwhile, the maximum of the strain solution decreases. Finally, we observe numerically that all these solutions approach a limit. Figures 10-12 and Figures 13-15 show similar behavior for cases $\eta = 0.2$ and $\eta = 0.4$. So even if initially the distance of the middle pair of atoms is in the elliptic region ($\eta = 0.2$ or 0.4) the coarse-grained solution (i.e. position, velocity and strain) approaches the fine-grid solution. We note that physically the pair of atoms with a larger strain will attract each other and quickly move to the hyperbolic region.

Case II. The defect occupies the whole interval $[0.4, 0.6]$. 

Figure 6: Time evolution of the discrete solution of (5) with $\eta = 0.2$ and the numerical viscosity $\mu = 0.01$. 
Figures 16-24 are parallel to Figures 7-15 in Case I. But the defect region is now wider. Again, Figure 16 depicts the time evolution of the position, velocity, strain and stress of particles under two different mesh size and $\eta = 0.1$. Figures 17-18 indicate the temporally averaged solution (velocity, strain) approaches a limit as $\ell$ or the mesh decreases. Cases with $\eta = 0.2$ and $\eta = 0.4$ appear different. Unlike Case I the strain stays in the middle elliptic region ($\eta = 0.2$ or $\eta = 0.4$) for much longer time. This may cause the growth of the solution (as we see in Figures 19 and 22). Figures 20-21 and Figures 23-24 do not seem to reach any limit, especially in the middle defect part. We observe that near the boundary of the elliptic region the magnitude of the strain increases when the mesh is refined. The velocity does not seem to converge as well when the mesh is refined. In the case of $\eta = 0.2$ it seems that the velocity solution when $\ell = 2$ is close to that when $\ell = 8$, while the velocity solution when $\ell = 4$ is close to that when $\ell = 16$. Consequently no limit is reached. In the case of $\eta = 0.4$ the solutions are quite in a clutter and they do not converge when decreasing $\ell$ or the mesh size.

3.3 Conclusion

Based on the computational results we claim that when the strain is in the convex region (or quickly evolves to the convex region) of the interacting potential the coarse-grained approximate solution presents a good approximation to the original fine-grid solution in a temporal average sense. On the other hand if the strain is in the non-convex region of the potential energy for a certain period of time then it does not seem possible that the coarse-grained approximation (of velocity and strain) would be sufficient for simulating dynamical properties of the material.

Remark: We may consider spatial averaging as well, for example, applying windowed and weighted spatial averages as in [13] for a first order hyperbolic system. In this case we see that the coarse-grained solution approaches the fine-grid solution if the strain is in the hyperbolic region. However, similarly as in the case of temporal averaging this is not true if the strain stays in the elliptic region for a certain time.

Acknowledgment. The work began when the second author was visiting Department of Mathematics of National University of Singapore. PP thanks to the NUS for its hospitality and the support. PL’s research is partially supported by the Singapore academic research grant R-146-000-053-112.

References


Figure 7: Time evolution of the solution in the case of $N = 1024$ and $\eta = 0.1$ with $\ell = 1$ and $\ell = 16$, respectively.

Figure 8: Time average of the velocity and strain at $T = 0.05$ with $\eta = 0.1$ and $\ell = 64, 32, 16, 8, 4$ and $2$.

Figure 9: Time average of the velocity and strain at $T = 0.1$ with $\eta = 0.1$ and $\ell = 64, 32, 16, 8, 4$ and $2$. 
Figure 10: Time evolution of the solution in the case of $N = 1024$ and $\eta = 0.2$ with $\ell = 1$ and $\ell = 16$, respectively.

Figure 11: Time average of the velocity and strain at $T = 0.05$ with $\eta = 0.2$ and $\ell = 64, 32, 16, 8, 4$ and $2$.

Figure 12: Time average of the velocity and strain at $T = 0.1$ with $\eta = 0.2$ and $\ell = 64, 32, 16, 8, 4$ and $2$. 
Figure 13: Time evolution of the solution in the case of $N = 1024$ and $\eta = 0.4$ with $\ell = 1$ and $\ell = 16$, respectively.

Figure 14: Time average of the velocity and strain at $T = 0.05$ with $\eta = 0.4$ and $\ell = 64, 32, 16, 8, 4$ and 2.

Figure 15: Time average of the velocity and strain at $T = 0.1$ with $\eta = 0.4$ and $\ell = 64, 32, 16, 8, 4$ and 2.
Figure 16: Time evolution of the solution in the case of $N = 1024$ and $\eta = 0.1$ with $\ell = 1$ and $\ell = 16$, respectively.

Figure 17: Time average of the velocity and strain at $T = 0.05$ with $\eta = 0.1$ and $\ell = 32, 16, 8, 4$ and 2.

Figure 18: Time average of the velocity and strain at $T = 0.1$ with $\eta = 0.1$ and $\ell = 32, 16, 8, 4$ and 2.
Figure 19: Time evolution of the solution in the case of $N = 1024$ and $\eta = 0.2$ with $\ell = 1$ and $\ell = 16$, respectively.

Figure 20: Time average of the velocity and strain at $T = 0.05$ with $\eta = 0.2$ and $\ell = 32, 16, 8, 4$ and 2.

Figure 21: Time average of the velocity and strain at $T = 0.1$ with $\eta = 0.2$ and $\ell = 32, 16, 8, 4$ and 2.
Figure 22: Time evolution of the solution in the case of $N = 1024$ and $\eta = 0.4$ with $\ell = 1$ and $\ell = 16$, respectively.

Figure 23: Time average of the velocity and strain at $T = 0.05$ with $\eta = 0.4$ and $\ell = 32, 16, 8, 4$ and 2.

Figure 24: Time average of the velocity and strain at $T = 0.1$ with $\eta = 0.4$ and $\ell = 32, 16, 8, 4$ and 2.