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Multiple Time Scale Algorithm for Multiscale Material Modeling

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Abstract: This paper presents a novel multiple time scale algorithm integrated with the concurrent atomic/atom-based continuum modeling, which involves molecular dynamic (MD) simulation and coarse-grained molecular dynamic (CG-MD) simulation. To capture the key features of the solution region while still considering the computational efficiency, we decompose it into two sub-regions in space and utilize the central difference method with different time steps for different subregions to march on in time. Usually, the solution region contains a critical field and a non-critical far field. For the critical field (named atomic region) modeled by MD simulation, a relatively small time step is used to update the solutions; for the far field (named atom-based continuum region) modeled by CG-MD simulation, we adopt a relatively large time step to reduce the computational efforts and thereby it leads to an acceleration of such simulations. Here, we solve a wave propagation problem to demonstrate the capability and feasibility of this algorithm. The results show that the wave can propagate across the interface between atomic region and atom-based continuum region smoothly without inducing any spurious wave reflection. Also, the effects of nonlocality and nonlinearity, introduced unintentionally by the interatomic potential, will be discussed.

Keywords: Multiple time scale algorithm; Multiple length scale modeling; Molecular dynamic simulation; Wave propagation; Nonlocality and nonlinearity

1 Introduction

Molecular dynamic (MD) simulation has established itself as a widely employed simulation technique for the study of material behaviors at nanoscale. Unfortunately, the extension of MD into computational science over a realistic range of length and time is limited, due to the large number of particles involved as well as the complex nature of their interactions. The limitations are also imposed by

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the requirement of smallness of the time step, even though one may be primarily interested in events that occur over a much longer time scale. The emergence of multiple length and time scale approach, along with the development of massively parallel computers, remarkably expands the realm of modeling and simulation from nanoscale to microscale.

The past several years have witnessed the explosive growth of interest in multiple length scale theories and simulations. One common approach is named concurrent multiscale modeling method, which incorporates MD with continuum theory and addresses the problem in a single theoretical framework. Among the concurrent multiscale methods, the coupling of length scale method (CLSM) was a pioneering work developed by Abraham et al. (Abraham and Broughton 1998), and by Rudd and Broughton (Rudd 2001), which incorporated the coupling of quantum mechanics approximation, MD, and FE method. Xiao and Belytschko (Xiao and Belytschko 2004) developed the bridging-domain method (BDM), in which the continuum and molecular domains were overlapped in a bridging sub-domain. The bridging scale method (BSM), developed by Wagner and Liu (Wagner and Liu 2003), used a form of the Langevin equation to constrain the interface between the fine and coarse scales. Shen and Atluri (S.P. Shen and Atluri 2004) developed the multiscale simulation technique based on the meshless local Petrov-Galerkin method, in which several alternate time-dependent interfacial conditions, between the atomic and continuum regions, are systematically studied by decomposing the displacement of atoms in the equivalent continuum region into long and short wavelength components. Ma et al. (J. Ma et al. 2006) used the generalized interpolation material point method (GIMP) and the coupling between GIMP and MD is achieved by enforcing compatible deformation, force and energy fields in the transition region between GIMP and MD. Quasicontinuum (QC) method, developed by Tadmor et al. (Tadmor, Ortiz and Phillips 1996) and extended by Knap and Oritz (Knap and Ortiz 2001), aims to reproduce the results of standard lattice statics based on energy minimization. It is worthwhile to mention that the Atomistic Field Theory (AFT) proposed by Chen (Chen and Lee 2005, Chen 2006, Chen 2009), with its corresponding numerical algorithm (Lee, Wang and Chen 2009, Wang and Lee 2011), is another successful example in concurrent multiscale material modeling and simulation.

Accompanying the multiple length scale study, a great deal of interest has been focused on increasing the time step in MD simulation. Anderson (Andersen 1983) and Ryckaert et al. (Ryckaert, Ciccotti and Berendsen 1977) proposed SHAKE and RATTLE algorithms based on the constrain of bond lengths. Although the application of these algorithms allows for a modest increase in the time step, the accuracy of the solutions may be adversely affected. Another idea is to introduce a

hierarchy of time steps corresponding to the hierarchy of frequencies in the system. Teleman and Jonsson (Olle Teleman and Jönsson 1986) introduced an algorithm whereby the slower degrees of freedom are held constant for a number of smaller time steps which are used for the faster degrees of freedom. However, this method has been shown to lead to a loss of accuracy as time marching on. The Ewald summation method is a well-known technique for computing electrostatic interactions. It is worthwhile to mention that Procacci et al. (Procacci et al. 1997) and Kawata and Mikami (Kawata and Mikami 2000) have proposed efficient multiple-time-step methods for Ewald summations. For the system consisting of light and heavy particles, the maximum time step that can be used to integrate the equations of motion must be chosen to insure accurate integration for the light particles. This implies that a very small time step is needed. Tuckerman and Berne (Mark E. Tuckerman, Glenn J. Martyna and Berne 1990, Mark E. Tuckerman, Bruce J. Berne and Rossi 1991) propose a reference system propagator algorithm (RESPA), which allows one to use a time step appropriate for the heavy particles. These methods have been shown to reach a simulation time much longer than that in direct MD while preserving full atomic detail. However, the advantages and efficiencies of these methods are still questionable when they are extended into a realistic range of length and time.

In this paper, we propose a novel multiple-time-scale algorithm based on the splitting of the solution space into an atomic region and an atom-based continuum region, following by solving a wave propagation problem in multi-element crystalline solid, which has more than one kind of atom in the unit cell. Accordingly, the atomic region is modeled by MD simulation; the atom-based continuum region is modeled by CG-MD simulation, in which the interatomic forces are calculated as in MD simulation, instead of the nodal forces integrated from the stress-strain relation. The nonlocal force-calculation procedure overcomes the force mismatch at the interface and enables a seamless scale transition from fully atomic resolution to continuum description. This procedure will be described in detail in the following sections.

2 Multiple Length Scale Modeling

Our previous works (Wang and Lee 2010, Wang et al. 2012) have presented the theoretical framework for the concurrent atomic/atom-based continuum modeling. Compared with many other multiscale methods, ours is naturally suitable for the multi-physics analysis of multi-element crystal material. Here, we only briefly review our multiscale method and its corresponding numerical implementation.

The idea is to bridge MD and CG-MD simulations, and employ them to model the critical field and the non-critical far field respectively. The governing equations of

MD simulation and CG-MD simulation may be expressed symbolically as

$$m^i \ddot{\mathbf{u}}^i = \mathbf{f}^i(\mathbf{u}, \mathbf{U}, t) \tag{1}$$

$$M_I^\alpha \ddot{\mathbf{U}}_I^\alpha = \mathbf{F}_I^\alpha(\mathbf{U}, \mathbf{u}, t) \tag{2}$$

The key point here is how to calculate the interatomic force for these two governing equations.

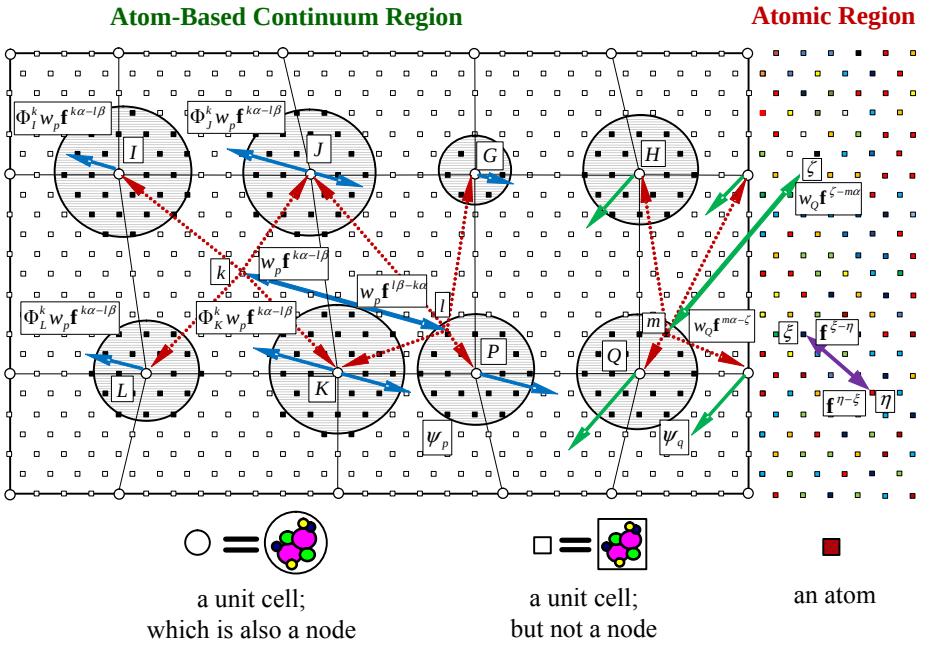


Figure 1: The schematic of multiple length scale modeling

Consider a crystalline material system consisting of two regions: an atomic region and an atom-based continuum region, as shown in Figure 1. Since the crystalline material is distinguished from other states of matter by a periodic arrangement of the atoms, it can then be represented as a collection of repeated unit cells and a group of discrete and distinct atoms situated within each unit cell. As depicted in Figure 1, the atomic region is shown with colorful points which are atoms, and of course as a special case, atoms may be grouped as unit cells; the atom-based continuum region is shown with a mesh filled with unit cells (although the problem is three-dimensional (3D), only a 2D mesh is shown here for simplicity). It is emphasized that, although this region is coined as the atom-based continuum region,

we never lose the sight of atoms. In the atom-based continuum region, it is seen that there are: (1) a finite element mesh constructed by elements and nodes (for example, Nodes I,J,K,L,G,H,P,Q); (2) a cluster (the grey circle) associated with each node (for example, clusters ψ_P and ψ_Q); (3) representative unit cells which belong to certain clusters (for example, unit cell $l$and m); (4) unit cells which do not belong to any clusters (for example, unit cell k).

CG-MD simulation is the foundation of our multiple length scale modeling. In the atom-based continuum region, an atom in general does not have its individuality – it only serves as a messenger, i.e., it transfers the force to its surrounding nodes. By borrowing the idea from finite element method, we adopt an assumption

$$\mathbf{u}^{k\alpha} = \sum_N \Phi_N^k \mathbf{U}_N^\alpha \tag{3}$$

where $\mathbf{u}^{k\alpha}$ is the displacement vector of the $\alpha-th$ atom in the $k-th$ unit cell; Φ_N^k is the $N-th$ shape function evaluated at the location of the $k-th$ unit cell; $\mathbf{U}_N^\alpha$ is the nodal value of the displacement vector of the $\alpha-th$ atom in the $N-th$ node of the element where the $k-th$ unit cell resides. In other words, the $\alpha-th$ atom in the $k-th$ unit cell is just a follower unless the $k-th$ unit cell is a node. At this junction, let $\mathbf{f}^{k\alpha}$be the interatomic force acting on the $\alpha-th$ atom in the $k-th$ unit cell. The virtual work done by $\mathbf{f}^{k\alpha}$is

$$\mathbf{f}^{k\alpha}\cdot\delta\mathbf{u}^{k\alpha} = \mathbf{f}^{k\alpha}\cdot\delta\left\{\sum_N \Phi_N^k \mathbf{U}_N^\alpha\right\} = \sum_N \left\{\Phi_N^k \mathbf{f}^{k\alpha}\right\}\cdot\delta\mathbf{U}_N^\alpha \triangleq \sum_N \mathbf{F}_N^\alpha\cdot\delta\mathbf{U}_N^\alpha \tag{4}$$

Therefore, the nodal force contributed by the atomic force can be obtained as

$$\mathbf{F}_N^\alpha = \Phi_N^k \mathbf{f}^{k\alpha} \tag{5}$$

To balance the computational efficiency and the numerical accuracy, we adopt the cluster-based summation rule (Knap and Ortiz 2001, Eidel and Stukowski 2009) for force calculations. Cluster ψ_P can be expressed as $\psi_P = \{l : |\mathbf{X}_l - \mathbf{X}_P| \le R_P\}$, where l represents a generic unit cell whose distance from Node P is less than or equal toR_P, the radius of cluster ψ_P. There is a weight associated with each cluster, e.g., w_P is the weight of ψ_P. For each node (for example Node P), one may find the number of unit cells, N_P and n_P, which belong to Node P through shape functions and cluster ψ_P, respectively. Then, we can calculate the weight as $w_P = N_P/n_P$. It is noticed that, in the calculation of interatomic forces, there are two extreme cases: (1) nodal integration - $n_P = 1 \Rightarrow w_P = N_P$ and (2) all pair calculation - $n_P = N_p \Rightarrow w_P = 1$.

Between two distinct atoms in the atom-based continuum region, at least one of them must belong to a cluster, i.e., in the representative unit cell, the interatomic force acting on atoms $k\alpha$ and $l\beta$can be calculated respectively as $w_P\mathbf{f}^{k\alpha-l\beta}$and $w_P\mathbf{f}^{l\beta-k\alpha} = -w_P\mathbf{f}^{k\alpha-l\beta}$ and then the nodal forces can be obtained from (5) (cf. Figure 1).

On the other hand, any atom in the atomic region has its own degree of freedom, and hence it takes the force and then follows the Newton's law. Between two distinct atoms ξ and η in the atomic region, the interatomic force is calculated and treated as in MD simulation, i.e., the derivation from the interatomic potential with respect to position.

Between two atoms, one in the atom-based continuum region and the other in the atomic region, the interatomic force acting on atoms $m\alpha$ and ζcan be calculated respectively as$w_Q\mathbf{f}^{m\alpha-\zeta}$ and $w_Q\mathbf{f}^{\zeta-m\alpha} = -w_Q\mathbf{f}^{m\alpha-\zeta}$. Then $w_Q\mathbf{f}^{m\alpha-\zeta}$ multiplied by the shape functions will be distributed to the corresponding nodes (cf. Figure 1).

The governing equations (1) and (2) are second order nonlinear ordinary differential equations and therefore we can implement central difference method to approximate the solutions by marching on with large and small time steps in atom-based continuum region and atomic region, respectively. In the following section, we will illustrate the multiple time scale algorithm step by step.

3 Multiple Time Scale Algorithm

Actually, in the arena of continuum mechanics, many researchers have explored the use of different time steps based on FE domain decomposition for large-scale structural dynamics. Since the time step of the explicit time integration is usually governed by either a stability condition (Cauchy condition) or an accuracy requirement determined by $\Delta t \leq \Delta t_{cr} = L_{\min}/v$ (where $L_{\min}$ is the minimum size of all elements; v is the longitudinal wave speed), the minimum time step is forced to be used for the entire domain with a consequence of a huge computational waste. Belytschko et al. (Belytschko, Yen and Mullen 1979, P. Smolinski, S. Sleith and T. Belytschko 1996, Liu and Belytschko 1982) were the first to propose the multi-time step integration method, also referred to as the sub-cycling method. They used different time steps to update the kinematic quantities in different sub-domains. Along the boundary between two sub-domains, an interface condition is required to ensure a match of displacement fields on both sides of the two sub-domains. In this work, we use different time steps for atomic region and atom-based continuum region. However, there is no overlapping between these two regions, which means there is no single atom belonging to both regions, and therefore there is no need to have an interface condition. Here we formulate a multiple time scale algorithm for

the central difference method and couple it with the previously mentioned multiple length scale modeling.

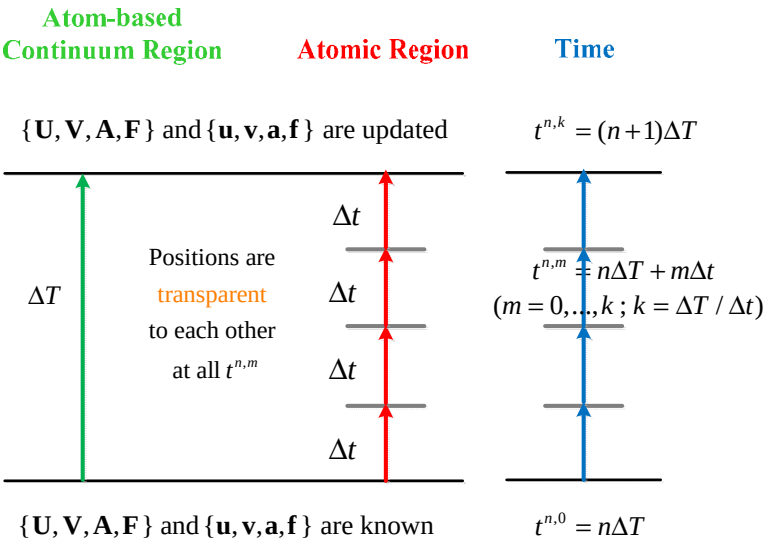


Figure 2: Representation of time steps for the Atom-based Continuum region and the Atomic region

Figure 2 shows the time steps, ΔT *and* Δt, and the marching for both atom-based continuum region and atomic region, respectively. Let **U**, **V**, **A** and **F** represent the position, velocity, acceleration and force, respectively, in the atom-based continuum region; similarly, let **u**, **v**, **a** and **f** represent the position, velocity, acceleration and force, respectively, in the atomic region. Let the large time step be k times the small time step, i.e., $\Delta T = k\Delta t$. The superscript n and m of $t^{n,m}$ are used to number the updated steps in the atom-based continuum region and the atomic region, respectively. Therefore, time can be calculated as $t^{n,m} = n\Delta T + m\Delta t$, where $m = 0, ..., k$. At each time step in atom-based continuum region, the current time can be simplified as $t^{n,0} = n\Delta T$ and the updated time can be simplified as $t^{n,k} = t^{n+1,0} = n\Delta T + k\Delta t = (n+1)\Delta T$. The algorithm can now be implemented as follows:

Step 0: Initial conditions

Assume $\mathbf{U}^{0,0}$, $\mathbf{V}^{0,0}$, $\mathbf{u}^{0,0}$, and $\mathbf{v}^{0,0}$ are known at time $t = t^{0,0} = 0$. Then, $\mathbf{F}^{0,0}$, $\mathbf{f}^{0,0}$, $\mathbf{A}^{0,0}$ and $\mathbf{a}^{0,0}$ can be obtained from eq. (1) and eq. (2).

Step 1: Time update for the atom-based continuum region

At time $t = t^{n,0} = n\Delta T$, $\mathbf{U}^{n,0}$, $\mathbf{V}^{n,0}$, $\mathbf{A}^{n,0}$ and $\mathbf{u}^{n,0}$, $\mathbf{v}^{n,0}$, $\mathbf{a}^{n,0}$ are known from the previous step or from **Step 0**.

Step 2: Time update for the atomic region, $t = t^{n,m} = n\Delta T + m\Delta t$

Step 3: Update the displacement vectors for both regions

In the atom-based continuum region, we perform the Taylor series expansion for the displacement vector, i.e.,

$$\begin{aligned}\mathbf{U}(t) &= \mathbf{U}(n\Delta T + \tau) \\ &= \mathbf{U}(n\Delta T) + \tau\dot{\mathbf{U}}(n\Delta T) + \frac{1}{2!}\tau^2\ddot{\mathbf{U}}(n\Delta T) + \frac{1}{3!}\tau^3\mathbf{U}(n\Delta T) + ... \\ &\approx \mathbf{U}^{n,0} + \tau\mathbf{V}^{n,0} + \frac{1}{2}\tau^2\mathbf{A}^{n,0}\end{aligned} \tag{6}$$

Then we may express $\mathbf{U}^{n,m} = \mathbf{U}(n\Delta T + m\Delta t)$ as

$$\mathbf{U}^{n,m} = \mathbf{U}^{n,0} + m\Delta t\mathbf{V}^{n,0} + \frac{1}{2}(m\Delta t)^2\mathbf{A}^{n,0} \tag{7}$$

Similarly, we may express the displacement vector in the atomic region as

$$\mathbf{u}^{n,m+1} = \mathbf{u}^{n,m} + \Delta t\mathbf{v}^{n,m} + \frac{1}{2}(\Delta t)^2\mathbf{a}^{n,m} \tag{8}$$

Step 4: Compute the interatomic force and acceleration for atomic region

Recall that the two force vectors **F**and **f** , as well as the two acceleration vectors **A**and **a**, are the functions of both **U**and **u**. Also, it is noticed that the two displacement vectors are updated at the same time for each small time step, which means they are transparent to each other at all $t^{n,m}$. Then, the acceleration vector can be written as

$$\mathbf{a}^{n,m+1} = \mathbf{a}(\mathbf{u}^{n,m+1}, \mathbf{U}^{n,m+1}, t^{n,m+1}) \tag{9}$$

Step 5: Update the velocity vector for atomic region

According to the procedure of central difference method, the velocity vector can march on as

$$\mathbf{v}^{n,m+1} = \mathbf{v}^{n,m} + \frac{1}{2}\Delta t(\mathbf{a}^{n,m} + \mathbf{a}^{n,m+1}) \tag{10}$$

Step 6: Update counter: $m \leftarrow m + 1$

Step 7: Go to step 2 unless $m = k$**, i.e.,** $t = (n+1)\Delta T$

Step 8: Compute the interatomic force and acceleration vectors for atom-based continuum region

Following the same idea in **Step 4**, the acceleration vector can be obtained as

$$\mathbf{A}^{n+1,0} = \mathbf{A}(\mathbf{U}^{n+1,0}, \mathbf{u}^{n+1,0}, t^{n+1,0}) \tag{11}$$

Step 9: Update the velocity vector for the atom-based continuum region

$$\mathbf{V}^{n+1,0} = \mathbf{V}^{n,0} + \frac{1}{2}\Delta T(\mathbf{A}^{n,0} + \mathbf{A}^{n+1,0}) \tag{12}$$

Step 10: Update counter: $n \leftarrow n+1$

Step 11: Output the results; if simulation not complete, go to Step 1

4 Wave Propagation

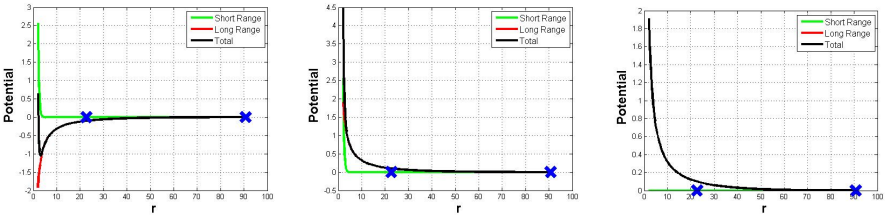
To test the performance of the schemes described above, we simulate wave propagation across the interface between the atomic region and the atom-based continuum region.

The interatomic potential is the only "constitutive equation" needed here, which renders almost all material properties accessible and involves the interaction between all atoms. For MgO, the typical single crystal in the class of rocksalt, we employ the Coulomb-Buckingham potential, i.e.,

$$V^{ij} = \frac{q^i q^j}{r^{ij}} + A^{ij} e^{-\frac{r^{ij}}{B^{ij}}} - C^{ij}\left(r^{ij}\right)^{-6} + D^{ij}\left(r^{ij}\right)^{-12} \tag{13}$$

where A^{ij}, B^{ij}, C^{ij}, and D^{ij} are material constants between atom i and atom j, and $r^{ij} = \left\|r^i - r^j\right\|$. In eq. (13), the first term on the right hand side is the Coulomb potential, which is a long range potential, and all the other three terms describe the Buckingham potential, which is a short range potential. Table 1 lists the corresponding numerical values in the Buckingham potential. It is clarified here that all of the units used in this paper are atomic units. Figure 3 depicts the variations of interatomic potentials as a function of position, including long range interaction and short range interaction. The first cross symbol points the range for short interaction and the second one for long interaction. This clearly exhibits how the nonlocal procedure introduced by the calculation of the interatomic potential.

Figure 4 illustrates three models (including the cross-sectional view, front view, and boundary conditions) studied in this paper. Model 1 is a pure MD model, consisting only atoms, and simulated by MD simulation; model 2 and model 3 consist



(a) (b) (c)

Figure 3: Interatomic potential for (a) Mg-O (b) O-O and (c) Mg-Mg.

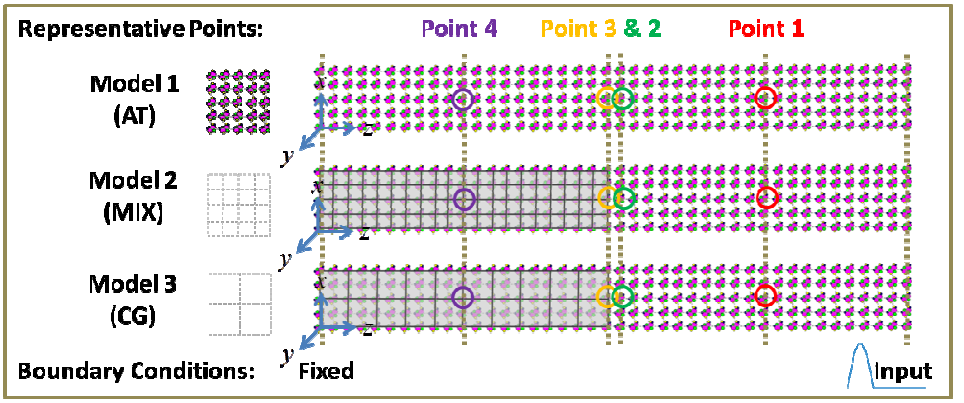


Figure 4: Computational models of a clamped MgO specimen under an impulsive loading and the positions of the selected representative points.

Table 1: Database for MgO

	A	B	C	D	Short Range	Long Range
Mg-O	47.2	0.566	0	0	12*a	4*12*a
O-O	350.88	0.414	54.09	2463.2		
Mg-Mg	0	0	0	0		

both atoms and elements, simulated by the proposed multiple length scale modeling method (cf Section 2). For atom-based continuum region, when the finest mesh is used, i.e., Model 2, any unit cell is a finite element node, which means there is no unit cell within the elements and the model is identical to a full-blown MD model (Model 1); when the coarse mesh is used, i.e., Model 3, the majority of the degrees of freedom can be eliminated and hence the computational cost can be reduced. The sizes of these three models are the same, i.e., $(4a, 4a, 41a)$, and a is the lattice constant for MgO ($a = 1.889726$ Bohr). Here we select four representative points: Point 1 $(2a, 2a, 31a)$, Point 2 $(2a, 2a, 21a)$, Point 3 $(2a, 2a, 20a)$ and Point 4 $(2a, 2a, 10a)$.

As verifications, the result obtained from MD simulation (Model 1) is considered as a standard and "exact" solution. Consider five cases and define NTR as the time step ratio, i.e., $NTR = \Delta T/\Delta t$: (1) Case AT for Model 1, (2) Case MIX-1 for Model 2 with $NTR = 1$, (3) Case MIX-4 for Model 2 with $NTR = 4$, (4) Case CG-1 for Model 3 with $NTR = 1$, and (5) Case CG-4 for Model 3 with $NTR = 4$. The displacement responses along z-axis of Point 1, Point 2 and Point 4 are shown in Fig. 5 (a)-(c), respectively; and the total energy (kinetic energy plus potential energy) as function of time is plotted in Fig. 5(d). It is seen that the displacements of the representative points for the last four cases are in good agreement with case 1 (MD results). Moreover, the results demonstrate that the total energy is conserved as long as the material system is free of external disturbances. These results unmistakably serve as verifications of our approach and the corresponding computer code that we developed.

For case 5, characterized by multiple length scale (constructed by atomic region and atom-based continuum region) and multiple time scale ($NTR = 4$), the displacement responses of the representative points in acoustic mode are shown in Fig. 6 (a) and the variations of kinetic energy, potential energy and total energy as functions of time are shown in Fig. 6 (b). The results show that the displacement responses of Point 2 and Point 3 (very close to each other but belong to different regions, cf. Fig. 4) are almost identical with a slight time delay; this means the wave in acoustic mode propagates through the interface between the atomic region and atom-based continuum region smoothly without any reflection or dispersion.

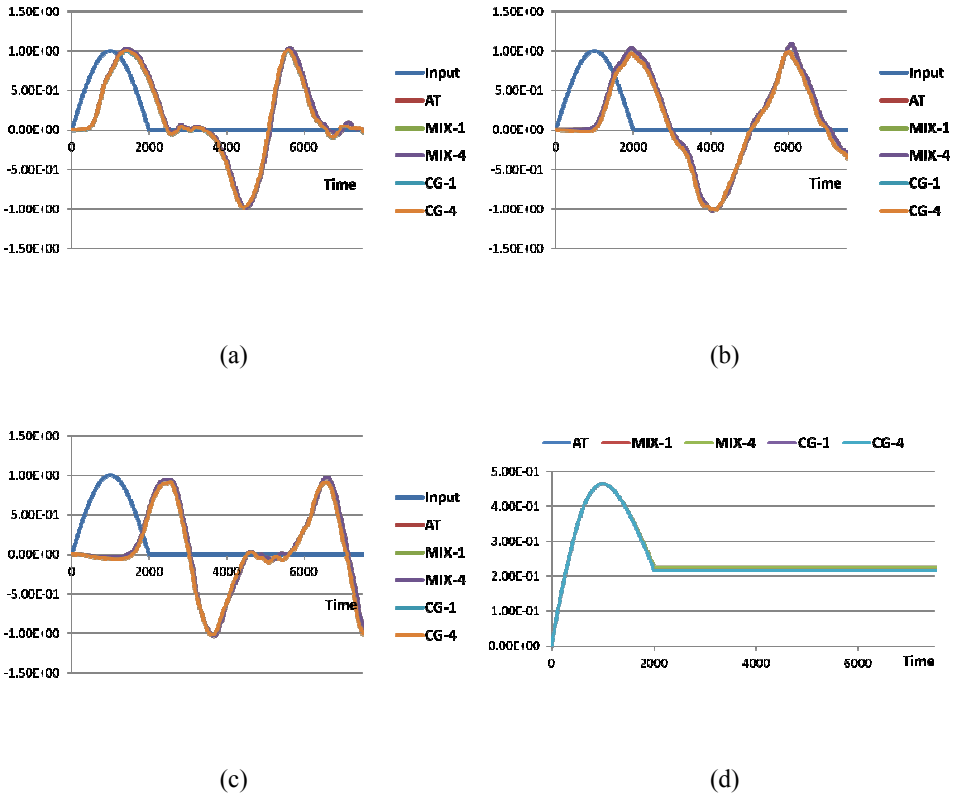


Figure 5: Displacement response of (a) Point 1, (b) Point 2, (c) Point 4 and (d) total energy

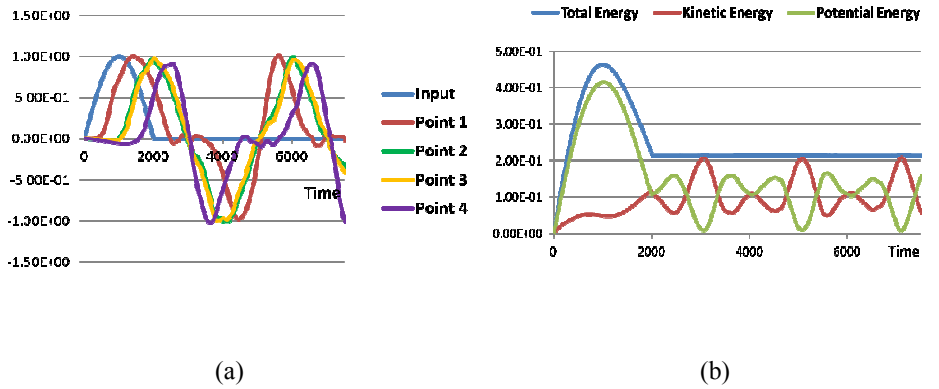


Figure 6: (a) Displacement responses in acoustic mode of Point 1, Point 2, Point 3 and Point 4; and (b) energies variations

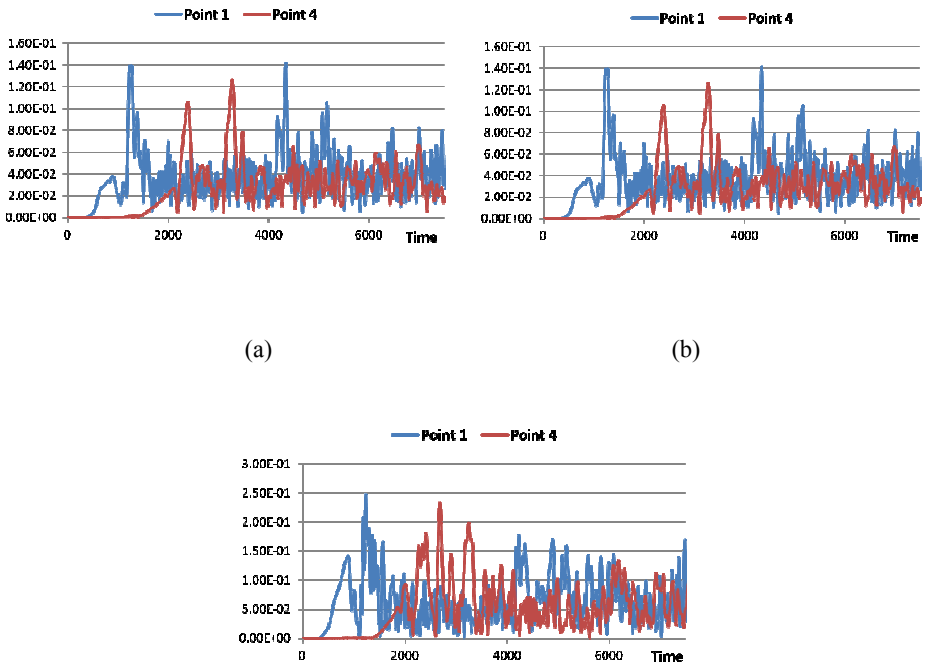


Figure 7: Displacement responses in optical mode along (a) x-axis, (b) y-axis, and (c) z-axis

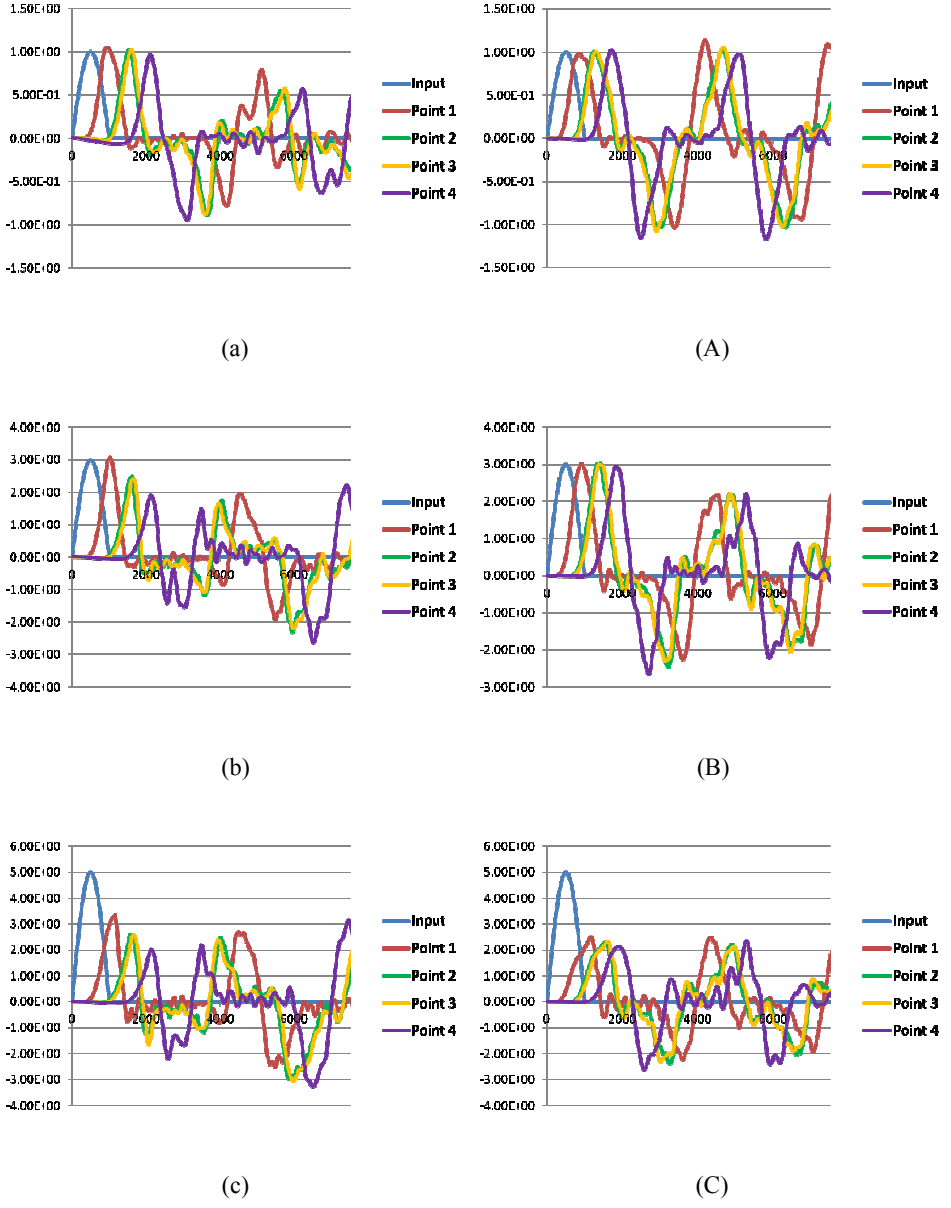


Figure 8: Displacement responses subject to impulse with magnitude equals to (a, A) 1, (b, B) 3, and (c, C) 5

The reason is that the interatomic force calculation only depends on the positions of atoms within the interaction range. This nonlocal procedure overcomes the force mismatch at the interface and enables a seamless length scale transition from fully atomic resolution to continuum description. Since our theory is ready for the simulation of material system with multi-elements, the wave propagation in optical mode can also be investigated. Figure 7 (a)-(c) show the displacement responses of the representative points in optical mode along x-axis, y-axis, and z-axis, respectively. Compared with the responses in acoustic mode, the frequencies in optical mode are much higher. Since the position of Point 1 is nearer than Point 4 to the boundary where the input is applied, the response of Point 1 starts earlier than that of Point 4. The magnitude of optical response along z-axis is larger than that along the other two directions. The results along x-axis and y-axis are exactly the same since there is a 90-degree rotational symmetry about the z-axis. Actually this verifies our computer code again.

Furthermore, we explore the displacement responses subject to the impulse with different magnitudes 1, 3, and 5, and the corresponding results are shown in Figure 8(a)-(c), respectively. When the input magnitude equals to 1, the wave at different points can achieve as high as that of the input one by one in order (cf. Fig. 8(a)). However, when the input magnitude increases to 3 or 5, the wave peaks decay more and more (cf. Fig. 8(b)-(c)). Although the total energy is not depicted here, we want to point out that it is still conserved after the input loading finished for these two situations, which means there is no damping in the system. To explore this hidden mechanism, we artificially reduce the ranges of short and long interactions from $12a$ to $6a$and from $48a$ to $12a$ respectively; and the results are shown in Figure 8(A)-(C). It is seen that the decay phenomena disappear when the magnitude of the input equals to 3, but the wave peaks in Figure 8(C) still cannot achieve the same height as the input when the magnitude of the input equals to 5. It is because the nonlocality and the nonlinearity have been unintentionally introduced in the expression of interatomic potential. We may now conclude that the nonlocal and nonlinear effects play a significant role in MD and CG-MD simulations.

5 Conclusions

In this paper, we have proposed a new theory which can handle the **M**ultiple length scale modeling coupled with **M**ultiple time scale algorithm for **M**ulti-physics simulation of **M**ulti-elements material system. It may be abbreviated as **4M** theory. By employing the 4M theory, we investigate the wave propagation characteristics. The results show that the wave can propagate across the interface between the atomic region and the atom-based continuum region without any spurious reflection or dispersion. Although no versatile results shown here, our theory and its corresponding

computer code are general enough. We will present more interesting phenomena in the future.

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