Multiscale Coupling of Molecular Dynamics and Peridynamics

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Abstract
We propose a multiscale computational model coupling molecular dynamics and peridynamics. The multiscale model is based on previously developed multiscale micromorphic theory. In the proposed multiscale approach, we divide a body into atomistic region and macroscale region. Molecular dynamics is used to simulate atomistic region, and Peridynamics is used to simulate macroscale region; both can capture non-local interactions at respect scales. A transition zone is introduced as a messenger to transfer information between different regions or scales. We employ the “supercell” developed in the previous multiscale theory as transition element, and it is coined as the adaptive multiscale element due to its ability of carrying and passing information between distinct scales. With the adaptive multiscale element, both top-down and bottom-up approaches of communication can be clearly realized and characterized. To mitigate the issue of numerical wave reflection at multiscale boundary, a filter is constructed in a simple manner near the interface. Examples of 1-D and 2-D wave propagation from atomistic region to macro region are demonstrated. The mechanical wave can transit through the interface smoothly without unphysical consequences, and the filtering process is proved to be efficient.

Keywords: Multiscale simulation, Molecular Dynamics, Peridynamics, Solid Mechanics

1. Introduction

Computer technology has been transforming scientific and engineering researches. The ever powerful computer and advanced algorithms open up opportunities to help us see the world in completely new perspectives. For example, the state-of-the-art computational theory and technology, such as ab initio computation and molecular dynamics [6, 9, 3], enable us to observe and predict the motion of electrons and atoms with indomitable resolution. Compare with experimental study, computer simulation is fast, cheaper, more efficient, informative, and flexible, which greatly expands the frontier of many disciplines including materials science, biology, chemistry, etc. The state-of-the-art exascale supercomputer is capable of handling a molecular system up to sub-millimeter with 110 billion (1.1 × 10^{11}) atoms [7]. However, simulation of a molecular system of macroscale size with 6.022 × 10^{23} atoms above is still out of reach in engineering practice, not to mention the capacity of common purpose computers. First principle calculation is even more limited in spatial and time scales because of calculation of electronic structures. Another challenge is how to analyze and extract useful information from large amount of data that is generated from the computer simulation. In engineering research and developments, phenomenological models based finite element analysis and finite difference analysis provide practical tools of simulating macroscopic problems in continuum scale. By virtue of interpolation and discretization, requirements on computer capacity is greatly alleviated. However, macroscale calculation usually employs homogenized field variables and adopts empirical assumptions, such as constitutive law, in which some detailed information is lost, making it difficult to understand microscale mechanics and physics of materials, for instance microscale materials defect motions.

The limitations of computational model in each scale motivated various multiscale simulations, concurrent or hierarchical. The goal of a multiscale model is to combine physical theories or mathematical models from different scales

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in a single framework, and solve the problem in distinct or simultaneous scales depending on the problems of interest. The possibility of scale division is based on two factors. First, physical nature of materials manifests itself in multiple scales of space and time. Materials defects and flaws are typical multiscale phenomena. For example, microscopic dislocation largely determines the macroscale strength of the material; highly localized region around the crack tip where is characterized with bond breaking and strong discontinuity, but the region where is away from the crack tip may only have moderate deformation. Second, reliable coupling techniques are required to transfer information among different scales. Cross-scale communication is one of the most challenging problems in computational physics and materials, because quantities in different scales have distinct properties. For examples, force in microscale is in terms of point-wised interaction between two particles, while in macroscale, it may have a continuous distributed form; and temperature is a concept in macroscale, and the corresponding microscale quantity is the random velocity of particles.

Several multiscale models have attracted attention for their success in practice. Among them, the macroscopic, atomistic, ab initio dynamics(MAAD)[1, 2] method is one of the earliest works, which spans three scales from quantum mechanics to continuum mechanics. It has been applied to solve dynamical fracture problem of silicon. On the other hand, the issue of numerical wave reflection at interscale boundary can be observed in this method. The quasicontinuum method[26, 19, 20, 8] is another widely recognized model, where representative atoms are selected to replace full atomistic representation or calculation, and it has been successful in solving some quasi-static problems such as nano indentation. However, it is restricted to static and quasi-static problems without characterization of dynamics. In addition, the mismatch of the impedance at the interscale boundary induces a so-called “ghost force”. To resolve the inter-scale boundary mismatch problem, Bridging scale method [31, 16, 17, 14] provides a procedure that can realize the scale transition by a process of projection with minimizing least square error, and it introduces an impedance force that may largely alleviated the inter-scale boundary wave reflection. The coupled atomistic and discrete dislocation(CADD) [21, 22] is advantageous to simulate dislocation-type of defects, and it may involve a priori knowledge of slip systems for dislocation detection and passing through interfaces. The recently proposed Multiscale Crystal Defect Dynamics (MCDD) [12] employs a similar idea by using information of the lattice microstructure to construct multiscale method but in a much broader context. Other successful multiscale models include concurrent atomistic continuum method(CAC)[4, 32], and the perfectly matched multiscale simulation (PMMS) method[27, 11], etc.

An ideal multiscale method needs to have a two-way cross-scale information communication passage. This is what lack in all existing multiscale methods. The bottom-up approach is relatively straightforward, where information from microscale is properly collected and interpreted to describe macroscale phenomena. For example, macroscale displacement field is averaged or homogenized from atomistic displacements; stress and temperature can be calculated from atomistic forces and random velocities according to statistical mechanics. On the other hand, the top-down message passing is more challenging, and it requires uncanny physical insights. Specifically, top-down approach may be illustrated as the response of a molecular system when macroscale boundary condition such as traction is enforced. This procedure is not trivial, because a single-scale model cannot describe both molecular system and macroscale boundary conditions. To resolve this issue, recently, the present authors proposed a physical model with multiscale structure and dynamics [13, 28, 29]. The model is derived from and equivalent to classical molecular dynamics, but macroscopic quantities such as traction are incorporated into microscale model versus multiscale structure design, and thus the top-down message passing becomes natural.

This work is to further establish a computational paradigm based on the previous multiscale molecular dynamics theory. By taking advantage of the previous physical multiscale theory, an adaptive multiscale element is constructed as a messenger to translate information between regions of different scales. The message transition is smooth due to the clearly defined top-down and bottom-up characterizations. In atomistic region, molecular dynamics is the natural choice. In macroscopic region, several models can be employed depending on the problem of interest. For example, finite element method can be used in continuum field modeling, and meshfree methods [15, 10] may be more suitable for the materials with strong nonlocal interactions. In this work, we choose peridynamics [23, 18, 24, 25] in macroscale modeling because that it is a nonlocal theory that has similar dynamical structure as molecular dynamics. The non-local balance law provides a seamless connection to atomistic region. To solve the problem of spurious wave reflection in the cross-scale boundary, we introduce a filter near the multiscale interface. The procedure of filtering high-frequency wave on the interface is natural and adaptive without need of cumbersome ad hoc treatment. Due to the intrinsic interscale coupling properties of the multiscale model, mechanical as well as thermodynamical quantities in both scales can be readily described and transferred among different scales without loss, and sophisticated
The paper is arranged in four sections. Following the introduction, the framework of the multiscale computational model is presented in Section 2, which includes the general picture of the model, introducing the transition zone, review of peridynamics and the construction of the filter. Numerical algorithm is discussed subsequently. In Section 3, we shall employ the multiscale method to compute in two numerical examples in order to validate the model. The first example is an 1-D wave propagation problem, the process of wave transition through across-scale boundary is demonstrated, and the filtering technique is also illustrated. The second example is a 2-D wave propagation, and it further proves the promising application of the multiscale method. Summary and outlook are given in the last Section.

2. Multiscale coupling model

The multiscale coupling model consists of three parts: atomistic region, macro region and a transition zone responsible for translating information between two regions, as shown in Fig1(a). The atomistic region is described by classical molecular dynamics. Interatomic potential is used to derive nonlocal forces between atoms or molecules. Macro region usually requires empirical constitutive relation. Many methods can be chosen in this region depending on the problem of interest. In this work, we adopt peridynamics to be consistent with atomistic region due to their similar non-local behaviors, and the constitutive relation is based on Cauchy-Born rule. The formulation will be briefly introduced subsequently.

The essential part of the multiscale model is the transition zone. To ensure a reliable passage of information between macro and atomistic regions, several conditions need to be taken into account. First, in the bottom-up procedure, atomistic information such as force and displacement should be sensed by transition zone and interpreted to macro domain. Specifically, macroscale only captures low-frequency waves with coarse resolution, and high-frequency atomistic vibration should be filtered out otherwise it will reflect back to the atomistic region. Second, in the top-down procedure, macroscale information such as stress, strain and displacement should also be properly interpreted to atomistic domain. The previous multiscale theory[28, 29] is employed here to characterize the top-down approach. The basic unit “supercell” can carry both atomistic and macroscale information, which makes it a good candidate of transition element. In this computational model, we rename it as “adaptive multiscale element”. We briefly review the theory and the properties of “supercell” in the following subsection.

2.1. Microscale modeling: Multiscale molecular dynamics

As shown in Fig 1(a), the transition zone has atomistic resolution same as atomistic region. However, we divide atoms in this zone into several supercells. Each supercell is viewed as a material point on macroscale which has shape as an assemble of atoms. In addition, each atom inside the supercell is free to move as internal degree of freedom. Given the property of shape, the supercell is able to describe macroscale motions such as deformation and cell-level displacement. Therefore, it is possible to apply associated macroscale force field such as stress on the supercell. On the other hand, with the atomistic resolution, all information of atomistic scale is retained. As a consequence, the supercell has multiscale structure and property. The detailed discussion of supercell can be found in [28]. Here we briefly summarize the formulation.

The atomistic position \( \mathbf{r}_i(t) \) at current time is composed of

\[
\mathbf{r}_i(t) = \mathbf{r}_a(t) + \mathbf{\phi}_a(t) \cdot \mathbf{s}_i(t)
\]

where \( \mathbf{r}_a \) is the center of mass of \( \alpha \)-th cell calculated as,

\[
\mathbf{r}_a = \frac{\sum_i m_i \mathbf{r}_i}{\sum_i m_i}
\]

with \( m_i \) the mass of \( i \)-th atom in \( \alpha \)-th cell. The motion of the center of mass represents rigid body translation of the supercell. \( \mathbf{\phi}_a \) is the total deformation gradient of \( \alpha \)-th cell and is uniform throughout the cell. \( \mathbf{s}_i \) is the internal degree of freedom which represents the atomistic distribution inside the cell. \( \mathbf{\phi}_a \cdot \mathbf{s}_i \) is the relative position comparing to the center of mass. This operation is different from Cauchy-Born rule, where the vector of relative postion is \( \mathbf{\phi}_a \cdot \mathbf{s}_i^0 \) and \( \mathbf{s}_i^0 \)
is in referential configuration. Cauchy-Born rule gives a uniform deformation, but changing $s_i$ with time makes $\phi \cdot s_i$ fully recover the atomistic motion and the Eq. 1 valid. $\phi$ can be further decomposed to

$$\phi_i(t) = \chi_i(t) \cdot F_o(t)$$  \hspace{1cm} (3)

where $F_o$ is related to macroscale continuum deformation and depending on the centers of mass among supercells[28]. $\chi_i$ is an independent part of deformation including stretch and rotation. By introducing center of mass and deformation gradient, each supercell obtains the properties of a material point in macroscale continuum mechanics. The internal degrees of freedom is then, enable the interaction between particles from atomistic domain.

The mechanical environment of a supercell is shown in Fig.1(b). Two force fields from different scales drive the motions of the cell. First part is the interaction of surrounding atoms which is from atomistic region or other supercells. Second part is stress or traction on the interface acted by macroscale region. We characterize these two external forces by external potential energies as,

$$V_{\alpha}^{atom} = \sum_{i,j \neq \alpha} \varphi(r_{ij})$$  \hspace{1cm} (4)

$$V_{\alpha}^{surf} = -S_{\alpha}^{0 \sigma_0} \cdot r_\alpha$$  \hspace{1cm} (5)

where $i$ and $j$ index atoms from different cells; $\varphi$ is the pair potential, and $r_{ij}$ is the distance between $i$-th and $j$-th atoms. $S_{\alpha}^{0 \sigma_0}$ is the surface exposed to traction $\vec{T}_\alpha$, which are both in the referential configuration.

Thus the total effect is

$$V_{\alpha}^{ext} = V_{\alpha}^{atom} + V_{\alpha}^{surf}$$  \hspace{1cm} (6)

On the other hand, the internal potential energy has similar form of $V_{\alpha}^{atom}$ which is,

$$V_{\alpha}^{int} = \frac{1}{2} \sum_{i,j \neq \alpha} \varphi(r_{ij})$$  \hspace{1cm} (7)

but here the indices $i$ and $j$ represent atoms in the same cell and there is an $\frac{1}{2}$ factor.

The kinetic energy is calculated from Eq. (1) as[28]

$$K_\alpha = \frac{1}{2} \sum_i m_i \dot{r}_i \cdot \dot{r}_i$$

$$= K_\alpha^{rigid} + K_\alpha^{cell} + K_\alpha^{atom}$$

$$= \frac{1}{2} M_\alpha \dot{r}_\alpha \cdot \dot{r}_\alpha + \frac{1}{2} \dot{r}_\alpha \cdot \phi_\alpha \cdot \phi_\alpha : J_\alpha + \frac{1}{2} C_\alpha : \sum_i m_i \dot{s}_i \otimes \dot{s}_i$$  \hspace{1cm} (8)

where $M_\alpha$ is the mass of the whole cell; $C_\alpha = \phi_\alpha^T \phi_\alpha$ is the right Cauchy-Green tensor, $J_\alpha = \sum_i m_i \dot{s}_i \otimes \dot{s}_i$ is the inertia tensor which is approximately constant in time. Originally, additional cross terms are expected in the above equation. But they are negligible so that we get rid of them to simplify the derivation. Readers may find the detailed discussion in [28].

The Lagrangian for $\alpha$-th cell can be written as,

$$L_\alpha = K_\alpha - V_\alpha$$

$$= K_\alpha^{rigid} + K_\alpha^{cell} + K_\alpha^{atom} - V_\alpha^{int} - V_\alpha^{ext}$$

$$= \frac{1}{2} M_\alpha \dot{r}_\alpha \cdot \dot{r}_\alpha + \frac{1}{2} \dot{r}_\alpha \cdot \phi_\alpha \cdot \phi_\alpha : J_\alpha + \frac{1}{2} C_\alpha : \sum_i m_i \dot{s}_i \otimes \dot{s}_i$$

$$- \frac{1}{2} \sum_{i,j \neq \alpha} \varphi(r_{ij}) - \sum_{i,j \neq \alpha} \varphi(r_{ij}) + S_{\alpha}^{0 \sigma_0} \cdot r_\alpha$$  \hspace{1cm} (9)
where
\[ M_a \mathbf{r}_a = \sum_{i \in a, j \in a} \mathbf{f}_{ij} + S_{ij} \mathbf{I}_a \]  
(10)
\[ \dot{\phi}_a \cdot \mathbf{J}_a = \left( \mathbf{\mathcal{P}}^{\text{int}}_a - \mathbf{\mathcal{P}}^{\text{ext}}_a \right) \Omega_a^0 \]  
(11)
\[ m_i \mathbf{C}_a \cdot \ddot{s}_i = \sum_j \mathbf{f}_{ij} \cdot \dot{\phi}_a - m_i \mathbf{C}_a \cdot \dot{s}_i \]  
(12)
where \( \mathbf{f}_{ij} \) is the interaction on i-th atom from j-th atom; \( \Omega_a^0 \) is the volume of the supercell in the referential configuration; and
\[ \mathbf{\mathcal{P}}^{\text{int}}_a = \frac{1}{\Omega_a^0} \left( \frac{1}{2} \sum_{i \in a} \mathbf{s}_i \otimes \mathbf{s}_i - \dot{\phi}_a \cdot \sum_{i \in a} m_i \dot{s}_i \otimes \dot{s}_i \right) \]  
(13)
\[ \mathbf{\mathcal{P}}^{\text{ext}}_a = \frac{1}{\Omega_a^0} \sum_{i \in a, j \in a} \mathbf{f}_{ij} \otimes \mathbf{s}_i \]  
(14)
are defined as internal and external first Piola-Kirchhoff (PK-I) stresses. The equations of motion have the general form of \( \ddot{\mathbf{r}} = \dot{\mathbf{f}} \). The general masses are \( M_a, J_a \) and \( m_a \mathbf{C}_a \) for three equations, respectively. The driving force for rigid body translation \( \mathbf{r}_a \) consists of two parts from atomistic interaction and macroscale surface traction. The deformation of the cell is driven by external PK-I stress while resisted by internal PK-I stress. Internal motion is induced by atomistic interactions and damped if macroscale velocity \( \mathbf{C}_a \) exists.

The adaptive nature of the supercell is due to the capability of carrying information or boundary conditions from different scales. The atomistic interaction influences motions of all scales including rigid body translation, deformation and internal degrees of freedom as seen in Eqs. (10)–(12), while macroscale information such as traction and displacement can be readily applied to Eq. (10). Moreover, we can apply an equilibrium stress state on a supercell by replacing \( \mathbf{\mathcal{P}}^{\text{ext}}_a \) in Eq. (11) with a prescribed value \( \mathbf{\mathcal{P}}^{\text{ext}}_a \). Therefore, the adaptive multiscale element is a good candidate as an messenger in transition zone for the multiscale model.

### 2.2. Macroscale modeling: Peridynamics

Peridynamics [23, 18, 24, 25] is a nonlocal computational formulation of continuum mechanics. From multiscale perspective, it may be viewed as a coarse grain model. Different from classical continuum mechanics, in peridynamics, the interaction between material points is nonlocal, i.e. for a fixed material point \( \mathbf{r}_a \) in the current configuration, it can interact with neighboring particles \( \mathbf{r}_b \) within a compact support called as horizon, which is similar to the concept of cutoff range in molecular dynamics. Here we denote the material point of interest as \( \alpha \) to be consistent with the center of mass in an adaptive multiscale element, and all other particles in the horizon as \( \beta = 1, 2, \ldots, N \). The uppercase is used to denote the quantities in the referential configuration. \( \mathcal{H}_a \) is used to denote the horizon. Interactions from material points outside the horizon are set to zero. The deformation state of a material point \( \alpha \) is associated with

\[ \mathbf{K}_a := \int_{\mathcal{H}_a} \omega(||R_a||)R_{a\beta} \otimes R_{a\beta} dV_{\beta} \approx \sum_{\beta=1}^N \omega(||R_a||)R_{a\beta} \otimes R_{a\beta} \Delta V_{\beta} \]  
(15)
where \( R_{a\beta} = R_\beta - R_a \). The shape tensor is basically a moment tensor or loosely speaking a moment of inertia tensor.
We then can define a two point nonlocal second order tensor \( \mathbf{N} \) as

\[
\mathbf{N}_{\alpha} = \sum_{\beta=1}^{N} \omega(||\mathbf{R}_{\alpha}||) \mathbf{r}_{\alpha\beta} \otimes \mathbf{R}_{\alpha\beta} \Delta V_{\beta},
\]

(16)

where \( \mathbf{r}_{\alpha\beta} = \mathbf{r}_{\beta} - \mathbf{r}_{\alpha} \). When we refer the peridynamics as a coarse grain model, we imply that the following Cauchy-Born rule is hold in each horizon,

\[
\mathbf{r}_{\alpha\beta} = \mathbf{F}_{\alpha} \mathbf{R}_{\alpha\beta}
\]

(17)

By substituting Eq. (17) into (16), we obtain the expression for the discrete non-local deformation gradient,

\[
\mathbf{F}_{\alpha} = \mathbf{N}_{\alpha} \mathbf{K}_{\alpha}^{-1} = \left( \sum_{\beta=1}^{N} \omega(||\mathbf{R}_{\alpha}||) \mathbf{r}_{\alpha\beta} \otimes \mathbf{R}_{\alpha\beta} \Delta V_{\beta} \right) \mathbf{K}_{\alpha}^{-1}.
\]

(18)

Considering the state-based peridynamics, we denote the force state at material point \( \alpha \) as \( \mathbf{T}_{\alpha}(\mathbf{R}_{\alpha}, t) \), which can determined by the stress state as the point [25] as

\[
\mathbf{T}_{\alpha} < \mathbf{R}_{\beta} - \mathbf{r}_{\alpha} >= \omega(||\mathbf{R}_{\alpha}||) \mathbf{P}_{\alpha} \cdot \mathbf{R}_{\alpha\beta} \mathbf{K}_{\alpha}^{-1}
\]

(19)

where \( \mathbf{P}_{\alpha} \) is the first Piola-Kirchhoff stress at the material point \( \alpha \).

There are two ways to generate local stress: (1) Based on atomistic potential, and (2) Based on macroscale potential. We shall discuss them as follows:

1) **Stress derived from the atomistic potential**

In this case, each peridynamics point is associated with an atomistic unit cell (see Fig. ??). The elastic energy density at each peridynamics point is

\[
W = \frac{1}{2} \sum_{i=1}^{N_b} \varphi'(r_i)
\]

where \( \varphi(r_i) \) is the atomistic potential, and \( r_i \) is the atomistic bond length in the deformed configuration. Based on the Cauchy-Born rule, we can calculate the PK-I stress by taking derivative of elastic energy density with respect to deformation gradient,

\[
\mathbf{P}_{\alpha} = \frac{\partial W}{\partial \mathbf{F}} \bigg|_{\mathbf{F} = \mathbf{F}_{\alpha}} = \frac{1}{2\Omega_k} \sum_{k=1}^{N_b} \varphi'(r_k) \frac{\mathbf{r}_k \otimes \mathbf{r}_k}{r_k}
\]

(20)

The calculation is inside an unit cell. \( k = 1, \ldots, N_b \), where \( N_b \) is the number of bonds in a unit cell. \( \varphi(r_k) \) is the pair potential of \( k \)-th bond. \( \mathbf{r}_k \) and \( \mathbf{R}_k \) are bond vectors in current and referential configuration, respectively. Cauchy-Born rule states that \( \mathbf{r}_k = \mathbf{F}_{\alpha} \cdot \mathbf{R}_k \). Therefore, if we have the deformation gradient in a material point, we can calculate the first Piola-Kirchhoff stress at the macroscale material point \( \alpha \).

The advantage of the Cauchy-Born based peridynamics is that it does not need to introduce any ad hoc the bond breaking criterion, as the state-based peridynamics usually does, which is often inconsistent with the constitutive relation. In the proposed method, we assume that the **macroscale peridynamics bond breaking is associated with the microscale bond breaking**. For instance, if the atomistic bond between \( \mathbf{R}_0 \) and \( \mathbf{R}_1 \) is broken, we assume that the bond between two macroscale points \( \mathbf{P}_0 \) and \( \mathbf{P}_1 \) is broken. The rule is assumed for the any other points in the horizon, because the macroscale horizon is a scaled copy of microscale unit cell, which may contain first, second, and higher order neighbors.

2) **Stress derived from the bond-based peridynamics**

In this case, we adopt the basic assumption of the bond-based peridynamics by assuming that there exists macroscale potential, i.e.

\[
\Psi(r_{\alpha\beta}) = \frac{c(||\mathbf{R}_{\alpha\beta}||)^2}{2} \mathbf{r}_{\alpha\beta} \cdot \mathbf{R}_{\alpha\beta}
\]
Figure 1: (a) The multiscale model consists three part: atomistic region, macro region and transition zone. The essential part is the transition zone, which is served as a messenger to translate information from both regions. A filter is constructed near the interface to solve the issue of high-frequency wave reflection. (b) The adaptive multiscale element in the transition zone. This element is an assemble of atoms which has macroscale properties such as shape and average displacement while the atomistic resolution is retained. The element is capable of carrying and translating information from different scales.

Figure 2: The Cauchy-Born rule based multiscale peridynamics
where
\[
s = \frac{\|r_{\alpha\beta}\| - \|R_{\alpha\beta}\|}{\|R_{\alpha\beta}\|} = \frac{r_{\alpha\beta} - R_{\alpha\beta}}{R_{\alpha\beta}}, \quad \eta_{\alpha\beta} := r_{\alpha\beta} - R_{\alpha\beta}.
\]

Therefore, the elastic energy density at the material point \( \alpha \) will be
\[
W = \frac{1}{2\Delta V_0} \sum_{\beta=1}^{N} \Psi(r_{\alpha\beta}).
\]

By applying the Cauchy-Born rule again, i.e.
\[
r_{\alpha\beta} = F_{\alpha\beta} R_{\alpha\beta},
\]
we have
\[
\mathbf{P}_\alpha = \frac{\partial W}{\partial \mathbf{F}} \bigg|_{\mathbf{F} = \mathbf{F}_\alpha} = \frac{1}{2\Delta V_0} \sum_{\beta=1}^{N} \Psi'(r_{\alpha\beta}) \frac{r_{\alpha\beta} \otimes R_{\alpha\beta}}{r_{\alpha\beta}},
\]
where
\[
\Psi'(r_{\alpha\beta}) = \frac{c(R_{\alpha\beta}) \mu}{R_{\alpha\beta}},
\]
where the function \( \mu \) is a material strength function,
\[
\mu = \begin{cases} 1 & s < s_0 \\ 0 & s \geq 0 \end{cases} \quad \text{and} \quad s_0 = \frac{10G_0}{c\sigma\delta^S},
\]
where \( \delta \) is the radius of the horizon, and \( G_0 \) is the material fracture energy release rate.

After determining the stress state at every peridynamics particles, we can establish a unified formulation for peridynamics based on the so-called state-based peridynamics formulation. Considering the balance of linear momentum at the material point \( \mathbf{r}_\alpha \), we have the following nonlocal balance equation,
\[
\rho_\alpha \dot{\mathbf{r}}_\alpha = \mathbf{L}(\mathbf{R}_\alpha, t) + \rho_\alpha \mathbf{b}(\mathbf{R}_\alpha)
\]
where
\[
\mathbf{L}(\mathbf{R}_\alpha, t) = \int_{\mathcal{H}_\alpha} \left( \mathbf{T}_\alpha < \mathbf{R}_\beta - \mathbf{R}_\alpha > - \mathbf{T}_\beta < \mathbf{R}_\alpha - \mathbf{R}_\alpha > \right) d\mathbf{V}_\beta
\]
is the force vector acting on \( \alpha \)-th point by neighboring points \( \beta \). The counterpart in classical continuum mechanics is \( \nabla_{\mathbf{R}} \cdot \mathbf{P}_\alpha \) which is a differential form. \( \mathbf{P}_\alpha \) is the PK-I stress in continuum mechanics. Technically, it is much easier to solve the integral form than differential form. Thus the main work left is to evaluate the force vector. In practice, since the domain is consist of discretized material points, the integral can be replaced by a summation,
\[
\mathbf{L}(\mathbf{R}_\alpha, t) = \sum_{\beta=1}^{N} \left( \mathbf{T}_\alpha < \mathbf{R}_\beta - \mathbf{R}_\alpha > - \mathbf{T}_\beta < \mathbf{R}_\alpha - \mathbf{R}_\beta > \right) \Delta \mathbf{V}_\beta.
\]

### 2.3. Construction of the filter

A common issue of multiscale methods is the reflection of high-frequency waves on the interface. Due to the larger lattice spacing of the macroscale domain, high-frequency wave components cannot be recognized. Therefore, as a result of energy conservation, high-frequency signals will be reflected back to the atomistic domain. The issue of reflection is demonstrated in Fig.3. When the wave passes the interface, the low-frequency wave transits smoothly, but the reflection of high-frequency components can be observed. Note that high and low frequencies are relative concepts compared with lattice spacings of both atomistic and macro domain. Low frequency means the wavelength is longer than intrinsic lattice spacing of macro domain, while high frequency is where the wavelength in between the intrinsic lattice spacings of the domains.
To solve the issue of reflection, we introduce a filter in the transition zone near the surface of macro domain as previously demonstrated in Fig. 1(a). The filter is similar as transition element in shape, which is also an assemble of atoms. The construction of the filter includes two steps as is shown in Fig. 4. First, we allow all wave components enter the filter. In this step, the filter is basically same as transition element, where atoms in the filter are free to move as any transition element. The motion is controlled by original dynamical Eqs. 10–12. Second step is a process of homogenization. The atomistic positions are set to an average value. The equivalent manipulation is to replace $s_i$ with its initial value $s_i^0$. Thus the homogenized atomistic position is

$$r_i = r_o + \phi \cdot s_i^0$$  (25)

The replacement is effective in Eqs. 10–11, but Eq. 12 is eliminated. It is like the internal degrees of freedom are frozen and only macroscale motions are allowed, i.e. particles are adhered on the uniform deformation of the supercell. This is an energy release process. The interesting fact of the adaptive multiscale element is that we can lock any of the three scale variables to meet the need of different resolutions. The treatment of directly sweeping the high frequency components is brutal but effective. When the waves enter the filter, a “smooth” uniform displacement is taken to replace the waves. Theoretically, all high-frequency waves are expected to be cleaned while the low-frequency components are transmitted to the macro domain. We will demonstrate the process in the numerical examples.

2.4. Implementation

The transition zone is introduced to translate information between different regions. In a mechanical system, force(stress) and displacement(strain) are two basic sets of quantities. As we discussed in last section, the adaptive multiscale element is capable of carrying all these information from both regions. Thus the message translation is seamless without unphysical consequences. We briefly state the two options of message passing on the interface as follow,

1. Traction-Force interchange. In this case, the transition zone is a separate part. The traction from macro domain acts on the transition elements, while at the same time the macro domain gets the reaction. These action and reaction has the form of macroscale traction, which is incorporated in Eq. 10. On the other side, atomistic domain interact with transition zone by atomistic forces. The procedure is concurrent in time, i.e. three domains evolve at the same time.

2. Displacement interchange. In this case, the transition zone can be treated as an overlap of both macro and atomistic domains. In MD updates, the transition elements are parts of atomistic domain. And the centers of mass are automatically updated due to the global motion of the assemble(element). The updated centers of mass are then passed to the macro domain as displacement boundary condition. Similarly, the updated macroscale displacements

Figure 3: Illustration of wave reflection. Due to the larger lattice spacing, the macro region may not be able to recognize the high-frequency components. If the total energy is conserved without releasing, these high-frequency components will reflect back to the atomistic region.
Figure 4: Construction of the filter. Step I: The filter has the same function as transition element, where all wave components propagate into the element. Step II: Homogenization. Displacements are averaged inside the filter. In practice, we set the internal variable $s_i$ to its initial value $s_i^0$, which produces a uniform total deformation.

are used by transition elements as centers of mass, while the shape and internal variables are still free of motion, as in Eqs.11~12. Meanwhile, the atomistic region updates based on the new atomic positions in transition zone.

An appropriate integration scheme is necessary for updating the quantities and facilitate the exchange of information. The advantage of the multiscale structure is not only in space but also in time. An efficient strategy is choosing larger time steps for macroscale and smaller steps for atomistic scale. There are two levels of computational cycles. The two regions are in the first level. Based on different approaches of force-traction or displacement interchange, parallel and serial algorithms can be used[28] separately. The second level is the three quantities of the adaptive multiscale element in transition zone, which are $r_i$, $\phi_i$, and $s_i$. Therefore, we have five scale variables which provide us plenty of combinations and great flexibility for choosing step sizes during time integration. On the second level, both parallel and serial algorithm are applicable based on different conditions and requirements. Velocity verlet[30] and predictor-corrector[5] are among popular integrators in particle methods. We employ them in implementing our multiscale model. Velocity verlet is used in calculating macro region, atomistic region and the centers of mass $r_i$ of transition element. Predictor-corrector is used to calculate $\phi_i$ and $s_i$ of transition element. As an example, the MD update is stated as follow,

\[
\begin{align*}
    r_i^{n+1} &= r_i^n + v_i^n \Delta t_i + \frac{1}{2} a_i^n \Delta t_i^2 \\
    v_i^{n+1} &= \frac{v_i^{n+1} + v_i^n}{2} \\
    a_i^{n+1} &= \frac{f_i^{n+1}}{m_i} + \frac{1}{2} \left( \frac{f_i^n - f_i^{n+1}}{\Delta t_i} + \frac{f_i^{n+1} + f_i^{n+2}}{2 \Delta t_i} \right)
\end{align*}
\]

In the second step, we need to evaluate force based on the new position $r_i^{n+1}$. For centers of mass of transition element and the macroscale material points, we replace $r_i$ by $r_o$ in the above equations.

We organize the general procedure of implementation in the following table,
• Determine the specific problem of interest, e.g. wave or crack propagation, etc.
• Set up parameters of the system, e.g. material, model dimension, time steps, etc.
• Initialize the whole system: initial displacement, velocity, boundary condition, etc.
• Select the type of communication: force-traction/displacement.
• Update atomistic region: Velocity-verlet by Eqs.26~28.
• Update transition zone:
  - Velocity-verlet for \( r \) in Eq.10;
  - Predictor-corrector for \( \phi \) and \( s \) in Eqs.11~12;
• Update macro region: Velocity-verlet by Eqs.26~28.
• Exchange of information:
  - Force-traction: atomic forces \( \rightarrow \) transition elements \( \rightarrow \) macroscale traction
  - Displacement: atomistic displacements \( \rightarrow \) transition zone \( \rightarrow \) macro displacements 
    \( \rightarrow \) transition zone \( \rightarrow \) atomistic displacements

3. Numerical Validation

In this section, we present two examples of 1-D and 2-D wave propagation to validate the adaptive multiscale model. Displacement exchange is demonstrated in these examples. Pairwise Morse potential is used to model the atomistic interaction, which is

\[
\varphi(r) = D(e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)})
\]  

(29)

The pair force is derived as

\[
f(r) = -\frac{\partial \varphi(r)}{\partial r} = 2D\alpha(e^{-2\alpha(r-r_0)} - e^{-\alpha(r-r_0)})
\]  

(30)

where the constants \( D = 0.0965 \) eV, \( \alpha = 2.71/\text{Å} \) and \( r_0 = 2.878 \) Å.

3.1. 1-D wave propagation

In the 1-D problem, Aluminum with an atomic weigh of 26.98 u is selected as the material under studying. The lattice space is \( a_0 = 2.878 \) Å. Each adaptive multiscale element has 5 atoms, and each peridynamical material points is chosen the same size of the multiscale element. The atomistic region consists of 475 atoms. 5 multiscale elements are located in the transition zone. A total 150 material points are assigned to the macro region. The model is shown in Fig.5. An initial Gaussian displacement is applied as,

\[
u(x, t = 0) = \begin{cases} 
  Ae^{-\frac{x^2}{2\sigma^2}} & x \leq L_c \\
  0 & x > L_c
\end{cases}
\]  

(31)

with \( A=0.01, \sigma = 200, b=0.08, \) and \( H=\sigma/5, \) in angstrom. The initial displacement is truncated at \( L_c = 4\sigma. \) The exponential term in Eq.31 is the low-frequency wave which is expected to pass through the transition zone to the
macro region. The cosine term is the high-frequency component which should be appropriately filtered and the associated energy should be released. Time steps for atomistic and macro regions are $\Delta t_a = 0.001$ and $\Delta t_m = 0.006$, respectively. For the transition elements, time steps are chosen as $\Delta t_s = 0.001$, $\Delta t_q = 0.002$ and $\Delta t_r = 0.002$. All units are in picosecond. The above selection of step sizes is just a demonstration. Practically, different combinations can be considered as long as they are fully tested to avoid lead or lag in time between different regions. During the updates, each scale or region includes several substeps. The number of substeps should be tested to ensure smooth transition.

**Figure 5:** 1-D model setup with an Gaussian initial displacement of magnitude 0.01. From left to right: atomistic domain ($0 \leq x < 1367$), transition zone ($1367 \leq x < 1439$) and macro domain ($1439 \leq x < 3598$). All units are in angstrom.

Fig.6(a) and (b) show the procedure of wave propagation without filter in transition zone. When macroscale time steps are smaller than 2250, the whole wave is in the atomistic domain. We can clearly distinguish the low- and high- frequency components of the wave. When it propagates to the macro domain, the low-frequency wave is almost entirely transmitted. However, without filter, the high-frequency component is reflected back to the atomistic domain since macro region cannot recognize this signal.

As we discussed in last section, constructing filter is simple and straightforward. In this example, we pick out 3 multiscale elements in the transition zone as filters. Fig.7 shows the location of the wave at $t=5000$ when filter is turned on. Compare with Fig.6(b), reflection of high-frequency components is largely mitigated. We may increase the size of the filter to further tune up the result.

To better exam the passage of information in the procedure, we plot the normalized energy of each region in macroscale time steps. Fig.8(a) shows the evolution of elastic energy in the atomistic region with and without filter, respectively. When the macro time steps are between 2300 and 4300, the wave transits from atomistic and macro domain. Ideally, total energy in atomistic domain should be damped off after 4300 macro time steps, as observed in the energy curve with filter. However, when the filter is turned off, we find a small amount of residual energy which is not the case in reality. The filter is capable of getting rid of more than 90% residual energy. The comparison of energy evolutions of both regions is shown in Fig.8(b). During the transition process, energy in atomistic region decreases but increases in macro region. Before and after the transition, energies are all constant with normalized value of 0 and 1.
Figure 6: Displacement at (a) $t=2250$ and (b) $t=5000$ with units of macroscale step size. No filter is placed in the transition zone.

Figure 7: Displacement at $t=5000$ with filter in the transition zone.
3.2. 2-D wave propagation

In the 2-D example, the hexagonal close-packed (HCP) plane is employed as a 2-D model. The material is aluminum with an atomistic weight of 26.98 u same as the 1-D model. The lattice constant is $a_0 = 2.878 \text{ Å}$. Same Morse potential is used for 2-D lattice. The shape of the multiscale elements in transition zone and material points in macro region is shown in Fig.9. Each multiscale element includes 9 atoms. The distance from the center of each element to the nearest neighbor is $3a_0$. The entire model is a rectangle as shown in Fig.10. A atomistic region is located at the center with 150×150 atoms. The size is calculated as $150 \times 75 \sqrt{3}a_0^2$ according to the lattice pattern. The transition zone surrounding the atomistic domain has a thickness of 5 multiscale element, in which a 2-element thickness is assigned as filter. Outside the atomistic region and the transition zone, a macro region with 160×160 material points except the central area, or a size of $480 \times 240 \sqrt{3}a_0^2$ is constructed. Similar as 1-D problem, an initial Gaussian wave in polar coordinate is applied as

$$u(r, t = 0) = \begin{cases} 
Ae^{-\frac{r^2}{2\sigma^2}}(1 + b \cos(\frac{2\pi r}{H})) & r \leq L_c \\
0 & r > L_c \end{cases}$$

(32)

Figure 8: Evolution of energy in each domain.

Figure 9: Shape of the multiscale elements in transition zone and material points in macro region.
Fig. 11(a)–(f) shows the history when the wave propagate from atomistic region into the macro region. Fig. 11(a) is the initial wave as mentioned above. Fig. 11(b) is the snapshot when the whole wave is still inside the atomistic domain. Two separate rings are formed with higher magnitude of the inner ring and lower magnitude of the outer ring. Subsequently, the outer ring passes the interface where the multiscale elements are located to aid the transition. As shown in Fig. 11(c), the interface does not cause any mismatch or discontinuity, and the outer ring is smoothly distributed on both sides of the interface. Fig. 11(d) is the time instance when the inner ring is passing the interface. We can see that even the with high magnitude and abrupt slope, the inner ring still passes under control. When the whole wave passes the interface, as is shown in Fig. 11(e), minimum residual is observed in atomistic domain even sharp corners are existed on the interface. Note that the rings will be damped when they expand the radius due to the energy conservation. In Fig. 11(e), the outer ring disappeared first. Subsequently, the inner ring is further propagating and damping in the macro domain.

![Image of initial model setup](image)

Figure 10: Initial model setup of the 2-D case. Inside is the atomistic region with rectangular shape. A larger macro region surrounds the atomistic region. Initial Gaussian wave is applied with a magnitude of 0.01.

4. Summary and Discussions

In this work, based on the multiscale micromorphic molecular dynamics theory, we proposed a multiscale computational model that can couple molecular dynamics and peridynamics. By properly constructing multiscale structure, we can incorporate macroscale quantities such as traction into the multiscale model, which makes the system capable of carrying both atomistic and macro scale information. By taking the advantage of the multiscale structure, we introduce an adaptive multiscale element to serve as a messenger on the interface or transition zone that is responsible for transferring information between different regions (scales) back and forth. We introduce the Cauchy-Born rule into peridynamics such that we can obtain the non-local macroscale constitutive relation through both atomistic potentials as well as phenomenological force potential.

By doing so, we have demonstrated that the proposed multiscale method is capable of passing basic mechanical information including force and displacement through the cross-scale interface seamlessly, which is ensured by the adaptive nature of the transition element. Construction of the filter near the interface provide a simple way to smooth out high-frequency wave without sophisticated or ad hoc numerical treatment; thus the issue of reflection is greatly mitigated. The proposed multiscale model is based on fundamental physical principles, which renders the subsequent mathematical structure simple and straightforward; more importantly, it provides insights and profound understandings on multiscale mechanics and physics.
Figure 11: History of wave propagation.

(a) $t=0$

(b) $t=320$

(c) $t=680$

(d) $t=1000$

(e) $t=1400$

(f) $t=1720$
To validate the proposed multiscale coupling method, we have implemented and analyzed two numerical examples of 1-D and 2-D wave propagation, respectively. The numerical results show that low-frequency wave can be smoothly transmitted smoothly through the cross-scale boundary, and the high-frequency wave can be filtered by turning on and off the filter. The energy evolution is monitored and observed in both cases and in regions of different scales, and the energy profile provided solid evidence for the efficiency of filtering process. The 2-D example further demonstrated the detailed message transition process through the multiscale interface.

References