Molecular dynamics-smoothed molecular dynamics (MD-SMD) adaptive coupling method with seamless transition

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SUMMARY

Smoothed molecular dynamics (SMD) method is a recently proposed efficient molecular simulation method by introducing one set of background mesh and mapping process into molecular dynamics (MD) flow chart. SMD can sharply enlarge MD time step size while maintaining global accuracy. MD-SMD coupling method was proposed to improve the capability to describe local atom disorders. The coupling method is greatly improved in this paper in two essential aspects. Firstly, a transition scheme is proposed to avoid artificial wave reflection at the interface of MD and SMD regions. The new transition scheme has simple formulation and high efficiency, and the wave reflection can be well suppressed. Secondly, an adaptive scheme is proposed to automatically identify the regions requiring MD simulation. Two adaptive criteria, the centrosymmetry parameter criterion and the displacement criterion, are also proposed. It is found that both the two criteria can achieve good accuracy but the efficiency of the displacement criterion is much better. The coupling method does not demand reduction in mesh size near the interface, and a multiple time stepping scheme is adopted to ensure high efficiency. Numerical results including wave propagation, nano-indentation, and crack propagation validate the method and show nice accuracy. Copyright © 2016 John Wiley & Sons, Ltd.

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1. INTRODUCTION

Wide applications of molecular dynamics (MD) method in various problems, such as nanowire [1], composites [2, 3], and extreme loading [4, 5], encourage researches on improving MD theories. Even with large-scale computing devices, a typical MD computation is still limited to sub-microns and nano-seconds. Efforts on increasing applicable spatial and temporal scales of MD method are one essential aspect in MD theory development.

One category of improving schemes is concurrent multiscale methods. Concurrent multiscale methods divide the whole domain into atomic regions and continuum regions. MD method or molecular mechanics method are adopted in atomic regions. Finite element method, finite difference method, mesh-free particle methods, etc., are adopted in continuum regions. A transition region (or called handshaking region) is used to connect atomic regions and continuum regions, and special techniques are always adopted in the transition region to avoid artificial effects due to mismatch between two kinds of descriptions. Typical concurrent multiscale methods include the coupled atomic and discrete dislocation method [6], the heterogeneous multiscale method [7], the bridging scale method [8, 9], the bridging domain method [10], the continuum stress and atomic force blending method [11], and combination of MD and continuum-based finite element analysis [12]. Readers can refer to, for example, [13–15] for a detailed review of concurrent multiscale methods.

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Another category of improving schemes is to reduce atomic degrees of freedom by introducing appropriate approximation to atomic potential or forces. The quasi-continuum (QC) method [16] is very successful in this aspect. The Cauchy–Born rule was introduced in QC method to calculate far-field elastic deformation. The coarse-grained molecular dynamics [17] is another pioneer work. Eidel and Stukowski [18] further developed QC method into a variational formulation with sampling energy in clusters. Liu et al. [19] proposed the atomic finite element method by computing finite element nodal forces directly from atomic potential. Xu et al. [20] improved the Cauchy–Born rule and proposed the hyperelastic-plastic constitutive model based on atomic potential. To and his collaborators [21, 22] proposed multi-resolution molecular mechanics/multi-resolution molecular dynamics (MMM/MMD) framework based on precise sampling atomic potential in finite elements. Representative atoms, sampling atoms, and non-sampling atoms were carefully classified in MMM/MMD framework so that high accuracy can be assured.

Smoothed molecular dynamics (SMD) method, as proposed in our previous work [23], can be classified into the second category of multiscale methods. SMD method is based on traditional MD method, and an extra background mesh is introduced. The atomic equations of motion are assembled onto mesh nodes to construct nodal equations of motion. Then the nodal equations are solved, and the atomic variables are updated with nodal increments. Different from MD method, the factor controlling the critical time step size in SMD method is the background mesh size. Much larger time step size, even one order higher than MD critical time step size, therefore, can be adopted in SMD method, but the overall accuracy is still well maintained [23]. The essence in enlarging time step size is smoothing out high-frequency atomic motions, so the name ‘smoothed’ molecular dynamics is used. SMD method with adaptive mesh refinement [24] and parallel SMD method [25] were developed to increase the efficiency and the applicable scale.

As high-frequency motions are smoothed, local atom disorders are not well described by standard SMD method. An improving scheme is to couple MD method and SMD method [23]. MD method is used for the regions where local atom disorders may happen, and SMD method is used for other regions. Typical examples such as nano-indentation and crack problem indicate that the coupling scheme can describe local atom disorders well and save computational resources. As the flow charts of MD and SMD methods are very similar except for the mapping process between atoms and background mesh nodes, the coupling is very straightforward and simple.

In the original MD-SMD coupling method, the MD region must be identified at the beginning of computation, which may reduce the flexibility and the efficiency of the coupling method. Dislocations emission process, which is a common process in nano-indentation and ductile fracture problems, requires that MD regions move along with dislocations. Designating a very large MD region will decrease the efficiency, but an initially small region has limited capability to describe the emission process.

An adaptive coupling method is proposed in this paper. MD regions and SMD regions are automatically converted to each other based on criteria calculated in the deformation. The MD-SMD coupling method is also improved by careful treatment of high-frequency motions at MD-SMD interface. Section 2 depicts SMD theory and MD-SMD coupling method in detail. The multiple-time-step (MTS) integration scheme is also introduced. Then the new technique for suppressing interface phonon reflection is developed in Section 3. The new technique is verified with one-dimensional and two-dimensional wave propagation examples. The adaptive coupling scheme is developed in Section 4, and the focus is on effective and efficient criteria. Then the entire MD-SMD adaptive coupling method is validated in Section 5 with benchmark examples.

2. SMOOTHED MOLECULAR DYNAMICS METHOD AND COUPLING METHODOLOGY

2.1. Smoothed molecular dynamics method

Classical MD method solves the following momentum equations

\[ m_i \ddot{r}_i = F_i = F_i^{\text{int}} + F_i^{\text{ext}}, \quad i = 1, 2, \ldots, n_{\text{atom}}. \]  

(1)
where \( m_i \) is atom mass, \( \mathbf{r}_i \) is atomic position vector, and \( \mathbf{F}_i \) is atomic force. The atom index \( i \) runs from one to the number of total atoms \( n_{\text{atom}} \). The superscript ‘int’ and ‘ext’ denote, respectively, the internal part and the external part of atomic forces, and the superposed dot denotes derivative with respect to time.

Molecular dynamics equations are usually solved with explicit time integration because of huge number of degrees of freedom. The time step size, therefore, is critical to computational efficiency. MD time step is controlled by atomic motions of highest frequency, so it is usually as small as femtoseconds.

Based on MD solution process, SMD method introduces one set of background finite element mesh and maps variables between atoms and nodal sites. Instead of solving momentum equations on atoms sites, SMD method maps Equation (1) onto nodes and constructs momentum equations on nodes as follows:

\[
M_I \ddot{\mathbf{r}}_I = \mathbf{F}_I, \quad I = 1, 2, \ldots, n_{\text{node}},
\]

where \( n_{\text{node}} \) is the number of total nodes, the nodal mass

\[
M_I = \sum_{i=1}^{n_a} N_I(\mathbf{r}_i)m_i,
\]

and the nodal force

\[
\mathbf{F}_I = \sum_{i=1}^{n_a} N_I(\mathbf{r}_i)\mathbf{F}_i.
\]

\( N_I(\mathbf{r}_i) \) is the standard finite element shape function. The summations in Equations (3) and (4) are calculated for all the atoms associated with node \( I \), that is, all the atoms in the elements node \( I \) links. Readers can refer to [23] for detailed derivation from Equation (1) to Equation (2). The number of associated atoms is denoted by \( n_a \). The nodal momentum \( \mathbf{p}_I \) can be calculated similarly to nodal mass and nodal force,

\[
\mathbf{p}_I = \sum_{i=1}^{n_a} N_I(\mathbf{r}_i)m_i\dot{\mathbf{r}}_i.
\]

So the atoms in SMD method play the role of quadrature points in finite element method. The process to calculate nodal momentum equations is almost the same as the assembling process in finite element method.

Smoothed molecular dynamics solution employs explicit time integration. At the beginning of each SMD step, atomic variables, including atom mass, atom momentum, and atom force, are assembled to nodal sites to obtain nodal variables. After solving momentum Equation (2), nodal velocities are updated with nodal accelerations. Then atomic velocities and atomic positions are updated, respectively, by nodal accelerations and nodal velocities. In other words, any increments of atomic variables are interpolated with increments of nodal variables

\[
\Delta g_i = \sum_{I=1}^{n_e} N_I(\mathbf{r}_i) \Delta g_I,
\]

where \( g_i \) and \( g_I \) are atomic variables and nodal variables, respectively. \( n_e \) is the number of nodes in one element. The background mesh can be viewed as deforming in the same way with the atoms inside each time step. At the end of each SMD step, the deformed background mesh is abandoned, and an undeformed mesh will be used at the beginning of next step. Reusing undeformed background mesh avoids possible numerical difficulties associated with element distortion.

Through the assembling and interpolation process between atoms and background mesh nodes, the controlling factor for critical time step size is altered to the background element size. SMD time
step size can therefore be much larger than MD time step size if the element size is much larger than atom spacing. The enlargement of time step size can be attributed to ‘freezing’ high-frequency motions, so that low-frequency motions allow larger time step size. It can be proved that SMD results will degenerate to MD results if the element size is small enough that any two atoms do not share nodes. Theoretically speaking, any type of mesh can be used as background mesh, but a uniform mesh with eight-noded cuboid element is most frequently used for reducing computational burden.

2.2. Multiple-time-step coupling of molecular dynamics and smoothed molecular dynamics methods

Smoothed molecular dynamics method is capable of using much larger time step size. Results of SMD method will be accurate if the deformation is gradual and high-frequency motions have little influence on the global results, but the description of local atom disorders is usually much influenced by suppressing high-frequency motions. Coupling MD method and SMD method is a natural way to achieve both high efficiency and nice accuracy. Based on the similar idea of concurrent multiscale methods, MD-SMD coupling method employs different simulation methods for different kinds of regions. MD method is used for the regions where atom disorders may happen, for example, the region under indentor or the region around crack tip. SMD method is used for the other regions.

As shown in our previous work [23], coupling between MD and SMD is straightforward owing to their similarities in flow charts. No mesh size reduction is required near the interface. A multiple-time-step (MTS) coupling technique was also developed. The emphasis of the present paper is on improvements of suppressing phonon reflections and adaptive coupling, but the entire flow chart of MTS MD-SMD coupling method is also listed in the succeeding texts for the completeness.

It is assumed that the variables at or before step \( n \) have been known. The following flow chart advances all the variables to time level \( t^{n+1} \). The velocity-Verlet scheme is chosen for time integration although any integration schemes popular in MD method can be adopted. The time step size for SMD region and for MD region satisfies \( \Delta t_{\text{SMD}} = m \Delta t_{\text{MD}} \). The outside cycle is for SMD region, and the inside cycle is for MD region. The symbol \( n + [i] \) is to indicate the time level \( t = t^n + i \cdot \Delta t_{\text{MD}} \). So \( n + [m] = n + 1 \). The atoms inside MD region are abbreviated as ‘MD atoms’, and those inside SMD region are denoted as ‘SMD atoms’.

1. Assemble nodal masses \( M^n_I \) (Equation (3)), nodal forces \( F^n_I \) (Equation (4)), and nodal momenta \( p^n_I \) (Equation (5)) from SMD atoms.
2. Solve Equation (2) for nodal accelerations \( \dot{r}^n_I \).
3. Loop for \( k = 0, 1, 2, \ldots, m - 1 \).
   (a) Update atomic velocities from step \( n + [k] \) to step \( n + [k + 1/2] \).
      - For atoms in MD region,
        \[
        \dot{r}^{n+[k+1/2]}_i = \dot{r}^{n+[k]}_i + \frac{\Delta t_{\text{MD}}}{2} \ddot{r}^{n+[k]}_i.
        \] (7)
      - For atoms in SMD region,
        \[
        \dot{r}^{n+[k+1/2]}_j = \dot{r}^{n+[k]}_j + \frac{\Delta t_{\text{MD}}}{2} \sum_{I=1}^{N} N_I (r^n_I) \ddot{r}^n_j.
        \] (8)
      - For nodes in SMD region,
        \[
        \dot{r}^{n+[k+1/2]}_I = \dot{r}^{n+[k]}_I + \frac{\Delta t_{\text{MD}}}{2} \ddot{r}^n_I.
        \] (9)

Updating variables of SMD atoms is based on the consideration that the forces exerted on MD atoms include contribution from SMD atoms. Ghost forces may arise if SMD atoms are not updated concurrently with MD atoms. It should be noted that only velocities and positions of SMD atoms are updated but not forces and accelerations.
Because updating atomic forces is the most time-consuming process in molecular simulation, advancing velocities and positions in inner cycles will influence little on the efficiency.

(b) Update atomic positions from step \( n + [k] \) to step \( n + [k + 1] \).

- For MD atoms,
  \[
  r_i^{n+[k+1]} = r_i^{n+[k]} + \Delta t_{\text{MD}} F_i^{n+[k+1/2]}. \tag{10}
  \]

- For SMD atoms,
  \[
  r_j^{n+[k+1]} = r_j^{n+[k]} + \Delta t_{\text{MD}} \sum_{l=1}^{n_c} N_l (r_j^n) \dot r_I^{n+[k+1/2]}. \tag{11}
  \]

(c) Compute forces \( F_i^{n+[k+1]} \) and then accelerations \( \ddot r_i^{n+[k+1]} \) of MD atoms at step \( n + [k + 1] \).

(d) Update atomic velocities from step \( n + [k + 1/2] \) to step \( n + [k + 1] \).

- For MD atoms,
  \[
  \dot r_i^{n+[k+1]} = \dot r_i^{n+[k+1/2]} + \frac{\Delta t_{\text{MD}}}{2} \ddot r_i^{n+[k+1]}. \tag{12}
  \]

- For SMD atoms,
  \[
  \dot r_j^{n+[k+1]} = \dot r_j^{n+[k+1/2]} + \frac{\Delta t_{\text{MD}}}{2} \sum_{l=1}^{n_c} N_l (r_j^n) \ddot r_I^n. \tag{13}
  \]

For nodes in SMD region,

\[
\ddot r_I^{n+[k+1]} = \ddot r_I^{n+[k+1/2]} + \frac{\Delta t_{\text{MD}}}{2} \ddot r_I^n. \tag{14}
\]

4. Reverse the velocities of SMD atoms to step \( n + 1/2 \) for later correction,

\[
\dot r_j^{n+1/2} = \dot r_j^{n+1} - \frac{\Delta t_{\text{SM}}}{2} \sum_{l=1}^{n_c} N_l (r_j^n) \ddot r_I^n. \tag{15}
\]

5. Compute new atomic forces \( F_j^{n+1} \) of SMD atoms at time level \( t^{n+1} \). Assemble nodal forces \( F_j^{n+1} \) (Equation (4)) from SMD atoms and then update nodal accelerations \( \ddot r_j^{n+1} \).

6. Advance the velocity of SMD atoms to step \( n + 1 \). The positions of SMD atoms after inner loop are the positions at step \( n + 1 \).

\[
\dot r_j^{n+1} = \dot r_j^{n+1/2} + \frac{\Delta t_{\text{SM}}}{2} \sum_{l=1}^{n_c} N_l (r_j^n) \ddot r_I^{n+1}. \tag{16}
\]

3. SEAMLESS COUPLING BY SUPPRESSING PHONON REFLECTIONS

3.1. Theory

One of the essential issues in coupling method is seamless transition between different regions. As SMD method can only describe waves whose lengths are not less than the element size, suppressing phonon reflection at the interface has to be considered when high-frequency waves propagate from MD region into SMD region. Otherwise, some artificial phenomena such as material melting...
may happen. A new scheme is proposed in this paper by utilizing SMD characteristics and frequency decomposition.

The new scheme applies damping forces only on high-frequency motions of the atoms in the regions surrounding MD-SMD interface, which is illustrated as the ‘transition region’ in Figure 1. The damping force $F^d_i$ is in the following form:

$$F^d_i = -m_i \frac{\dot{r}^\text{high}_i}{\Delta t_{MD}},$$  \hspace{1cm} (17)

which is derived by assuming that high-frequency motions should be eliminated in one MD time step. The assembling and interpolation process in SMD time stepping actually extracts low-frequency components from the entire atom motions. The high-frequency components can therefore be separated directly from SMD interpolations,

$$\dot{r}^\text{high}_i \approx \dot{r}_i^* = \dot{r}_i - \sum_{l=1}^{n_e} N_l(r_i) \dot{r}_I,$$  \hspace{1cm} (18)

where $\dot{r}_i^* = \sum_{l=1}^{n_e} N_l \dot{r}_I$ is the interpolated velocities. As the damping forces are exerted on MD atoms, atomic masses and momenta should be assembled to the background mesh nodes in transition region to calculate $\dot{r}_i^*$. The forces of the atoms in the transition region are appended with damping forces (Equation (17)), but these atoms are still advanced with MD flow chart.

In practical implementation, we reduce the magnitude of damping force but enlarge the transition region beyond one layer of atoms to avoid possible numerical problems aroused by sharp decrease in atomic velocity in one single step. Equation (17) is modified to the following form:

$$F^d_i = -\alpha m_i \frac{\dot{r}^\text{high}_i}{\Delta t_{MD}},$$  \hspace{1cm} (19)

which implies that high-frequency motions will be removed in $1/\alpha$ steps instead of in one single step. The value of coefficient $\alpha$ is estimated with the wave speed $c$, the time step size, and the size of the transition region $L$ as follows:

$$\alpha = \frac{c \Delta t_{MD}}{\lambda L},$$  \hspace{1cm} (20)

where $\lambda$ is a user-defined parameter. We recommend the range $[0.2, 0.5]$ for $\lambda$ based on computation tests, and it is found that the value $\lambda = 0.35$ is an appropriate value for all the following verification examples.

The essence of the proposed transition scheme is decomposition of frequencies. SMD characteristics ensure a simple but effective decomposition without additional computational cost. The aforementioned scheme can also be extended to other concurrent multiscale methods for seamless coupling.

Figure 1. Molecular dynamics–smoothed molecular dynamics (MD-SMD) coupling with transition scheme.
3.2. Verification with one-dimensional wave propagation problem

A one-dimensional example [8] is calculated to verify the seamless coupling technique. The harmonic potential is adopted, and one atom only interacts with its nearest left and right neighbors. All the values are given in reduced units. Initial displacements are given by:

\[
u(x, t = 0) = \begin{cases} 
A e^{-\left(\frac{x}{\sigma}\right)^2} e^{-\left(\frac{r_c}{\sigma}\right)^2} & 1 + b \cos \left(\frac{2\pi x}{H}\right), \\
0, & x \leq r_c \\
& x > r_c,
\end{cases}
\]

where \(A\) decides the amplitude of the wave, and \(b\) and \(H\), respectively, determines the proportion and the frequency of high-frequency components. Parameters are chosen as \(\sigma = 40\), \(A = 0.01\), \(b = 0.1\), \(H = \sigma/4\), and \(r_c = 5\sigma\).

One-dimensional computational model consists of 800 atoms, as shown in Figure 2. The left half part is MD region, and the right part is SMD region. The transition region is marked as \(\Omega_d\) in Figure 2. Initial displacement for one-dimensional wave propagation example. MD, molecular dynamics; SMD, smoothed molecular dynamics.

Figure 2. Initial displacement for one-dimensional wave propagation example. MD, molecular dynamics; SMD, smoothed molecular dynamics.

Figure 3. Results at \(t = 500\) with and without transition scheme. The length of damping region varies from \(L = 3\) to \(L = 9\).

Figure 4. Time history of residual energy in molecular dynamics (MD) region.
MD region in Figure 2. The size of background mesh is 5.0. The time steps are \( \Delta t_{MD} = 0.1 \) and \( \Delta t_{SMD} = 0.4 \). Three transition regions of different widths \( L = 3.0, 6.0, \) and 9.0 are examined. \( \alpha \) for each region is 0.0952, 0.0476, and 0.0317, respectively, based on Equation (20) as \( c = 1.0, \Delta t_{MD} = 0.1, \) and \( \lambda = 0.35 \).

As shown in Figure 3, serious high-frequency wave reflection appears in the case without transition scheme. Results also indicate that high-frequency motions can be well suppressed with the aforementioned transition scheme even when only three atoms are exerted damping forces \( (L = 3) \). Phonon reflection decreases significantly while increasing the width of damping region from \( L = 3 \) to \( L = 9 \). The total energy in MD region is plotted in Figure 4 for quantitative analysis. Nearly 67% energy is reflected to MD region if the transition scheme is not used, while the residual energy drops to only 6% for \( L = 3 \) and finally 0.6% for \( L = 9 \).

Another example with fixed transition region is calculated to study the effect of parameter \( \lambda \). The width of damping region is fixed at \( L = 20 \). Three different \( \alpha \) are chosen as 0.05, 0.0143, and 0.0083 corresponding to \( \lambda = 0.1, 0.35, \) and 0.6, respectively. All the other parameters are identical to the previous case except \( b = 0.2 \) to introduce more high-frequency motions. The initial displacements are shown in Figure 5. As shown in Figure 7, the case with \( \lambda = 0.35 \) obtains an appropriate solution with very little phonon reflection. The reflection in Figure 6 can be attributed to a sudden application of large damping forces as the parameter \( \alpha \) is relatively large, while the reflection in Figure 8 is due to inadequate absorption of high-frequency motions. The dashed lines in Figures 6–8 are reference lines only for comparison purpose. The value \( \lambda = 0.35 \) is used in the following examples.
3.3. **Quasi two-dimensional wave propagation problem**

Then a quasi two-dimensional wave propagation problem is calculated to further verify the transition scheme. A hexagonal lattice structure and the 12-6 Lennard–Johns potential are adopted. The in-plane motions are constrained, and only the out-of-plane motion \((u_z)\) is allowed. All the values are in reduced unit system. The initial \(z\)-displacement is given by:

\[
u_z(\tilde{r}_i, t = 0) = \begin{cases} 
A e^{-(\tilde{r}_i / \sigma)^2} e^{-(r_c / \sigma)^2} 
& \frac{1 + b \cos \left( \frac{2\pi \tilde{r}_i}{H} \right)}{1 - e^{-(r_c / \sigma)^2}}, \\
0, & \tilde{r}_i \leq r_c \\
& \frac{1}{\tilde{r}_i > r_c},
\end{cases}
\]

where \(\sigma = 20, A = 0.01, b = 0.1, H = \sigma / 4\), and \(r_c = 5\sigma\). \(\tilde{r}_i\) is defined as the algebraic summation of in-plane distance and transverse distance between atom \(i\) and the center. The model contains 1,249,641 atoms, and the transition region consists of 10 layers of atoms \((L = 11.2)\). The time steps are \(\Delta t_{\text{MD}} = 0.002\) and \(\Delta t_{\text{SMD}} = 0.008\), and the element size of background mesh is \(5a_0\), where \(a_0\) is the lattice constant.

Two MD-SMD region partitions are used for solving the quasi two-dimensional example. The first one, as shown in Figure 9, horizontally divides the whole region into one MD region and two SMD regions, and the transition region \(d\) is a narrow rectangular region. The transition scheme is only applied to the right MD-SMD interface, which is to compare the effects with and without transition scheme in one example. Results of the first computational model are shown in Figure 10. Serious reflections occur on the left MD-SMD interface, but no obvious reflections are observed on the right MD-SMD interface.

Then another region partition as shown in Figure 11 is calculated. Snapshots of atomic potential energy contour at \(t = 24\) are shown in Figures 12 and 13. The atom configurations along the line

![Figure 8](image-url)  
**Figure 8.** Results at \(t = 520\) with \(\alpha = 0.0083\) \((\lambda = 0.6)\). Arrows denote wave propagation direction.

![Figure 9](image-url)  
**Figure 9.** The first computational model for two-dimensional wave propagation example. MD, molecular dynamics; SMD, smoothed molecular dynamics.
Figure 10. Contour plot of atomic potential energy of the first model at $t = 32$.

Figure 11. The second computational model for two-dimensional wave propagation example. MD, molecular dynamics; SMD, smoothed molecular dynamics.

Figure 12. Contour plot of atomic potential energy of the second model without transition scheme at $t = 24$. 
A – A are shown in Figures 14 and 15. It is shown that the transition scheme can suppress most high-frequency reflections at MD-SMD interface, meanwhile low-frequency motions are not affected. The total energy of MD region (not including the atoms in transition region) is shown in Figure 16. More than 50% atomic energy is reflected to MD region if no transition scheme is adopted. But most of the high-frequency energy is absorbed with transition scheme even though it cannot be transferred into SMD region, and the energy curve with transition scheme is very close to that of MD results.

4. ADAPTIVE COUPLING METHOD

The original MD-SMD coupling method [23] requires designating different regions at the beginning of the computation. However, automatic identification and adaptive coupling is desired for practical problems, especially when local atom disorders are moving. As mentioned before, the coupling between MD and SMD method is simple and straightforward, and the only difference is whether the assembling and interpolation process is used or not. So it is quite convenient for coupling MD and SMD method adaptively. A schematic flow chart of adaptive coupling is shown in Figure 17. MD regions can be designated or not, and a background mesh covers the entire computational region at
the beginning of computation. At the beginning of every SMD step, all the elements of the background mesh are cycled to check whether the element may contain atom disorders so that MD computation is needed. If it is indicated that MD computation is required, then the atoms in the element are ‘MD atoms’, which means that the atomic variables will be updated with atomic forces or velocities directly. Otherwise, the atoms in the element are ‘SMD atoms’, which means that the atomic variables will be updated with nodal variable increments. A very narrow transition region of the width several atoms will surround SMD elements. Sub-step size $\Delta_{\text{MD}}$ will be applied to MD atoms, and a time step size $\Delta_{\text{SMD}}$ will be applied to SMD atoms.

According to the aforementioned discussion, the criterion to decide whether MD computation is needed is critical in adaptive coupling method. The criterion should indicate local atom disorder correctly, and it should also be stable to avoid frequent alternating between MD formula and SMD formula in one element. Two criteria are proposed in this paper. One is based on the centro-symmetry parameter (CSP), and the other is based on atomic displacements.

Centro-symmetry parameter is widely used to characterize various kinds of defects or surface atoms. The value of CSP is defined as follows [26]:

$$v^{\text{CSP}} = \sum_{j=1}^{n_{\text{S}}/2} |\Delta \mathbf{r}_{j} + \Delta \mathbf{r}_{j+n_{\text{S}}/2}|^2,$$

(23)
where \( n_\text{N} \) is the number of nearest neighbor atoms of the central atom for perfect lattice. \( \Delta r_j \) and \( \Delta r_{j+N/2} \) are the vectors pointing from the central atom to a pair of nearest neighbor atoms in the opposite direction. For atoms on centro-symmetric lattice sites, the CSP value will be zero. The CSP value will be obviously larger than zero if the lattice deviates from centro-symmetry, which implies that local atom disorders can be easily captured with CSP value. The CSP value of surface atom is also not zero, but it is usually much larger than that of disorder atoms.

The criterion based on CSP is given as follows:

\[
\varepsilon_{c}^{\text{CSP}} \geq \varepsilon_{\text{th}}^{\text{CSP}},
\]

where \( \varepsilon_{c}^{\text{CSP}} \) is the element CSP, which can be defined as the average of CSP values of all the atoms in the element. Spatial average over atoms is used to avoid influences of oscillations, which may be frequent in high-temperature problems. The mesh used for calculating criteria can be different from the mesh for updating atomic velocities and positions. \( \varepsilon_{\text{th}}^{\text{CSP}} \) is a threshold value.

The CSP criterion can be very accurate, but calculating CSP will be resource demanding. Another criterion based on SMD flow chart is proposed. The assembling and interpolation process in SMD flow chart smoothes local deformations, so that the difference of one variable before and after mapping process can indicate severe local deformations. The second criterion, that is the displacement criterion, records atom displacements and their values after assembling to nodes and then interpolating to atoms. The criterion is given by:

\[
\varepsilon_{e}^{\text{D}} = \| u_i - u_i^* \|_{\text{ave-e}} \geq \varepsilon_{\text{th}}^{\text{D}},
\]

where \( u_i \) is the displacement vector of atom \( i \) and \( u_i^* \) is SMD-interpolated displacement vector obtained from the assembling and interpolation process similar to Equations (5) and (6). The subscript ‘ave-e’ stands for averaging over all the atoms inside the element. \( \varepsilon_{\text{th}}^{\text{D}} \) is the threshold value.

The threshold value in the criterion plays an important role for accurate results as well as efficient computation. Generally speaking, numerical tests are needed to determine the threshold value. But for the current two criteria, a reasonable value may be selected based on the physical meaning of the criterion. As indicated in [26], face-centered cubic (FCC) metal material will remain centro-symmetric under homogeneous elastic deformation, and CSP value will obviously deviate from zero if dislocations or stack faults appear. Typical CSP value for defects is from 0.5\( \text{Å}^2 \) to less than 20\( \text{Å}^2 \) [26], so the threshold value for CSP criterion is selected as 0.5\( \text{Å}^2 \) in the following examples. The threshold value is 0.036 nm (around one-tenth of lattice constant) for displacement criterion, which is an approximate estimate for the displacement of an atom around the defect.

5. NUMERICAL EXAMPLES

Molecular dynamics–smoothed molecular dynamics adaptive coupling method with transition scheme is validated with nano-indentation and tension of cracked specimen. Copper crystal is used (lattice constant \( a_0 = 3.615 \text{Å} \)), and embedded atom potential [27] is adopted in the following examples.

5.1. Nano-indentation example

A copper block of the dimensions 40\( a_0 \times 40 a_0 \times 5 a_0 \) is indented by a soft indenter as shown in Figure 18. A cylindrical indenter whose axis along [0 0 1] direction is placed right above the copper block and moves along [0 1 0] direction. The atoms in the bottom two layers of the indented block are fixed throughout the simulation. Periodical boundary conditions are applied in [1 0 0] and [0 0 1] directions, and the upper surface of the block is free. The indenter interacts with the atoms by the following repelling force

\[
F(r) = \begin{cases} 
-K(r - R)^2, & r \leq R \\
0, & r > R, 
\end{cases}
\]
where $r$ is the distance between the center of the indenter and the atom, and $K$ is an indenter parameter. In this example, $R = 10a_0$ and $K = 10\text{eV/Å}^3$. The background mesh size is $5a_0$. The time steps are $\Delta t_{\text{MD}} = 10\text{ fs}$ and $\Delta t_{\text{SMD}} = 40\text{ fs}$. The width of the transition region is $2a_0$ and the parameter $\lambda = 0.35$. The copper block is relaxed for $10\text{ ps}$, and then the cylindrical indenter indents into the copper with constant velocity $1\text{ m/s}$.

As shown in Figure 19, the indentation forces obtained by MD-SMD adaptive coupling method agree well with MD results. The adaptive coupling method can capture the yielding point as well as describe the forces after yielding point accurately. As the model size is limited, the force-depth curves in the elastic regime are a little higher than MD curve because of the influence of SMD region. Both CSP criterion and displacement criterion can obtain accurate results, and the differences between results of two criteria are nearly negligible.

Configurations of copper block at various indentation depths are shown in Figure 20. CSP contour, which can indicate dislocations generated during indentation, is demonstrated in Figure 20. Partial dislocations nucleate below the indenter and emit downward as indentation progresses. Nucleation and emission of dislocations lead to the drop of indentation force, which corresponds to the yielding point. Results with CSP criterion are a little better than those with displacement criterion. But both the criteria can capture the nucleation and emission process well with only a little delay in the

![Figure 18. Nano-indentation example.](image1)

![Figure 19. Comparison of indentation forces between molecular dynamics (MD) results and the results of adaptive coupling method. SMD, smoothed molecular dynamics; CSP, centro-symmetry parameter.](image2)
emission process. The boundary of MD region (outer black line) and the boundary of the transition region (inner black line) are also plotted in Figure 20. It shows that MD region is enlarged automatically as the dislocations nucleate and emit. A small initial MD region is designated at the beginning in the example, although it is actually not necessary in the adaptive coupling method.

The computational cost of MD and adaptive coupling method is listed in Table I. Only about one-half of computational time is saved for adaptive coupling method, which is because the background mesh size is only $5a_0$ and $\Delta t_{\text{SMD}}$ is only four times of $\Delta t_{\text{MD}}$. The computational cost of adaptive coupling method relative to MD computational cost can be roughly estimated as follows:

$$c_r = \eta + (1 - \eta) \cdot \frac{\Delta t_{\text{MD}}}{\Delta t_{\text{SMD}}} \cdot (1 + \beta),$$

(27)

where $\eta$ is the average area fraction of MD region and $\beta$ is the ratio of the extra computational cost in one SMD time step to the cost in one MD step. For the current example with embedded atom potential, $\beta$ is around 35%. If $\eta = 1/6$ (i.e., MD region covers one-sixth of the total region), $c_r$ is about 0.45. The efficiency will be increased much if much larger SMD time step size is used, or MD region can be limited to a small range.

Table I. Computational cost of the nano-indentation example.

<table>
<thead>
<tr>
<th>Method</th>
<th>CPU time (s)</th>
<th>Ratio to MD cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>MD</td>
<td>10,597</td>
<td>1.0</td>
</tr>
<tr>
<td>MD-SMD, displacement criterion</td>
<td>5265</td>
<td>0.497</td>
</tr>
</tbody>
</table>

MD-SMD, molecular dynamics–smoothed molecular dynamics.

Figure 20. Comparison of configurations and centro-symmetry parameter (CSP) contours at various indentation depths. (a) Molecular dynamics (MD) results; (b) MD-smoothed molecular dynamics (SMD) results with CSP criterion; and (c) MD-SMD results with displacement criterion. The black lines in (b) and (c) indicate the borders of MD region and transition region.
5.2. Crack propagation example

The crack propagation example is shown in Figure 21. The model is of dimensions $50a_0 \times 104a_0 \times 5a_0$ and consists of 104,000 atoms. A $20a_0$-long crack is placed in the center of the model along [1 0 0] direction by excluding the interaction forces between two sides of the crack. SMD background mesh size is $10a_0$, and $\Delta t_{\text{MD}} = 10\,\text{fs}$ and $\Delta t_{\text{SMD}} = 100\,\text{fs}$. The width of transition region is $2a_0$ and the parameter $\lambda = 0.35$. Periodical boundary conditions are applied in [0 0 1] direction.

After relaxation for 10 ps, four layers of atoms on the top and the bottom of the model are moved, respectively, with upward and downward constant velocity 5 m/s. To reduce the vibration at the beginning of loading, ramped velocities along the tensile direction from $-5$ to 5 m/s are applied to the middle atoms as initial conditions.

Tensile forces of MD method and adaptive coupling method are shown in Figure 22, and the specimen configurations during tension are shown in Figure 23. MD-SMD curve with the displacement criterion matches well with MD curve, and the criterion can distinguish MD regions accurately. But the CSP distribution shows that only several atoms near the crack tip have large CSP values,
which indicates that the average CSP criterion is not suitable for this crack example. If the maximum CSP value in one element is used to determine whether the element should be simulated with MD formulation or SMD formulation, the results are also good (as shown in Figures 22 and 23). The displacement criterion is recommended as it works well for both the indentation example and the crack example.

The aforementioned two examples indicate that MD-SMD adaptive coupling method can obtain results very close to MD results. The overall performance of displacement criterion is better than that of CSP criterion, as the displacement criterion is more stable and much more efficient. The crack example demonstrates four times acceleration for adaptive coupling method with displacement criterion.

Figure 23. Comparison of configurations at different engineering strains. (a) Molecular dynamics (MD) results; (b) MD-smoothed molecular dynamics (SMD) results with centro-symmetry parameter criterion; and (c) MD-SMD results with displacement criterion. Color denotes region type: green for MD region, blue for SMD region, and red for transition region.
Table II. Computational cost of the crack propagation example.

<table>
<thead>
<tr>
<th>Method</th>
<th>CPU time (s)</th>
<th>Ratio to MD cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>MD</td>
<td>13,105</td>
<td>1.0</td>
</tr>
<tr>
<td>MD-SMD, displacement</td>
<td>3225</td>
<td>0.246</td>
</tr>
</tbody>
</table>

MD-SMD, molecular dynamics–smoothed molecular dynamics.

criterion when compared with MD computation, as shown in Table II. The numerical efficiency will be further increased if larger element size is adopted in SMD computation.

6. CONCLUSIONS

Smoothed molecular dynamics method is an efficient molecular simulation method, but it lacks good capability in describing local atom disorders. A much more accurate and efficient molecular simulation method by adaptively coupling MD and SMD methods is proposed in this paper. The regions where atom disorders may happen are automatically simulated with MD method, while the other far-field regions are simulated with SMD method. No mesh reduction near the interface is required owing to similarities between MD and SMD methods. Multiple time steps are adopted in MD and SMD regions to assure high efficiency.

The adaptive criteria are proposed and discussed in detail. One criterion is based on CSP, and the other is based on the differences between original MD displacements and smoothed displacements. Examples demonstrate that both the criteria can capture atom disorders and convert SMD computation to MD computation automatically. The displacement criterion is more preferred than the CSP criterion owing to much higher efficiency.

Seamless transition between MD region and SMD region is also focused on. A simple but effective transition scheme is proposed based on the characteristics of frequency decomposition of SMD method. Only the high-frequency motions are absorbed before entering into SMD region, and the low-frequency motions will not be influenced. The transition scheme is also very efficient.

Examples of wave propagation, nano-indentation, and tension of cracked specimen validate the entire method. Good agreements with MD results are obtained. Local atom disorders, such as nucleation and emission of dislocations, can be simulated accurately.

Extension of MD-SMD adaptive coupling method to much larger computational scale will be focused on in future. Combination of the coupling method with continuum-based methods is another future work. The proposed transition scheme, though utilizing SMD characteristics, can be extended to other concurrent multiscale methods to eliminate phonon reflections at the interfaces effectively and efficiently. The high-frequency motions are completely absorbed and no longer affect the remaining simulations in the present transition scheme. A future improvement may be recording the statistical information of high-frequency motions and reconstructing high-frequency motions when the wave propagates into another MD region.

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