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Adaptive smoothed molecular dynamics for multiscale modeling ☆

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ABSTRACT

In the smoothed molecular dynamics (SMD), the high frequency modes are eliminated from the motion of atoms to enlarge the time step significantly. In some situations, however, rearrangements or atoms disorder may occur. Hence, it is desirable to use MD in localized regions to capture the interesting high frequency motion, while use SMD elsewhere to save the computational cost. In this paper, an adaptive smoothed molecular dynamics (ASMD) is developed. During the simulation process, if the high frequency motions of atoms are dominant in a region, the background grid in the region is refined hierarchically until it is able to capture the high frequency motion of the atoms.

1. Introduction

With the rapid development of computer technology, computational methods have become more and more important for material design. The methods used in material research are dominated by molecular dynamics for nanoscale problems and finite element method (FEM) for macroscale problems. The molecular dynamics method is powerful in atomic simulations. Constrained by computer power, the size of the problem is limited to nanometer and nanoseconds. The traditional FEM is based on continuum law, and may encounter difficulties in tracking atoms phenomena. To cope with this problem, the smoothed molecular dynamics (SMD) was developed by the authors [1].

The basic idea of SMD comes from the material point method [2]. In SMD, atoms are rigidly attached to a background grid. The grid eliminates the high frequency modes from the motion of atoms while preserves their dominant low frequency modes. Consequently, the time step of molecular simulations could be enlarged significantly without loss of accuracy in situations where the high frequency modes possess negligible amplitudes and practical interests. However, the high frequency modes are important in situations where the rearrangement or discontinuities of the atomic lattices occur, such as in dislocation, crack, bond breakage and bound formation. To overcome this difficulty, a SMD–MD coupling scheme was developed [1], in which MD was used in localized regions while SMD was used elsewhere. However, the localized regions are required to be identified by users at the beginning of a simulation, and can not be changed during the simulation.

An adaptive smoothed molecular method (ASMD) is developed by introducing an adaptive background grid into SMD. An uniform background grid is used initially, and refined hierarchically to capture the high frequency motion of the atoms during the simulation process in regions where the high frequency motion of atoms is dominant.

2. Model and simulation

In many interesting applications, atomistic methods are only required in localized regions, and approaches that operate at larger length scales and longer time scales can be used elsewhere. The length scale and time scale of SMD are much larger than that of MD, and can be adjusted by adjusting the background grid. Therefore, we can establish an adaptive method by introducing an automatic adaption scheme into the background grid of SMD, and refine the grid automatically in localized regions while coarsen the grid automatically elsewhere.

2.1. Background grid

Unlike other multiscale method, such as the quasicontinuum method [3], the background grid used in SMD can be easily generated. The grid needs not to be graded down to atomic lattices, and the grid nodes need not to be coincided with atoms. The background grid could be refined hierarchically as shown in Fig. 1.

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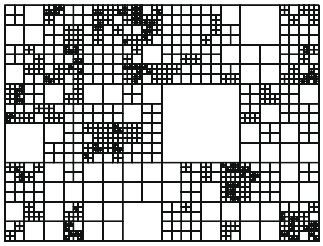

Fig. 1. Adaptive background mesh.

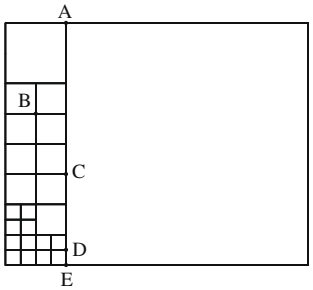

Fig. 2. The tie interface method.

2.2. Automatic adaption

To refine the gird automatically, an error estimator is required to identify the localized regions. The error estimator in a grid cell is defined as

$$\varepsilon_e = \frac{\sum_{i=1}^{N} \|\mathbf{F}_i - \mathbf{F}_i^*\|_2}{N} \quad (\|\mathbf{F}_i - \mathbf{F}_i^*\|_2 > \delta) \tag{1}$$

where $\mathbf{F}_i$ is the force of atom i calculated from the atomic potential, and $\mathbf{F}_i^*$ is the smoothed force of atom i obtained by mapping the grid nodal forces back to the atom. δ is the threshold, and N is the total number of atoms at which $\|\mathbf{F}_i - \mathbf{F}_i^*\|_2$ is larger than the threshold.

The cells whose error estimator ε_e are larger than a prescribed value of $\bar{\varepsilon}$ will be refined. When the ε_e of a parent cell and its child cells are less than $\bar{\varepsilon}$, the child cells are deleted and the parent cell is reused. the value of $\bar{\varepsilon}$ is very important to balance the solution accuracy and computational cost.

2.3. Mapping method

In SMD, the physical variables are mapped between atoms and grid nodes by using the traditional finite element (FE) shape functions. In ASMD, a node may be shared by cells with different size, such as the nodes C and D shown in Fig. 2. In this case, it is critical to guarantee the continuity of the variables between these cells. The tied interface method is used. For the inner nodes such as B, the variables can be mapped between atoms and the node by using the traditional 4-nodes FE shape functions. For the nodes share by cells with different size, such as nodes C and D, the variables are first mapped from atoms to nodes C and D by using the shape functions of the small cells, and then mapped from the nodes C and D to nodes A and E by using the shape functions of the large cell. The physical variables can be mapped back from the nodes A and E to atoms in a similar way. Therefore, the continuities of physical variables between adjacent cells are guaranteed.

3. Validation

To validate the proposed ASMD, the nanoindentation of single crystal copper, as shown in Fig. 3, is simulated. The rigid indenter is depressed at a constant velocity of 14.4 m/s in [001] direction

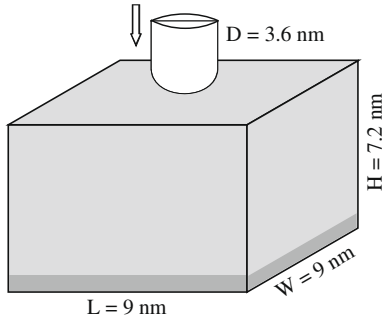

Fig. 3. Nanoindentation problem.

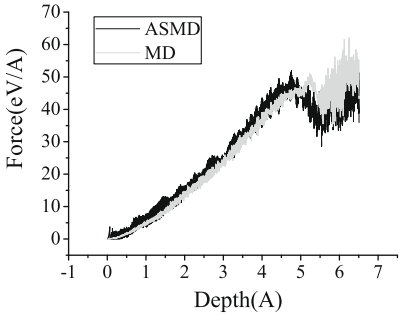

Fig. 4. Load vs. indenter displacement.

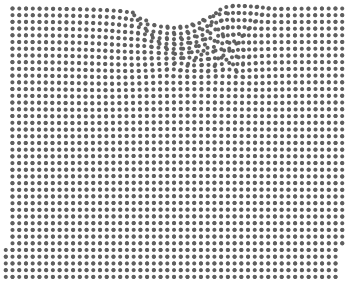

Fig. 5. Configuration obtained by MD.

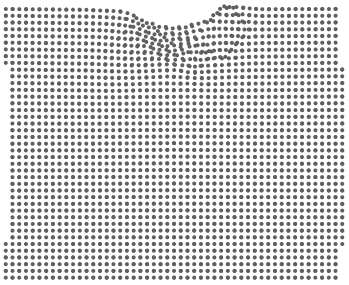

Fig. 6. Configuration obtained by ASMD.

and periodic boundary conditions are used in [100] and [010] direction. The atoms in the bottom layer are fixed. The $4 \times 4 \times 4$ background grid is used initially, and is refined automatically during the simulation.

The load–displacement curves and atom configurations obtained by using ASMD and MD are compared in Figs. 4–6. The dislocations are observed on the right side of the indenter in both MD and ASMD simulation.

The configuration of dislocations in Fig. 6 is a little bit different from Fig. 5, for the ASMD is a mixed method and the waves emitted from the indenter could be more or less reflected on the border of

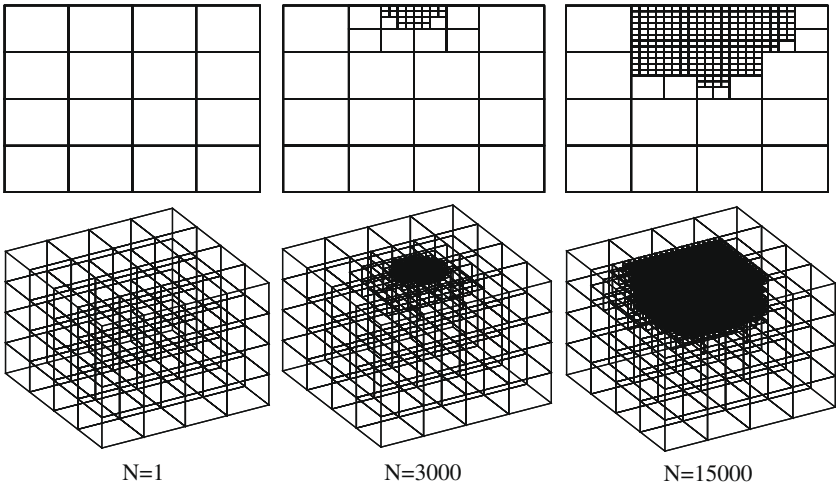

Fig. 7. The background mesh (*N* represents simulation steps).

MD–SMD. But the difference is not so great as shown in the figures. Because slight difference in 3D positions of atoms could induce great difference in 2D images of several slices of atoms under the indenter, which are used to represent atoms dislocations clearly.

In ASMD simulation, the background grid is refined adaptively in dislocation region so that the dislocation can be captured successfully. Fig. 7 shows the refining process of background grid during the simulation.

4. Conclusion

By developing an automatic adaption scheme, an adaptive SMD is proposed, which automatically refine the background grid in localized regions. Numerical results show that the proposed ASMD is able to capture the localized phenomena while operate at much larger length scales and much longer time scales elsewhere. Unlike other multiscale methods, the background cell in ASMD needs not to be graded down to the atomic lattices.

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