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An improved smoothed molecular dynamics method by alternating with molecular dynamics

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Highlights

- An alternating smoothed molecular dynamics (AltSMD) method is proposed.
- AltSMD can adopt much larger time step size than MD and achieve accurate results.
- Influences of parameters in AltSMD method are investigated in detail.
- A criterion for automatic alternating is proposed for AltSMD method.

Abstract

An effective method for nano-mechanics is presented by combining smoothed molecular dynamics (SMD) method and molecular dynamics (MD) method. SMD method was proposed in our previous work to sharply increase the feasible time step of MD. A set of background mesh was introduced in SMD and the equations of motion are solved on the background mesh nodes rather than on atom sites as in MD, which converts the controlling factor of critical time step size to the background mesh size. Much larger time step size, which can be one order larger than MD step size, can be adopted in SMD computation. But the application of SMD into problems with moving atom disorders and at finite temperature is still not satisfactory. An improvement scheme is proposed in this paper by alternating SMD computation and MD relaxation in the solution process. SMD is used at the beginning of the computation, then it is converted to MD relaxation whenever required. SMD computation continues after MD relaxation until next relaxation is needed. The conversion between MD and SMD is very convenient and straightforward owing to their similarities. The accuracy can be guaranteed by MD relaxation process, and the overall efficiency is better than MD efficiency since large time step size can be adopted in SMD computation. Examples of nano-indentation and nanowire tension validate the alternating SMD method. Influences of factors including the length of relaxation intervals and the number of MD relaxation steps are studied. A criterion automatically determining the alternating process is also proposed and validated.

Keywords: Molecular dynamics; Smoothed molecular dynamics; Multiscale computation; Nano-indentation; Nanowire

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1. Introduction

Molecular dynamics (MD) method is widely used in many scientific research fields such as fracture mechanics [1], nanowire mechanics [2,3], composites [4], and problems of extreme condition [5]. MD results have straightforward physical meaning, and a large amount of important information can be extracted. The applicable spatial scale and temporal scale of classical MD method, however, are still very limited even with fast-developed massive computing devices.

The limitation in spatial scale lies in that one point in MD method usually represents one atom, which can result in a system of millions of degrees of freedom (DOFs) in one computation. It is very costly to simulate as little as 1 μm^3 material, because the typical distance between atoms is of the order Å. Concurrent multiscale methods, which combine molecular dynamics and continuum-based modeling techniques, have been focused on to expand the spatial capability of MD. A typical concurrent multiscale method includes two kinds of regions. The core atomic region surrounds the crack tips, the dislocations or the contact lines where traditional continuum theory may fail. The continuum method is used in the far-field region. The computational cost in the far-field region therefore can be saved owing to the reduction of atomic DOFs. Handshaking region, or called the bridging region or the transition region, links the atomic region and the continuum region.

The idea of concurrent multiscale method can be traced back to the work of Kohlhoff et al. [6] in early 1990s. Other pioneer work includes Tan and Yang [7], Broughton et al. [1], Shilkrot et al. [8], E et al. [9], and the quasi-continuum method [10]. Rising interests in nano-mechanics and nano-electro-mechanical system encourage researchers to develop more accurate multiscale methods. Huge differences between discrete atomic system and continuum system may lead to mismatch on the interface of the two regions. Liu and his collaborators [11,12] proposed a bridging scale method, which can eliminate the wave reflection if high-frequency waves approach the interface. Xiao and Belytschko [13] proposed another method, called the bridging domain method, which bridged the two kinds of regions with Lagrangian multiplier and augmented Lagrangian multiplier methods. The mismatch between atomic region and continuum region was also recognized as "ghost force" in quasi-continuum method [10,14], which can be carefully eliminated from force terms. Fish et al. [15] blended the continuum equilibrium equation and the atomic force in the transition region, and the constraints in the interface region were implemented in the weak form.

Bridging the giant gap can also be dealt with by keeping the atomic potential or forces whilst reducing atomic DOFs by introducing continuum assumptions. The coarse-grained molecular dynamics [16] is a pioneer work in this field. The Cauchy–Born rule was adopted in quasi-continuum method [10] to convert atomic potential to the function of local deformation gradient. Quasi-continuum method was further improved by sampling atomic potential in clusters [17]. Liu et al. [18] proposed atomic finite element method (AFEM), which directly computed nodal forces in finite element method based on atomic potential. A linkage between atomic finite element and conventional finite element was also developed by non-local interaction. Biyikli et al. [19] proposed a multiresolution molecular dynamics framework based on sampling the atomic energy in finite elements. They carefully classified different kinds of representative atoms, sampling atoms and non-sampling atoms to improve the accuracy.

Recent investigations of concurrent multiscale methods focused more on finite-temperature problems. Dupuy et al. [20] developed finite temperature quasi-continuum method. The widely used Cauchy–Born rule in quasi-continuum method and other multiscale methods needs to be adjusted at finite temperature, and a quasi-harmonic assumption is always adopted to simplify the formulation. A finite temperature continuum theory [21] was constructed from finite temperature Cauchy–Born (FTCB) rule and Taylor expansion of atomic potential. Liu and Li [22] proposed a non-equilibrium multiscale model based on non-equilibrium MD and FTCB rule. Liu and Li [23] further combined FTCB rule and cohesive element to construct a multiscale interphase zone model, and applied the model into dynamic fracture problems. Fish et al. [24] proposed a generalized mathematical homogenization (GMH) model for finite temperature based on investigation of dynamic problem on unit cell coupled with thermo-mechanical continuum equations. Xiang et al. [25] investigated the atomic motions in a representative volume element (RVE) to construct thermo-mechanical constitutive equations. A separation of mechanical motion and thermal motion was employed, and the equations were constructed based on conservation laws. Originating from the heterogeneous multiscale method (HMM) [9], a concurrent method at finite temperature was developed and then successfully applied for brittle crack problems [26]. Anciaux et al. [27] focused on the bridging domain method, and they removed the thermal gradient in the continuum region by improving the coupling technique. Mathew et al. [28] separated the mechanical