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Chaos, Solitons and Fractals 30 (2006) 791–796
CHAOS SOLITONS & FRACTALS
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An atomistic simulation method combining molecular dynamics with finite element technique

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Accepted 30 August 2005

Abstract

A numerical method that combines molecular dynamics simulation and finite element analysis to simulate the mechanical behaviors of materials and structures at nano-scale is proposed. In this combined method, the initial atomistic model is transformed to continuum model, and an approximate solution is first obtained with the finite element method for the system under the specified boundary conditions and external loadings. Then the deformed continuum model is transformed back to form a new atomistic model, and molecular dynamics simulation is performed to quickly reach the final stable equilibrium state. An example is presented to demonstrate that the combination procedure is valid and efficient. This method can take advantages of both the efficiency of continuum mechanics method and the accuracy of atomistic simulation method.

1. Introduction

Molecular dynamics simulation can be considered as a computer experiment, which has some advantages over an actual experiment, especially at nano-scale. The interests in mechanical devices less than a micron in size for applications in nano-electro-mechanical systems [1] are growing. At nano-scale, it is possible to attain extremely high fundamental frequencies [2] while simultaneously preserving very small force constants. Many atomistic simulations, mainly using molecular dynamics method, have been carried out to investigate the mechanical behaviors of structures at nano-scale [3–6]. However, molecular dynamics method has its own shortcomings. The length size and time scale that molecular dynamics can simulate are very much limited. Current parallel super-computers can deal with up to billions of atoms, where the spatial size is still in sub-micro meters. Currently, the parallelization algorithm focuses only on spatial decomposition [7]. As to time scale, parallelization is very difficult, if not impossible. Some promising multiscale methods have been proposed [8–11]. These multiscale methods employ two strategies. One is hand-shaking regions. The

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doi:10.1016/j.chaos.2005.08.161

other is deducting continuum methods from atomistic information, such as quasi-continuum method. However, great difficulties still remain at the interfaces, computational cost and time scales.

Some interests focus on mechanical deformation of nano-structures. To check whether the system has reached an equilibrium state, some physical qualities, such as temperature and mechanical deformation, are computed and their variations with the time are monitored. When these quantities no longer vary with the time appreciably, then equilibrium is reached. The time to reach an equilibrium state depends on the initial state of the system, and how far it is initially from its equilibrium. In some cases, the final equilibrium state, rather than the process how the equilibrium is reached, is interested. From our previous work [12], it is found that for some mechanics problems at the nano-scale, continuum mechanics solutions, such as finite element method, can still give an indicative result, but an atomistic scale simulation is necessary to get more accurate results.

In this paper, our idea is to reach the equilibrium state more quickly by combining the finite element method and molecular dynamics simulation at two stages. The finite element computation is carried out at the first stage as a coarse simulation to obtain an interim state that is near to the expected final equilibrium state. At the second stage, molecular dynamics simulation is then carried out to reach the equilibrium state with much fewer time steps. In the following sections, the methodology is presented in detail and a case study is given.

2. Computational methodology

To start a molecular dynamics simulation we need to define the set of positions and velocities to assign initially to the particles. There are two ways to do this, starting from scratch and continuing a simulation. The former way is to create a set of initial positions and velocities. The positions are defined on an ideal lattice based on a certain crystal structure. Initial velocity can be defined from a Maxwell–Boltzmann distribution. Another way is to take the initial positions and velocities to be the final or any interim positions and velocities of a previous MD simulation.

Besides the above two ways to start or continue a molecular dynamics simulation, here we present a new way: starting from the result of a previous finite element analysis (FEA). Our scheme to do the combination of finite element method and molecular dynamics is shown in Fig. 1. In this figure, the left route is for general molecular dynamics simulation, and the right route is flowchart we proposed to combine molecular dynamics with finite element method. The proposed method is still an atomistic simulation method. The finite element method is employed to accelerate the speed

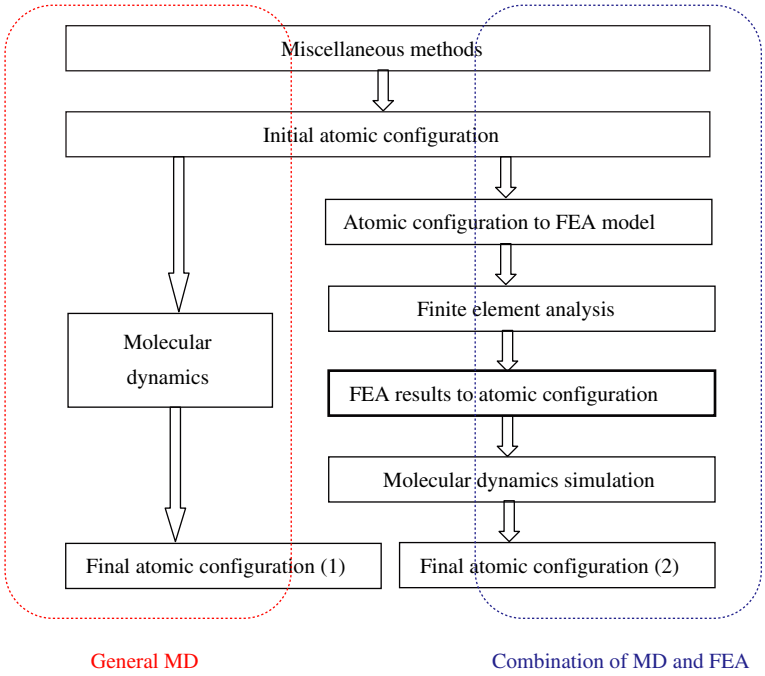

Fig. 1. Schematic flowchart of FEA/MD combination method.

of molecular dynamics simulation to reach the equilibrium state. It is not a direct coupling method of FEM and MD, which means that finite element simulation and molecular dynamics simulation is the proposed method is serial, not concurrent.

Here we present our combination method in a way that contrasts with general direct molecular dynamics simulation method. First, an initial atomic configuration for the system to be simulated is obtained with miscellaneous methods. This configuration may be a free relaxation state of the system after some molecular dynamics integration steps. For this step, both methods are the same. For general MD, the second step is to do molecular dynamics simulation of the initial configuration subjected to external loadings and boundary conditions until the final equilibrium state is reached. For a specified system and simulation temperature, the maximum time-step of molecular dynamics simulation is fixed. The simulation step should be very large to reach the expected equilibrium state, thus very long CPU time is needed. The proposed idea is that a coarse result can be obtained using finite element method, CPU time of which is negligible compared with molecular dynamics simulation. The same external loadings and boundaries are applied during finite element simulation. The FEM result is coarse compared with direct full atomistic simulation, but much closer to the final equilibrium state than the initial configuration. Then molecular dynamics simulation starts from the result of finite element simulation, so it will take much fewer simulation steps to reach the final equilibrium state. The result is that the CPU time needed is much less than full direct atomistic simulation.

There are three main problems to be tackled. One is how the FEA is performed. The second is how to transform FEA result to MD atomic configuration. The third is that whether the MD result from this configuration is the same as the direct MD result.

To perform the finite element analysis, a geometry model must be created from atomic configuration. As shown in Fig. 2, the inner rectangle is connected by the centers of four corner atoms. However, it is not the correct geometry model for this atomic configuration. Physically, an atom is not a geometrical point; rather an atom occupies a volume in space. The volume of an atom can be calculated from crystal lattice constants. The geometrical size then can be decided by lattice constants and the number of lattice. The lattice constants can change with temperature and other conditions, and it can be computed from the initial atomic configuration. The number of lattice is related with the crystal structure. For our example shown, the numbers of lattice in the two directions are 3.5 and 2.5 respectively. The correct geometry model should be the outer rectangle in Fig. 2. The actual simulation is three-dimensional, but here the figure is two-dimensional only for clarity. All atoms lie inside the geometry model, which is important for our procedure. After the geometry model is decided, the finite element analysis can be performed under the given boundary conditions and external loadings. Some approximate materials parameters are used based on macro mechanics, or based on some previous atomic simulations, because accurate materials parameters for nano-structure are not known and are just what we want to investigate.

The FEA results include coordinates of nodes, node connections of elements, displacements of all nodes. As shown in Fig. 3, a mapping from initial atomic configuration to a new atomic configuration is created in accord to the deformation of the system. In finite element analysis, an important tool is interpolation functions (as known as shape functions). The same interpolation functions are used for the transformation from FEA results to atomic configuration needed for MD simulation. For each initial atom position, first which element it lies in is computed, then the interpolation functions is computed for this atom in the element. The displacement of the nodes of the element is known, so the

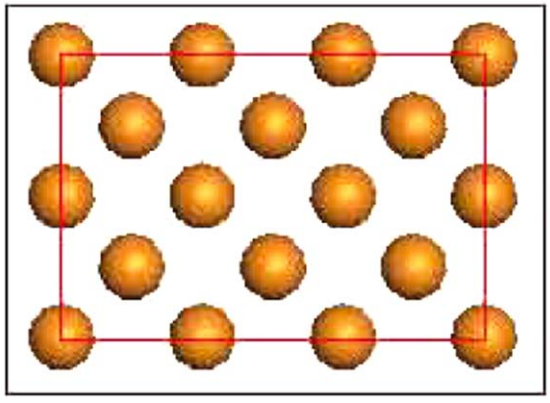

Fig. 2. From atomic configuration to geometry model.

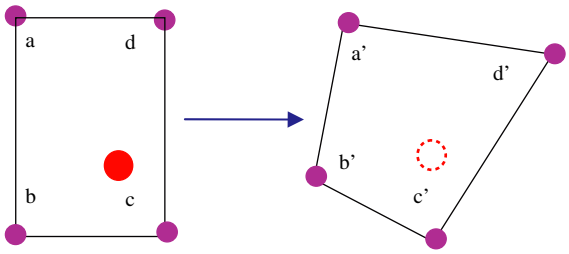

Fig. 3. Determine new atomic positions from FEA result.

displacement of the atom can be calculated. The new atomic configuration can then be obtained by adding the displacement of each atom to its initial position. Thus the FEA model is transformed to atomic model.

The continuum result is an approximate one due to small size effect at atomistic scale, but is much closer to the accurate solution than the initial atomic configuration. Molecular dynamics simulation can start from this configuration to save computational cost. Except the atomic positions, the phase space of atomic system includes atomic velocities. For above FEA computation, the temperature is not considered explicitly, but the properties of materials, such as elastic modulus, are dependent on temperatures. We assign random velocities to all the atoms with the appropriate Maxwell–Boltzmann distribution for the specified temperature. The molecular dynamics simulation continues from the atomic configuration derived from FEA results, under specified boundary conditions and external loading, to reach final stable atomic configuration. In the next section, an example is studied to validate the above proposed procedure, by contrasting with the result of direct molecular dynamics simulation.

3. One example case

A case as shown in Fig. 4 is studied. The aim is to investigate the extension properties of nano-rod using direct molecular dynamics simulation method and the combination method proposed in this paper. The size of the copper nano-rod is $5.5a \times 5.5a \times 110.5a$ (a is lattice constant, 0.3609 nm), or 1.98 nm × 1.98 nm × 39.88 nm. The total number of atoms is 13371. Its deformation under a uniform extension force is computed. Atoms of one layer at one end are fixed in length direction. An extension force of 11.82 nN is applied uniformly on the atoms of one layer at the other end. The temperature is 1.0 K.

First, molecular dynamics simulation is carried out from the ideal lattice configuration, which is free of external loading and boundary conditions. During this relaxation, the energy of the system will minimize, and the system will reach a stable equilibrium state, which is the initial atomic configuration of the following molecular dynamics simulation. Then, a finite element model is created from the initial atomic configuration. The geometry model is a cuboid. The nodes at one end are fixed in the length direction, which is in accord with the atomistic model. The extension force is applied at the other end. The deformation can be simulated using finite element techniques. The material parameters, elastic modulus and Poisson's ratio, are from our previous simulation. The properties of nano-structures are dependent on their sizes, so the parameters are approximate more or less.

Using our above presented method, we can obtain the atomic configuration from the result of FEA. Molecular dynamics simulation starts from this atomic configuration, under our given boundary conditions and extension loading.

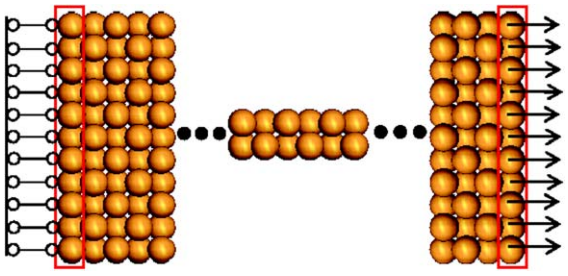

Fig. 4. Model of $5.5 \times 5.5 \times 110.5$ copper nano-rod under extension (The middle part is omitted just for clarity).

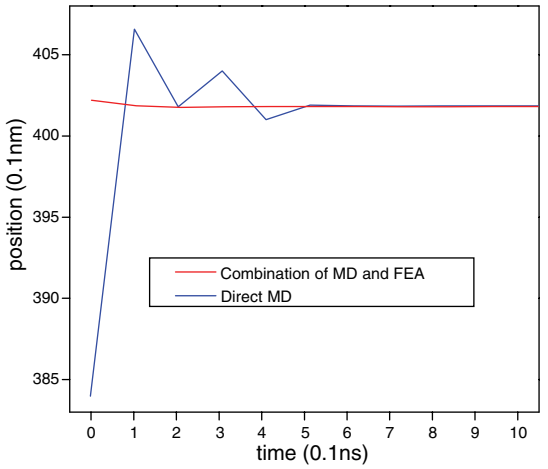

Fig. 5. The comparison of results from direct method and combination method.

As a comparison, direct molecular dynamics simulation is also carried out. The plot of the position of loading end as a function of simulation time is shown in Fig. 5. From Fig. 5, it is found that the two curves converge to the same value with the time, which means that the proposed combination method can obtain the same final equilibrium state as the direct molecular dynamics method. The simulation time to reach the equilibrium state is proportional to the integration steps of molecular dynamics, which is in accord with the computational CPU cost. From the Fig. 5, the direct method takes about 500,000 steps to reach equilibrium, while our combination method only takes about 100,000 steps, and the CPU of finite element simulation is negligible, which means that the new method cost only one fifth computational time. These results verify that the presented combination method is validate and efficient.

4. Concluding remarks

In this paper, an MD/FEA combination method to investigate the mechanical behaviors of nano-materials is proposed. This method can take advantages of both the efficiency of continuum mechanics method and the accuracy of atomistic simulation method. The case study proves that the combination method is validate and efficient. The computational cost is much reduced, while the accuracy of molecular dynamics simulation is kept. How much computational time can be saved depends on the result of the finite element analysis. The FEA result can be considered as an interim state between initial system model and final system state under external loadings and boundary conditions.

Acknowledgement

The project is supported by the National Basic Research Program of China under the grant no. 2006CB300404 and by the Scientific Research Foundation for the Returned Overseas Chinese Scholars, State Education Ministry.

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