

Review on Multi-scale Simulation Methods

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Abstract. It is by now widely recognized that not only natural but also synthetic materials are inherently of hierarchical, multi-scale character important properties and material responses can arise at a myriad of length scales ranging from atomic to microscopic to mesoscopic to macroscopic. In this article, several multi-scale research methods were introduced, focusing on the basic principles of some comparatively advanced ones. Then their advantages and disadvantages were discussed. Finally, the future development of this method was predicted.

1. Introduction

It is recognized that the material deformation and the ring of damage originate from the microscopic and atomic dimensions of the material in a large number of material and structural destruction events. The properties of the material depend on the atomic structure and the microstructure of the material [1]. In order to understand the material's deformation and destructive characteristics, we just can not focus on the macro-scale surface phenomenon. Instead, we should carry out multi-scale analysis, this includes macro-scale, mesoscale, micro-scale and even atomic-scale analytical methods. In such scales and levels, not only we could find out the causes of the problems and the basic model of research object's destruction and deformation, but also we could avoid the bad results that appearance of the outside covered the real reasons. Multi-scale analysis is important for the discovery of new mechanisms, the introduction of new methods, the improvement of materials, and the design of new materials.

2. Main analysis idea of multi-scale research

The study of multi-scale materials is to develop an effective method to make the related physical variables at different scales quantitatively related to the geometric parameters, such as stress, strain, electric field strength, electric displacement, ply thickness, etc. According to the quantitative analysis, we can simultaneously obtain the evolution of stress and strain in the microstructure and the macroscopic stress-strain curve. In this way, the deformation and break analysis of the material can be performed and the constitutive relationship of the material can be obtained. This constitutive relationship is a more precise one in which the deformation and stress of the material are coordinated at each scale. The classification of multi-scale research methods in various physics branches is different, paper [2] divides multi-scale research methods into two basic categories: serial and parallel.

The first type is serial multi-scale research method. It means, according to different time or space scales, the actual problem is divided into multiple levels, and appropriate parameters are chosen to achieve the links between different levels. According to the problems we studied, we get equivalence step-by-step from the microstructure to the macrostructure, finally the macro-equivalent properties of



the material are obtained from the bottom to up, then invert the solved macroscopic physics, we can obtain the microscopic physics from top to bottom. Based on the analysis of all levels, starting from the requirements of macro performance, we get optimization design of each layer of the material structure. In a specific analysis of a certain level, the relationship between the performance parameters of adjacent levels and the important structural parameters can be established by theoretical analysis methods or numerical simulation methods. Between different scales, some key parameters was selected for information transfer, this method is suitable for the situation where the coupling of variable groups is not so strong between different scales.

The second category is the parallel multi-scale research method. This method is mainly for numerical simulation, and it means we will simultaneously consider multiple simulations of different scales in one computational experiment. For example in a computational region of the continuous medium model the mesoscale, micro-scale, and even nanoscale will simultaneous be introduced to establish certain mathematical relationships [3]. In general, this method uses a continuous medium model in the general area, in some key areas, such as the crack tip, molecular mechanics models and even quantum mechanical models are used. The connection of the area is realized by a certain coupling method, so that the calculation amount is greatly reduced and the parallel calculation of multiple scales is realized while ensuring the accuracy [4]. This method is applicable when the coupling between the certain scale variable group is strong.

Table 1. Main methods of multi-scale analysis

Serial multi-scale research method	Parallel multi-scale research method
Finite Element Method (FEM), Extended Finite Element Method (XFEM), Boundary Element Method (BEM), Finite Volume Method (FVM), Discrete Element Method (DEM), Meshless Method, Asymptotic expansion of homogenization , Cellular Method, Voronoi Cell Finite Element Method (VCFEM), Fast Fourier Transform Model (FFT Model), Density Functional Theory (DFT), Ab Initio Molecular Dynamics (AIMD), Monte Carlo Simulation (MC), Molecular Dynamics (MD), Atomic-scale Finite Element Method (AFEM), Peridynamics (PD), Coarse Granulation method (CG),etc.	Multi-scale Finite Element Method (MsFEM) Multi-scale Finite Volume method (MsFV), Extended Multi-scale Finite Element Method (EMsFEM), Macroscopic Atomistic Ab initio Dynamics MAAD, Coupled Atomistic Discrete Dislocations (CADD), Continuous medium-molecular dynamics stacking method, Bridged Scale Method (BSM), Bridged Domain Method (BDM), Quasi Continuum method (QC), Coarse Grained Molecular Dynamics (CGMD), Heterogeneous Multi-scale Method (HMM), etc.

2.1. Molecular Dynamics method (MD)

In classical molecular dynamics, each atom under the action of a potential field force is considered to be moved by Newton's law. It generally does not consider the effects of electronic motion. Although its accuracy is not as good as that based on the first principle of quantum mechanics, as long as the vibration frequency of atoms is not very large, this treatment is a good approximation to the molecular system. It has the advantages of simple program and less calculation, compared to considering the first principle of quantum mechanics.

Molecular dynamics generally adopts Cartesian coordinates. In a simulation system, the position of any point i in the interacting material points with a total of N can be represented by the radial vector

r_i of the material point and the projections x_i , y_i , and z_i on the three mutually perpendicular axes. the differential equation of motion with N particles can be written as follows using the Lagrange function L :

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{r}_i} - \frac{\partial L}{\partial r_i} = 0, \quad i = 1, 2, \dots, N \quad (1)$$

In the above formula, the Lagrange function L is a function of the particle position vectors r_i and \dot{r}_i . For a free non-interacting particle system with a total of N , the Lagrange function that satisfies its requirements can be represented by the function T :

$$L = T = \sum_{i=1}^N \frac{m_i}{2} (\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2) = \sum_{i=1}^N \frac{m_i \dot{r}_i^2}{2} \quad (2)$$

Considering the particle interactions, the potential energy function U must be added to the formula, it depends on the interaction between atoms. After calculation, we can get the classical molecular dynamics equation expressed by Newton's second law:

$$m_i \ddot{r}_i = - \frac{\partial U(r_1, r_2, \dots, r_n)}{\partial r_i} = F_i, \quad i = 1, 2, \dots, N \quad (3)$$

In the formula, the force F_i is the sum of the forces acting on i around the particle. It shows that if you know the potential energy function U , you can get the force F_i , so the potential energy function is the key to studying molecular dynamics, and it is also the focus of many articles. However, the process is complicated because of the complex quantum effects that occur within the atom, this quantum effect is the source of formation of binding energy and valence electrons. It also determines the formation, destruction, and spatial distribution of interatomic bonds. It can be seen that the method of molecular dynamics is to use the integral of differential equations of motion to calculate the properties of an atomic system. The specific approach is to obtain a numerical solution of the particle motion equation on a computer, so we should pay attention to its error range.

The molecular dynamics gives the material structure, deformation and motion law at the atomic scale, these laws are the foundation of various physical, chemical and biological phenomena. But it should be pointed out that various simulation methods also depends on the computer itself. Although the computing power of computers is increasing, it has not been possible to extend the research scope of molecular dynamics to the dimensions of continuous media for a long time.

2.2. Macroscopic atomistic ab initio dynamics (MAAD)

In practice, if the number of atoms considered in the calculation of molecular dynamics under computer conditions is several million atoms, then the material it contains is approximately $0.1 \mu\text{m}^3$. This shows that it is difficult to meet actual requirements only by the calculation of molecular dynamics. Therefore, we need to change the single-scale simulation method of molecular dynamics and couple atomic-scale simulations with analog scales of other spaces. The Macroscopic atomistic ab initio dynamics (MAAD) developed by Abraham and Broughton et al. has a groundbreaking significance [5, 6, 7]. The basic idea of this method is to connect tight-binding (TB), molecular dynamics (MD) and finite element methods (FEM) together in a unified way to perform calculations

with quantum, atomic, and macroscopic dimensions at the same time. When these three types of operations are performed simultaneously, on the one hand, the result of one operation is passed to the other two computing areas, and on the other hand, information received from other computing areas is also accepted. For example, in the study of crack propagation in solids, five areas were divided. They are the macroscopic continuous medium region using the finite element method, the molecular dynamics region, the crack tip region analyzed by the tight binding method, the handshake region between the finite element and the molecular dynamics region, and the handshake region between the molecular dynamics region and the crack tip region.

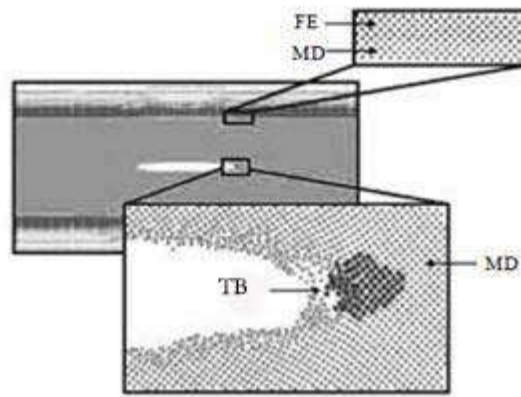


Figure 1. Tight binding (TB), molecular dynamics (MD) and finite element (FE) regions.

The Hamiltonian function of the total energy of the entire system is expressed as:

$$H_{tot} = H_{FE} + H_{FE/MD} + H_{MD} + H_{MD/TB} + H_{TB} \quad (4)$$

Each item represents the energy function of the respective area and the transition area.

$$H_{MD} = \frac{1}{2} \sum_{i=1}^n \frac{p_i^2}{m_i} + U(r_1, r_2, \dots, r_n) \quad (5)$$

$$H_{FE} = \frac{1}{2} \int_{\Omega} \varepsilon_{ij}(r) C_{ijkl} \varepsilon_{kl}(r) d\Omega + \frac{1}{2} \int_{\Omega} \rho(r) (\dot{u})^2 d\Omega \quad (6)$$

In the above formula, ε_{ij} is the second-order tensor, C_{ijkl} is the fourth-order elastic stiffness, ρ is the density, Ω is the volume of the material region, and \dot{u} is the particle velocity.

The total potential energy of the tightly bound zone can be expressed as:

$$U_{TB} = \sum_{n=1}^{Nocc} \varepsilon_n + \sum_{i,j(j>i)} V^{rep}(r_{ij}) \quad (7)$$

This formula can be understood as the total potential energy is the combined effect of the atomic attraction term ε_n and the repulsion term V_{rep} . See related papers for reference [8].

For the handshake area, the atomic region is on one side of the transition region, and the continuous media region described by the finite element mesh is on the other side. In the transition area, the nodes

of the finite element mesh are placed on the skeleton of the atom lattice. However, except for atoms on the interface, most of the atoms are not on the nodes of the finite element, its potential energy is determined by an interpolation function. When the interface changes to the continuous medium region, the size of the finite element becomes larger and larger, and finally fills the entire model space. Among them, a padding zone is arranged on the finite element region of the boundary, and a pseudo-atom zone is arranged in the zone, which coincides with the physical space of the finite element zone. The purpose of designing this padding zone is to provide a more realistic environment for real atoms on the other side of the boundary so that there are enough atomic atoms at the interface to provide atomic forces. MAAD adopts the weighted average method and its expression is:

$$H_{FE/MD} = \omega_{MD} H_{MD} + \omega_{EF} H_{EF} \quad (8)$$

$$H_{MD/TB} = \omega_{MD} H_{MD} + \omega_{TB} H_{TB} \quad (9)$$

In the above formula, ω represents a weighting factor, and its value is not strictly based on.

MAAD is the initial attempt in a multi-scale analysis method, and it get satisfactory results. In the multi-scale method developed later, although some methods and ideas of MAAD have been absorbed, there is little work that spans such a large scale at a time. MAAD can only be used when the temperature is absolutely zero, under this condition, the kinetic energy of the atom is zero and the system studied is a static system. Broughton, one of MAAD's founders, later proposed a coarse-grained multi-scale method with Rudd in 1988, this method emphasizes the coupling of molecular dynamics and contact media without taking the tight binding method into account [9, 10].

2.3. Quasi Continuum Method (QC)

The Quasi Continuum method (QC) was proposed by Tadmor and Ortiz et al. in 1996[11]. Its purpose is to build a complete atomic system without having to explicitly calculate every atom. The QC method defines two types of atoms: locally characterized atoms and non-locally characterized atoms, but not defining atomic scale regions and continuous media regions. However, in fact, non-local atomic regions should be understood as real atomic regions, and local atomic regions should be understood as finite element regions. The QC method also introduces spacer atoms for smoothly transferring the atomic region to a continuum area, the coordinate r_p is obtained by interpolating the positions of the finite element nodes, and the energy of the padding atoms is not included in the energy of the system. In order to avoid excessive calculation of the energy of interface atoms and finite element nodes, the energy of the finite element connected to the interface is calculated by the weighting method. The total energy of QC method is:

$$E_{QC} = \sum_{i \in (A,D)} E_i(r_A, r_I, r_P) + \sum_{\mu} \omega_{\mu} E_{\mu} \quad (10)$$

The first term in the formula denotes the energy of atoms in the atomic region and the interface. The second item represents the energy of the finite element, A is the atomic region, I is the interface region, P is the finite element number, and ω is the weighting function, the energy E of each unit is determined by the Cauchy-Born rule.

In addition to the several methods described above, there are some multi-scale simulation methods. Such as Coupled Atomistic Discrete Dislocations (CADD) by Shilkrot et al, or the methods on the table 1 [12- 19].

3. Prospects

People have long recognized the importance of multi-scale analysis, but the lack of related models and methods has led to multi-scale analysis that has only recently attracted widespread attention and formed a research boom. But so far, an effective multi-scale method that can span large scale ranges has not yet emerged, one of the keys is the lack of an effective method to quantitatively link the microstructure of the material with the macroscopic properties of the material.

Our future direction of development is: (1) Develop micro-scale, mesoscale and macro-scale analysis methods, so that we can link small-scale analysis with large-scale analysis to form a complete multi-scale analysis system. (2) Study more accurate coupling methods and develop multi-body potential functions to accurately describe the micro-mechanical effects of materials and improve the reliability of simulations. (3) Using more accurate and effective algorithms to reduce the amount of calculation while ensuring simulation results. (4) Extend the scope of application and realize the application in new materials. In recent years, the development of new materials is very rapid, multi-scale composite mechanics analysis method can effectively promote the development and design of new materials. However, the current multi-scale analysis method is more applied to the performance prediction of composite materials. How to use multi-scale mechanics to conduct micro-material design still needs further exploration.

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