International Journal on Recent Technologies in Mechanical and Electrical Engineering (IJRMEE) ISSN: 2349-7947
Volume: 3 Issue: 3 42 – 47

A review of multiscale methods and their applications in modeling and simulation of engineering problems

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Abstract—In this paper, molecular dynamics and some multiscale methods are reviewed, including the temperature-related homogenization technique for nanoscale continuum approaches and the bridging domain coupling method. Those methods have been applied to solve different engineering problems, such as materials science and material phase change problems.

Keywords-*multiscale, hierarchical, concurrent*

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To accelerate and foster maturation of technology that enables novel engineering materials and devices to become smaller, lighter, more lethal, more survivable, multi-functional, and autonomous, simulation techniques play an important role in exploiting revolutionary new concepts and engineering design procedures. Recent developments in nanotechnology demand that nano/micro scale building blocks will complement and enhance new engineering techniques in the relevant technology areas, including sensors, materials, systems, devices, and components. Therefore, an aggressive development of new computational methods and tools is required to address mechanical, structural, chemical, and electrical phenomena encountered in micro- and nanoscale structures, interfaces and bulk specimens.

Molecular dynamics (MD) has become one of the powerful tools for revealing complex physical phenomena at the nano- or atomic scale [1]. In the MD method, atoms are mathematically modeled as particles that follow the classical Lagrangian mechanics. Kinematics of atoms are updated via solving Newtonian equations of motion. MD modeling and simulation has been widely used to study mechanics of nanomaterials. For example, MD simulations were used to study the temperature effects on tensile mechanical properties of single tungsten nanowire [2], and it was observed that the elastic modulus, tensile strength, and strain of phase transition decreased with increase in temperature. In another research [3], mechanical properties of copper nanowire ranging from 2 to 20 nm (diameters) under different tensile loads were studied via MD simulations. It was found that mechanical responses, including yield strain, Young's modulus, and resilience, were directly related to the proportion of surface bulk type atoms presenting in each nano wire. MD simulations were also applied to study carbon nanotube (CNT) based devices. The mechanical behavior of nanotube-based oscillators was simulated by MD method [4]. In addition, Choi et al. [5] studied CNT reinforced aluminum composites under uniaxial tensile loading and investigated fracture mechanics at atomic scale considering plastic deformation and crack evolution inside the composite matrix material. The simulation results showed the contribution of CNT inclusions on the composite mechanical properties. Besides the mechanical properties, the thermal feature of CNT, including the heat transfer between CNT and its neighboring materials was simulated via MD [6]. MD simulations were also capable to describe the material failure phenomenon. Zhou et al. studied the crack propagation mechanisms of Al/SiC (silicon carbide) interfaces [7] with four crack propagation modes to determine the adhesive strength coefficient for various crack interface types. They also studied the effect of adhesive strength of interface on the mechanism of crack propagation along the interface of metal/ceramic nanocomposites.

MD modeling and simulation was also employed in other research fields of engineering. Due to difficulties in consistently machining ceramic in its ductile regime, caused by sudden and rapid tool wear, accurate understanding of tool wear mechanism of SiC is needed in order to identify measures to suppress wear so that the operational cost can be minimized. Goel et al. [8] conducted MD simulations to understand the tool wear mechanism of SiC, which is a material of great

technological interest for engineering applications. Their simulations showed that the abrasive action which resulted in locally high temperature and caused tool wear of SiC. In addition, they developed a novel method for quantitative assessment of the progression of diamond tool wear. Zhang et al. [9] employed MD to study the wetting behavior of three soil minerals of quartz, orthoclase and muscovite. The wetting process of the soil minerals were simulated and the contact angles were determined from the time average density profiles.

Molecular modeling and simulation are capable tools for material phase change problems. Wei et al. [10, 11] studied ice melting at the nanoscale. They found that the ice melting speed was very rapid at the beginning and then decreased with time at the nanoscale. Comparison of the ice melting speed at the nanoscale to the ones at the micro and macro scales is shown in Fig. 1, where the dotted lines represent the predicted ice melting speeds at the nano and micro length scales with larger time scales. It should be noted that not only were various length scales considered but also the corresponding time scales were considered in this case. The melting speed at the nano length/time scale was much faster than those at the microscale and macroscale. Furthermore, ice melting speeds decreased with time evolution. If only considering various length scales, the ice melting speed at the nano length scale decreased with time. At the micro time scale, melting speed was slower than that at the micro length scale. Similarly, at the macro time scale, the melting speeds at the micro and nano length scales were slower than those at the macro length scale. The results illustrate that the ice melting speed was scale dependent.

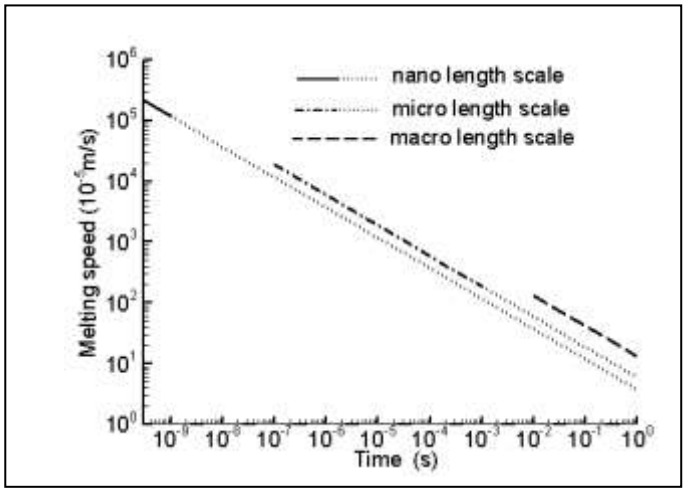

Figure 1. Ice melting speeds at various scales.

Although large molecular models containing millions or billions of atoms can be simulated with parallel computation, MD exhibits severe limitations with respect to both length and time scales. For example, even a cubic volume of 10^{-3} μm^3 may contain billions of atoms, and a typical time step in MD simulations is only about a femtosecond (~10^{-15} s). Such limitations prevent one from using MD in studying numerous phenomena such as material failure, which needs to be investigated at both large and small scales. At present, a complete modeling of micro/nano materials and devices using MD simulation is unrealistic using today's most powerful supercomputers. Therefore, the development of efficient numerical methods, which are capable of addressing various length and time scales, is very important. Such numerical methods are called multiscale methods. Multiscale methods can be divided into two classes: Hierarchical and concurrent multiscale methods. Most hierarchical models contain a continuum approximation based on the properties of a subscale model, such as a MD model. The intrinsic properties of the material are determined at the atomic level and embedded in the continuum model according to a homogenization procedure. Concurrent multiscale methods employ an appropriate model in different subdomains to treat each length scale simultaneously.

Hierarchical approaches have also been referred to as sequential, serial, or message-passing methods. Hierarchical multiscale modeling is one of the bridging methodologies for different scale models using statistical analysis methods, homogenization techniques, or optimization methods to distinguish the relevant cause-effect relations at the lower scale and to determine the relevant effects for the next higher scale. In other words, the hierarchical methodology attempts to piece together a hierarchy of computational approaches in which large scale models use the coarse-grained representations with information obtained from small scale models. This hierarchical modeling approach has proven effective in systems where the different scales are weakly coupled. A typical hierarchical multiscale method is the quasi-continuum method [12, 13], which employs energy minimization techniques. Indeed, most hierarchical methods employ homogenization techniques so that nanoscale continuum modeling can be achieved. A commonly used homogenization technique is the Cauchy-Born (CB) rule [14] with a hypothesis that assumes the lattice vectors deform as line elements within a locally homogeneous deformation. Arroyo and Belytschko [15] introduced a so-called "exponential Cauchy-Born rule" (ECB rule) to overcome the difficulties of conventional CB rule in approximating curved membranes

Hierarchical multiscale modeling has been applied to study novel materials in the area of materials science and engineering, such as composites, polymers, biomaterials and etc. Ghanbari and Naghdabadi [16] used a hierarchical multiscale modeling scheme to analyze cortical bone considering its nanostructure. Their method consists of two boundary value problems, one for macroscale and the other for microscale, and the two levels were coupled using the computational homogenization. At every material point in which the constitutive model is needed, a microscale boundary value problem is defined using a macroscopic kinematical quantity and solved. Using this method, they obtained the

mechanical properties of cortical bone with different mineral volume factions (MVF) and the results compared well with the available experimental data. Johnston and Harmandaris [17] developed a coarse-grained model for polystyrene on the gold surface using a hierarchical multiscale modeling approach. During the model verification, the density, structure, and conformational properties of coarse-grained films were found to be in excellent agreement with all-atom ones via MD simulations. The coarse-grained model was then used to study the structural and conformational properties of polystyrene films with various thickness and chain lengths. Zhang et al. [18] used the hierarchical multiscale approach to study the tensile strength of fiber-reinforced plastic matrix composites. The model couples phenomena across a wide range of length scales, starting from detailed micro-scale phenomena to macro-composite behavior. The proposed multiscale modeling involves the passing of key information from smaller to larger scales. The approach also employs the matrix plasticity at meso-scale to obtain the local stress transfer around a broken fiber.

In recent years, researchers are starting to implement hierarchical multiscale approaches to mechanical manufacturing processes. Welding is one of the most widely used manufacturing processes for joining mechanical components. During the welding process, the microstructure of the base material changes locally, and it leads to altering mechanical properties in the weld and the neighboring heat affected zone (HAZ). Wudtke et al. [19] presented a hierarchical multiscale method to capture the variation of the mechanical properties in the HAZ. In this model, micro-graphs of different points along the HAZ were used to build numerical representative volume elements (RVEs) which took into account different microstructure of the material in different locations. In addition, hierarchical modeling approach finds its application in the forming process of hexagonal close packed (hcp) materials that undergo abrupt grain reorientation due to twinning activity during forming process. He et al. [20] applied this hierarchical multiscale modeling approach in texture evolution during forming simulation of hexagonal materials like zirconium alloy to accurately capture the hardening behaviors of hcp metals during plastic deformation. Another hierarchical multiscale was developed to model the coupled evolutions of crystallographic texture and plastic anisotropy in sheet metal forming of polycrystalline metallic alloys [21]. In this hierarchical multiscale model, the homogenized micro-scale stress response given by the micro-scale model was approximated by an analytical plastic potential function.

Besides materials science, hierarchical multiscale modeling has also been extensively used in chemical engineering. Vlachos et al. [22] outlined a hierarchical multiscale simulation framework and discussed multiscale models based design of experiments to optimize the chemical information content of a detailed reaction mechanism. The design can be used to improve the fidelity and accuracy of reaction models. Chen and co-workers [23] demonstrated a hierarchical multiscale approach of steam reforming with models at both the atomic and molecular level. Wirth et al. [24] outlined a hierarchical multiscale approach to model the radiation damage. The approach was based on the past information on parameters and controlling mechanisms from different scales and the results illustrated a range of phenomena occurring during irradiation in the fusion environment.

In addition, there are more interesting applications of hierarchical multiscale modeling in engineering. Bretzner et al. [25] presented a system for hand tracking and hand posture recognition with multiscale color feature hierarchies for representing hand shape and particle filtering with hierarchical layered sampling for simultaneous tracking and recognition of hand states. Aarnes et al. [26] developed a hierarchical multiscale method for two-phase flow in highly heterogeneous porous media based on a mixed finite-element formulation. They also introduced adaptive strategies for the coarse grids to improve the accuracy of the multiscale solution and resulting very flexible with respect to the size and the geometry of coarse-grid cells. Lv et al. [27] presented a new hierarchical multiscale approach to the thermo-electromechanical behaviors of the smart materials composed of highly heterogeneous piezoelectric microstructures. Three types of multiscale numerical base functions were constructed to capture the small-scale information of thermal, electrical and mechanical fields, respectively. Yu et al. [28] developed a hierarchical multiscale model for all-vanadium microfluidic fuel cells with porous electrodes in which the diffusion coefficient was used as a bridge between the microscale, mesoscale, and macroscale models.

However, most homogenization techniques utilized in the proposed hierarchical multiscale models have the assumption of zero temperature. To consider temperature effects on the mechanics of materials, a temperature-related homogenization technique must be employed to derive the stress-strain relation in the continuum model. Xiao and Yang [29-31] developed a new homogenization technique, i.e. the temperature-dependent Cauchy-Born (TCB) rule. In the TCB rule, there are several assumptions: (1) the deformation is locally homogeneous; (2) the vibration of the atom is harmonic; (3) coupled vibration of different atoms is negligible; and (4) atoms have the same local vibration modes. The free energy, W_H, of a crystalline solid at a temperature of T within the continuum model can be expressed as

$$W_H(\mathbf{F},T) = \int_\Omega w_C(\mathbf{F})\,d\Omega + n\kappa_B T \int_\Omega \rho^q \ln\left[\hbar\left(\bar{D}(\mathbf{F}(\mathbf{X}))\right)^{1/2n} \Big/ \left(2\pi\kappa_B T\right)\right] d\Omega \quad (1)$$

where w_C is the potential energy per unit volume at zero temperature, n is the number of the degrees of freedom per

atom, κ_B is the Boltzmann constant, $\hbar = h/2\pi$ where h is Planck's constant. ρ^q is the number of atoms per unit volume, and $\bar{D}(\mathbf{F})$ is the determinant of the local dynamic matrix of an atom in the molecular structure subjected to a homogeneous deformation gradient **F**. With the TCB rule, the first Piola-Kirchhoff stress in the continuum model is then obtained from the free energy density, w_H, as

$$\mathbf{P}(\mathbf{F},T) = \partial w_H(\mathbf{F},T) / \partial \mathbf{F} \quad (2)$$

This equation serves as the constitutive relations in the continuum models. Xiao and Yang [29] has completed verification of the TCB model by performing stress analyses of various nanostructured materials at different temperatures. They implemented the TCB rule in the thermo-mechanical coupling model to study crack propagation in a nanoplate with an initial crack [30]. Once the crack propagates, some bonds in front of the crack tip are broken. The released energy results in a temperature increase in the surrounding domain around the crack tip. Furthermore, a temperature increase results in the reduction of cohesive traction in the cohesive zone in front of the crack tip. Consequently, the crack propagation speed increases gradually. Fig. 2 illustrates the temperature contour in the nanoplate during crack propagation. The temperature concentration occurs around the crack tip, and temperature propagates from the crack tip to the remaining domain

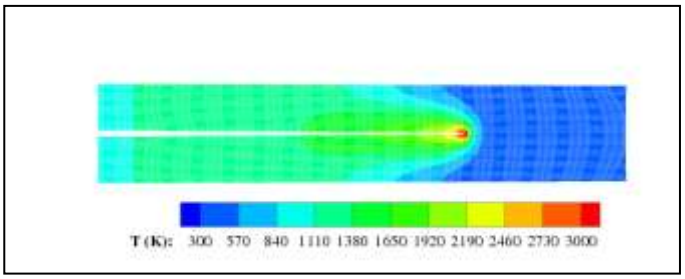

Figure 2. Temperature contour during crack propagation.

Concurrent approaches attempt to link methods appropriate at each scale together in a combined model where the different scales of the system are considered concurrently and communicate with some type of hand-shaking procedure. This approach is necessary for systems that are inherently multiscale, in other words, systems whose behavior at each scale depends strongly on what happens at the other scales. In a concurrent simulation, the system is often partitioned into domains characterized by different scales and physics. The challenge of the concurrent approach lies at the coupling between the different regions treated by different methods, and a successful multiscale model seeks a smooth coupling between these regions. Fish [32] reviewed several classes of existing concurrent schemes. In the Domain Bridging schemes, the continuum and discrete subdomains are overlapped and the Hamiltonian energy on the overlapped region is given as a weighted average of the continuum energy and the discrete energy. In the Local Enrichment schemes including the bridging scale method [33, 34], the solution is assumed to be the sum of coarse and fine approximations, $u = u^c + u^f$, whenever the coarse and fine domains overlap, and as u^f is enriched it converges to the fine scale description. Finally in the Multi-grid schemes, the high and low frequency responses are dealt with separately. The coarse scale model captures the low frequency response, and the fine scale model captures the high frequency corrections. The multiscale prolongation operator is then the sum of the classical smooth prolongation and the fine scale correction.

In a pioneering work, Abraham et al. [35, 36] developed a methodology called MAAD (Macro-Atomistic-Ab initio-Dynamics), in which a tight-binding quantum mechanical calculation is coupled with MD and, in turn, coupled with a finite element (FE) continuum model. A so-called handshake region was employed to couple different scales in the MAAD method to simulate crack propagation in silicon. Greco et al. [37] proposed a concurrent multiscale model for simulating crack propagation in fiber-reinforced composites, where both fiber/matrix interfacial debonding and matrix cracking were accounted for to accurately capture microscale effects. In addition, adaptivity was considered to be a crucial component of the method. A concurrent multiscale method in conjunction with a crack modeling framework was utilized for complete failure analysis of lightweight aggregate concrete (LWAC) [38]. Ghosh [39] developed an adaptive hierarchical-concurrent multilevel modeling framework for studying ductile fracture of heterogeneous metallic materials such as cast aluminum alloy. The model combines hierarchical models for homogenized constitutive modeling and concurrent models with scale transition in regions of localization and damage. This model can be easily adapted to a larger class of metal-matrix composites with micro-size particles/fibers and inter-particle spacing. It also provides a significant advantage with limited experimental data at smaller scales.

Although concurrent multiscale methods are advantageous in many applications, especially studies of material failure, several challenges are inherent to the simultaneous approach. The first fundamental challenge in the multi-scale approach is to account for the different fundamentals in each scale. For example in the atomistic theory, every individual particle is considered, whereas in the continuum theory the average is considered. The second challenge comes in the dispersion relation between the continuum and atomistic scales, wherein the dependence of the frequency on wave number is nonlinear in the atomistic model but linear in the continuum model, which affects velocities of the waves. Several methods have been introduced, including absorbing or non-reflecting boundary conditions, variational boundary conditions, blending methods and others [40]. In addition to these fundamental challenges, there is an inherent instability of concurrent atomistic/continuum displacement-coupling methods in fully

dynamic problems at finite temperature [41]. This led to demand of a new technique for coupling localized and non-localized material descriptions in a dynamic and stable way that did not require a well-defined Hamiltonian of the system.

Despite challenges in implementation, the concurrent multiscale approach remains a powerful tool in coupling the quantum, molecular, and continuum scales in engineering applications. Belytschko and Xiao developed a concurrent multiscale method, i.e. the bridging domain coupling method [42, 43]. In this method, the continuum domain overlaps the molecular domain via a bridging domain. A scaling of the molecular and continuum Hamiltonians is performed in the bridging domain, so that the total Hamiltonian of the system can be written as a linear combination of molecular and continuum Hamiltonians. Then, the equations of motion can be derived [42]. This method can efficiently eliminate wave reflection at the scale interfaces [43], and it has been proven to be stable [44]. Xiao and Hou [45] have successfully employed the bridging domain coupling method to model and simulate aluminum nanocomposites with embedded CNTs as shown in Fig. 3. They also studied crack propagation in nanocomposites. It was found that when the crack tip encountered the embedded CNT, the nanotube bridged the crack, and the crack propagation stopped as shown in Fig. 4. Consequently, failure stresses of nanocomposites were increased. Fracture of nanocomposites embedded with single-walled nanotubes (SWNTs), multi-walled nanotubes (MWNTs), and SWNT bundles were studied. They found that MWNTs have the best ability to resist crack propagation, while SWNTs have the least ability. Talebi et al. [46] employed the bridging domain coupling technique to model three dimensional cracks and dislocations at the atomic level. The multiscale method couples the molecular dynamics to extended finite element method and is based on linear weighting of the strain energy over the domain for cases of up to multi-million degrees of freedom. In this method, an atomic domain was placed on top of the three-dimensional extended finite element domain around the crack front. This configuration allowed the propagation and dislocations to be handled automatically in the region.

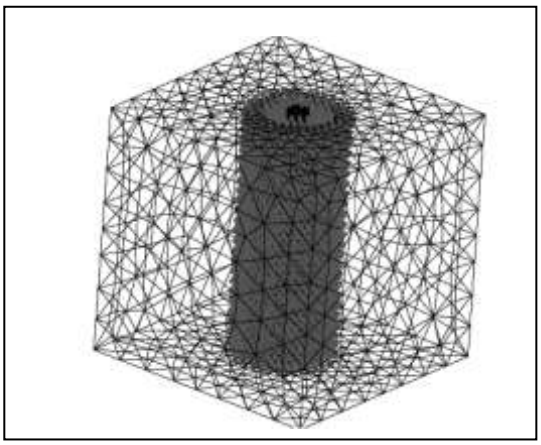

Figure 3. Multiscale model of a nanocomposite.

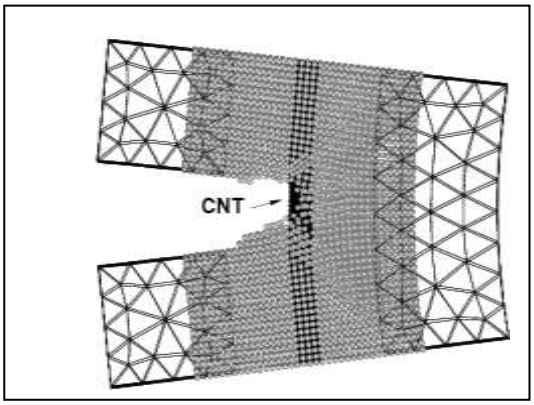

Figure 4. Side view of crack propagation in a nanocomposite.

In this paper, we reviewed molecular dynamics, hierarchical and concurrent multiscale methods and their applications in engineering community. Numerical methods have always been powerful tools in engineering system and process design. With the development of nano engineering, multiscale methods will be more and more attractive to engineers and scientists.

Acknowledgment

Zhang acknowledges support from NSFC (11272192).

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