



Multiresolution molecular mechanics: Statics



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ABSTRACT

This paper presents a new concurrent atomistic-continuum coupling method called the multiresolution molecular statics (MMS). By introducing a novel energy sampling framework, MMS aims at accurately and efficiently approximating the atomic energy of the system at different resolutions without the cumbersome interfacial treatment in existing methods. The key features of the MMS method are: (1) consistency with the atomistics framework, (2) consistency with the order of shape functions introduced, and (3) flexibility in energy approximation with respect to accuracy and efficiency. Under the energy sampling framework, several sampling schemes have been devised and tested for interface compatibility, and compared to existing methods. Sources of errors in the different approximations have been identified. The proposed MMS method demonstrates very good accuracy in solving crack propagation and surface relaxation problems when compared to full molecular statics.

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1. Introduction

Material defects such as dislocations and grain boundaries usually exist in localized regions but affect the overall mechanical behavior of materials. Such localized areas always involve more complicated deformations such as bond breaking and rearrangement and thus require atomistic modeling to resolve the details of the deformation mechanisms. However, atomistic simulations are limited by the size of the model simulated. The largest atomistic simulations performed with one of the fastest supercomputers in the world are on the order of 1 billion atoms, which only represent a small cube of 1 μm in size [1,2]. On the other hand, continuum mechanics techniques are developed for macroscale problems by describing the macroscale material behavior with empirical constitutive laws whose parameters are obtained from macroscale experiments. The constitutive laws require that variables such as temperature, displacement, and stress can be defined by an averaging process and that these variables are assumed to be smoothly varying continuous functions of position. Hence they represent the collective behavior of atoms, and thus continuum mechanics cannot accurately capture the deformation of discrete atoms. The mechanical deformation and failure of many engineering materials are characterized at multiple scales and the observed macroscopic behavior is governed by physics that occur on many different scales. Since atomistic simulations have the size limitation of scaling up to macroscale systems and continuum mechanics cannot accurately scale down to the atomistic description, a novel approach that combines

the best of these two approaches to simulate the behavior of materials at scales ranging from atomistic to macroscopic scales motivates the development of multiscale methods [3–28].

Capturing the interaction between the scales of interest is of main concern to multiscale modeling method. Concurrent methods that couple the atomistic region and continuum domain execute the entire simulation simultaneously and continually exchange information from one length scale to the other to ensure consistency among the field variables between the two simulation domains. Most concurrent coupling schemes employ a region where information passing between atomistic region and continuum domain is achieved. This region is usually referred to as the transition region or ‘handshake region’. It is in this region that requires special treatment due to the inherent incompatibility of the two subdomains: the non-local interaction of atomistics such as molecular statics (MS) and the local interaction of continuum mechanics such as finite element method (FEM). And various concurrent multiscale methods differ in the ways the approximations are made in the transition region [29,30].

Static methods are based on finding the configuration of mechanical equilibrium in the coupled atomistic-continuum system and assume quasistatic application of a mechanical load. Generally, concurrent methods can be classified into two groups depending on the equilibrium equations of the multiscale model: the energy-based schemes and the force-based approaches. Energy-based schemes usually minimize a well-defined energy functional of the multiscale system to obtain the force equilibrium rigorously. In contrast, force-based approaches abandon the use of energy functional and directly drive the physically-motivated forces on certain set of degrees of freedom to be zero by assuming that the energy minimization process is equivalent to finding the

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zero-force position of each degree of freedom. Among the energy-based coupling schemes, there are the quasicontinuum (QC) method [4,5], the ghost-force corrected QC method (QC-GFC) [6], the coupling of length scales (CLS) method [7], the bridging domain method (BDM) [15,28], the bridging scale method (BSM) [10,13,22–24], the energy-based cluster-based quasicontinuum method (CQC-E) [19] and the atomic-scale finite element method (AFEM) [12], just to name a few. Among the force-based coupling methods, there are the finite element-atomistic method (FEAt) [3], the coupled atomistic and discrete dislocations (CADD) [9,14], the atomistic-to-continuum (AtC) method [18,25–27], the force-based cluster-based quasicontinuum method (CQC-F) [8], the force-based version of quadrature rule type quasicontinuum method (QC-QR) [31,32] and the recently proposed atom collocation method (ACM) [21], just to name a few. As pointed out by Miller and Tadmor [29], the disadvantage of the energy-based method is that the non-physical side effects of the combined energy functional, usually termed “ghost force”, is extremely difficult to eliminate. On the other hand, the drawbacks of the force-based approach are that it can be slow to equilibrate, can converge to unstable equilibrium states, are non-conservative, and can be unstable numerically. For example, by introducing the cluster summation rule at the force level in the coarse-grained area, the CQC-F method was proposed to eliminate the non-local and local mismatch between atomistic region and continuum domain in the original QC method which employs the well-known Cauchy–Born (CB) rule in the continuum region. Then it is found in [19] that the forces in the CQC-F are non-conservative and the CQC-E is proposed by employing the same cluster summation rule on the energy-level to produce conservative forces and symmetric stiffness matrix [19]. Detailed discussions of various multiscale methods and existing issues can be found in several excellent review papers [29,30,33–35].

For energy-based methods employing continuum mechanics in the coarse-grained region, special weight functions have to be determined to weight the atomistic and continuum contributions in efforts to avoid double counting of energy. For example, the bridging domain method employs a partition-of-unity blending scheme to calculate the energy of the transition region. Some other energy weighting schemes are also employed in the QC method and the CLS method. For this type of energy-based methods, the well-known CB rule or other continuum constitutive laws are employed to approximate the energy of the coarse-grained area. However, the “non-local” dependence of energy in atomistic simulation is inconsistent with the “local” dependence of energy in continuum mechanics, which is independent of the definition of weight function introduced and thus they are incompatible in nature [12,36]. This is the exact reason why ghost force arises near the interface [30]. This local and non-local mismatch motivates the development of another type of energy-based multiscale method [19], which abandon the continuum mechanics description and keeps only the atomistic description in the coarse-grained area by employing a cluster summation rule as the weighting scheme to approximate the energy of the coarse-grained system. The cluster summation rule was first introduced in the force-based cluster-based QC method [8] to eliminate the interface mismatch and thus the ghost force problem arising in the quasicontinuum method. Recently, the same cluster summation rule was employed in the energy-based cluster-based QC method [19]. The cluster summation rule has the major advantage over the CB rule or other constitutive laws in that the internal interface between the atomistic region and the coarse-grained area does not occur. The reason why no interface occurs is that it used the same non-local sampling scheme to compute the force or energy in both domains. A disadvantage of the cluster-based approach is that, even for the case of nearest-neighbor interaction, it leads to large errors in energy that cannot be removed by increasing the cluster size when employed

with graded or non-smooth meshes as pointed out by Luskin and Ortner [37].

Motivated by eliminating the internal interface mismatch and, at the same time, accurately approximating the energy of the entire system, we propose a new concurrent energy-based multiscale method called the multiresolution molecular mechanics (MMM) method, which is based on a novel energy-sampling scheme. In this paper, we focus on statics and the static version of MMM is called multiresolution molecular statics (MMS). Compared to the cluster summation rule, the key ideas of the new sampling scheme are: (1) instead of sampling the energy of the coarse-grained area by weighting the energy of clusters centered around each element node or rep-atoms, a primary sampling atom and some secondary sampling atoms inside each element in the coarse-grained area are chosen and their energies are used to sample the energy of the element, and thus the energy in the coarse-grained area is sampled element-wise. (2) In the cluster summation rule, the weighting factors associated with each cluster are calculated by requiring that the cluster summation rule is exact only when the energy is piecewise linear. This introduces further assumption or approximation after shape functions have been introduced to reduce the degrees of freedom of the system. However, it is recognized that the energy distribution of the system will never be piecewise linear even with linear shape functions to control the deformation of ghost atoms since atoms that initially have the same neighboring environment and thus the same energy in the element should also have the same energy in the deformed configuration given that the linear shape function is employed. This may be the cause of additional error in the cluster summation rule by the additional assumption to calculate the associate weighting factors, and this additional error may be the reason why cluster summation rule introduces large errors that is independent of the cluster size. In contrast, the energy sampling is exact in the proposed scheme when the deformation is exactly linear, which is consistent with the shape function introduced. (3) The energy of rep-atoms is not included in the calculation of the atomic energy of each element but is considered separately, and hence more sampling flexibility can be introduced depending on the accuracy needed.

In this paper, statics is the focus and the method proposed will be called the multiresolution molecular statics (MMS) the rest of the paper. The structure of the paper is as follows. The general MMS formulations are developed in Section 2, followed by the comparison of accuracy between different sampling schemes in MMS in Section 3. Some benchmark tests employed in [30] are used here to test the interface compatibility of MMS and compare MMS with the existing multiscale methods in Section 4. This is followed by applications of MMS to 2D crack propagation and 3D surface relaxation problems in Section 5, where the accuracy of MMS are compared against standard molecular statics (MS).

2. Formulation of multiresolution molecular statics (MMS)

In the full atomistic model, Fig. 1(a), we assume that each atom has a site energy E_α . Let Π denote the energy of the full atomistic system, then

$$\Pi = \sum_{\alpha=1}^{N_A} E_\alpha(\mathbf{r}^{N_A}) - \sum_{\alpha=1}^{N_A} \mathbf{f}_\alpha^{\text{ext}} \cdot \mathbf{u}_\alpha \quad (1)$$

where N_A is the total number of atoms and $\mathbf{r}^{N_A} = (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_z, \dots, \mathbf{r}_{N_A})$ are defined as the set of atomic coordinates; $\mathbf{f}_\alpha^{\text{ext}}$ and \mathbf{u}_α are denoted as the external force vector and displacement vector for atom $\alpha \in N_A$, respectively. In order to deduce the equilibrium equations for atom $\alpha \in N_A$, the negative derivative of the total energy π with respect to \mathbf{r}_α , i.e. the force on atom α , must be zero. So $-\frac{\partial \Pi}{\partial \mathbf{r}_\alpha} = 0$ gives:

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