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A three-layer-mesh bridging domain for coupled atomistic–continuum simulations at finite temperature: Formulation and testing

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ABSTRACT

Although concurrent multiscale methods have been well developed for zero-temperature simulations, improvements are needed to meet challenges pertaining to finite-temperature simulations. Bridging domain method (BDM) is one of the most efficient and widely-used multiscale atomistic–continuum techniques. It is recently revealed that the BDM coupling algorithm has a cooling effect on the atoms in the bridging domain (BD), and application of thermostats to rectify the cooling effect in the original BDM formulation is unstable. We propose improvement of the BDM formulation for finite-temperature simulations by employing a three-layer mesh structure in the BD, consisting of coarse, meso, and atomic meshes. The proposed method uses a mesh-independent physics-based discrimination between thermal and mechanical waves to define and introduce a meso mesh that is independent of the finite-element (FE) mesh. Temperature stability in the BD is achieved by constraining only the mechanical part of atomic motion to the FE displacements while unconstrained thermal vibrations are thermostatted using local thermostats in the BD. The new architecture of three-layer-mesh BD effectively mitigates the temperature cooling effect encountered by the conventional BDM as well as suppresses the spurious mechanical wave reflection. Numerical simulations have shown the robustness and accuracy of the proposed multiscale method at finite temperature.

1. Introduction

Over the past few decades, computation has firmly established itself as a new approach in parallel to experiment and theory in understanding fundamental materials properties. Using supercomputers, which are accessible widely to academic community today, it is possible to carry out first-principles simulations of hundreds of atoms for tens of picoseconds and molecular dynamics (MD) simulations with interatomic potentials of millions of atoms for microseconds. However, these accessible length and time scales are still far short of the length scale and especially the time scale of real experiments. Some properties, for which convergence is very fast, e.g. those of point defects in periodic crystals, can be accurately calculated using first-principles techniques. However, the so-called strongly coupled multiscale systems have the properties whose convergence is very slow. These systems are typically associated with a long-range interaction, either electrostatic or elastic. As such, a process, which takes place in a small region, can be affected by the collective behavior of a very large number of atoms over long, sometimes even macroscopic distances. Also, in some cases, the detailed interactions of certain key atoms can influence the equilibrium configuration of potentially tens of thousands of atoms. Concurrent multiscale methods have

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been developed to circumvent the temporal and spatial limitations of all-atom simulations for modeling strongly coupled multiscale systems, in which the critical zones are limited to small parts of the problem domain while continuum description elsewhere. The fact that it is often unnecessary to use all-atom simulations to treat the whole problem domain is another motivation toward multiscale modeling. Processes involving bond formation, bond breaking, charge transfer, and nonlinear response are best handled with quantum/molecular mechanics while large and arbitrary geometries with wide-ranging boundary conditions can be readily handled with continuum mechanics [1].

The key to multiscale methods is to have an accurate and efficient algorithm that bridges seamlessly different scales. While sequential multiscale methods have enjoyed long-time success [2]; concurrent multiscale methods have been more challenging, as they need to adress a number of issues associated with energy transmission and changes in the constitutive description of a material across the interface between different models, such as spurious wave reflection. Different concurrent multiscale methods have been developed so far, including the quasicontinuum method (QM) [3,4], coarse-grained MD method (CGMD) [5,6], macroscopic–atomistic–ab initio dynamics (MAAD) method [7,8], bridging scale method (BSM) [9,10], bridging domain method (BDM) [11,12], and concurrent atomistic to continuum (AtC) coupling method [13]. In the QM, the entire model is viewed as an atomistic model while representative atoms and the Cauchy–Born rule are used to compute strain energy without using fully atomistic resolution everywhere. To eliminate the unnecessary atomistic degrees of freedom, representative atoms are selected to define finite elements for which the mechanical variables are calculated using finite-element (FE) interpolation and the Cauchy–Born rule. Accurate computation of the energy requires that the atoms be coincident with the finite element nodes in the critical fully-atomistic subdomain. Similarly, in the multiscale CGMD method, critical regions of the system are modeled with MD, while elsewhere is coarse grained for efficiency. The CGMD equations of motion smoothly match those of MD as the mesh size is reduced to the atomic scale since they are derived directly from finite-temperature MD through a statistical coarse graining procedure. In this method, the cross-over to atomistic domain for atomic-sized cells is completely smooth and no handshaking region between MD and CGMD regions is required. The MAAD couples a tight-binding (TB) quantum mechanics approximation with MD and in turn with a FE continuum model. In this method, atomistic and continuum models are coupled in a handshaking domain in which the two Hamiltonians are averaged. To reduce spurious reflections into the MD zone and to thermalize high-frequency phonons propagating through regions where the mesh spacing changes, the FE degrees of freedom are weakly coupled to a Brownian heat bath i.e. the random and dissipative terms are added to their equations of motion. The BSM couples MD and FE models without the need to mesh down the continuum model to the atomic scale by decomposing the displacement field into coarse and fine scales. It also eliminates the unwanted MD degrees of freedom by accounting for them in the form of an impedance force augmenting the standard MD equations of motion, so that high frequency waves which cannot be resolved by the FE model are dissipated naturally out of the MD region.

The concurrent multiscale methods have been mostly applied to study mechanics problems such as crack nucleation/propagation and crystal plasticity. One of the most popular multiscale methods is the BDM [11,12], which has been used in a number of interesting mechanics simulations [14–20]. The BDM is an overlapping domain decomposition scheme in which displacement/velocity compatibility between the atomistic and continuum domains is imposed using the Lagrange multipliers technique. In this regard, the BDM is similar to the earlier Arlequin method [21–24], which couples continuum models. In the BDM, similar to the BSM, the continuum model is not meshed down to the atomic scale since the positions of atoms and nodes are not necessarily identical in the BD. A uniform continuum mesh can be used, which does not correspond with atomic positions. To increase the efficiency, large finite elements can be used within the smoothly discretized meshes, without encountering the issues associated with rapid element-size changes. The BDM uses a so-called BD to couple MD and finite element (FE) models. Consequently, the quantities associated with the atoms and FE nodes need to be transferred between different models only in the BD. In this regard, the BDM is advantageous over the BSM, in which the FE mesh spans over the whole MD zone. Recently, an absorbing boundary condition [25] has been developed that enables application of the BDM with smaller bridging zones to further increase its efficiency. The BDM uses an effective but inexpensive algorithm [26] to remove spurious wave reflections whereas some other techniques [27–30,9] use computationally expensive time history kernels to obtain reflectionless boundary conditions. Furthermore, the BDM generally employs a linear scaling of the energies in the BD, in which the atomistic (continuum) energy is dominant near the purely atomistic (continuum) domain. This strategy provides a gradual transition from the molecular model to the continuum model, and alleviates the error that arises from dropping the atomistic energies from far-field atoms. Also, the BDM can be applied to nonlinear problems since it is not based on linearization.

In the BDM, the system is partitioned into three sub-domains (Fig. 1): atomistic, continuum, and BD. Displacement/velocity compatibility between atomistic and continuum scales in the BD is imposed using the Lagrange multipliers technique. The compatibility can be imposed stringently by associating one Lagrange multiplier with each degree of freedom of each atom in the BD, or it can be applied weakly by approximating the Lagrange multipliers from the finite element mesh i.e. one Lagrange multiplier is associated with each degree of freedom of each FE-node in the BD [12,17]. Application of L^2 and H^1 couplings in the BDM formulation has been investigated in [31,32]. It is found that L^2 coupling with a piecewise linear weight function, such as that used in this paper, is stable. One important step in the BDM is to diagonalize the Lagrange-multipliers constraint matrix using the row-sum technique, which is essential in eliminating spurious wave reflections at the interface of the atomistic and continuum domains [26]. The diagonalization step has also a positive side effect of reducing computational cost. According to use of the Lagrange multipliers in the BDM formulation, total Hamiltonian is divided into three parts: atomistic Hamiltonian, continuum Hamiltonian, and the Hamiltonian associated with the Lagrange multipliers.