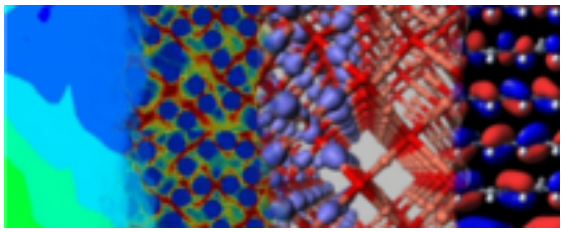

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Divide-and-Conquer Learn-on-the-Fly: A Hybrid Quantum-Classical Approach for Simulating the Nanomechanical Properties of Metallic Systems

Thursday, November 8, 2012 2:25 PM (25 minutes)

Simulations performed with the molecular dynamics (MD) method constitute an important tool in the study of the mechanical properties of nanoscale systems. The MD method is classical in nature and its main limitations stem from the empirical nature of the employed potentials, whose functional form is postulated a priori, and from not taking the electronic effects explicitly into account. In consequence, results obtained in such a strictly classical fashion do not neccessarily correctly model physical reality in all cases, particularly for systems that are far from equilibrium, such as nanostructures undergoing plastic deformation; i.e. classical potentials are said to lack transferability. The explicit inclusion of electronic effects offered by quantum-based approches, which start from first principles (ab initio) does yield a transferable description of the interatomic interactions; this, however, is associated with significant computational complexity, which prevents these approaches from being directly applied to systems involving more than several hundred atoms, and even then in practice the performed simulations are usually not dynamical. Hybrid (quantum-classical) approaches realize a compromise whereby a subset of the system (such as a region where bond-reorganization is taking place) is treated with a first-principles approach whilst the remainder undergoes classical MD. The Learn-on-the-Fly (LOTF) technique (Csanyi et al., PRL 93 (17), 2004) offers a particularly elegant way of embedding the results of quantum-mechanical calculations within an MD simulation, by periodically, locally re-parametrizing the empirical potential so that it reproduces the accurate forces obtained from first principles in the region of interest. In its original formulation it has been successfully applied to the fracture of silicon, where the classical Stillinger-Weber potential is shown to give qualitatively wrong predictions. We present Divide-and-Conquer Learn-on-The-Fly (Dziedzic et al., PRB 83 (22), 2011) –a generalization of LOTF, which is suitable for systems where the interaction range is longer, such as d-shell metals. We show how the force-matching stage can be recast to make the problem of simultaneously optimizing thousands of parameters in situ to match thousands of atomic forces computationally tractable. We demonstrate the feasibility of our approach on several examples: simulating nanoindentation and nanoscratching of Cu monocrystals, calculating the structure and properties of liquid Au and the structure of selected AuCu nanoclusters.

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