Linking Scales in Materials Simulation

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Abstract: Many problems in materials simulation require the linking of length scales, starting with electronic structure at subnanometer scales, passing through atomistic simulation at nanometer scales and proceeding to continuum properties on centimeter scales. We report two developments, one, self-consistent tight binding (SCTB) linking electronic to atomic scales and another, renormalized molecular dynamics (RNMD) linking molecular dynamics to continuum scales. SCTB uses a data base of first principles calculations (density functional theory, or quantum chemical methods available, for example from the Gaussian code) to fit a Hartree self consistent tight binding model of the electronic and atomic structure. The tight binding model is then used to simulate much bigger structures in direct, Car-Parinello type, dynamics calculations on much larger systems than could be studied by first principles methods. The tight binding model is thus a kind of tool for extrapolating the first principles results to larger scales. The main technical problems arise in the fitting which will be described. We report examples in the simulation of water, electrochemical interfaces and high temperature superconductors. RNMD begins with a molecular dynamics model and uses a generalization of the idea of potential of mean force to compute a mean force between two particles in the original simulation in which the high frequency components above a frequency cutoff have been averaged out. The resulting pair force represents the forces between particles correctly when the particles are more than a distance apart which scales, in simple cases, as the velocity of sound divided by the cutoff frequency. We use this renormalized force in a new simulation with a reduced density of renormalized particles, each representing a number of original particles equal to the ratio of the original density to the reduced density. We will report implementation in a Lennard Jones fluid and possibly in a model polymer system.

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