

Heat Capacity of the Atom – A Fundamental Problem in Molecular Dynamics

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Molecular Dynamics (MD) is used in computational heat transfer to determine the thermal response of nanostructures. With theoretical basis in statistical mechanics, MD relates the thermal energy of the atom to its momentum by the equipartition theorem. Momenta of atoms in an ensemble are determined by solving Newton's equations with inter-atomic forces derived from Lennard-Jones potentials. Statistical mechanics always assumes the atom has heat capacity as otherwise the momenta of the atoms cannot be related to their temperature.

In heat transfer simulations of bulk materials, MD simulates the continuum by imposing periodic boundary conditions (PBC) on an ensemble of atoms having heat capacity in submicron computation boxes. MD simulations of the bulk are valid because atoms in the bulk do indeed have heat capacity

MD simulations of heat transfer in discrete nanostructures differ from that in the bulk because of quantum mechanics (QM). Unlike statistical mechanics, QM precludes atoms from having heat capacity at the nanoscale. Indeed, the difference between QM and statistical mechanics is of fundamental significance in the MD of nanoscale heat transfer. By QM, atoms in discrete nanostructures lacking heat capacity cannot conserve heat by an increase in temperature, and therefore the classical Fourier heat conduction equation that depends on temperature has no meaning. Nevertheless, MD simulations of discrete nanostructures having heat capacity abound the literature. Although consistent with statistical mechanics, MD of discrete nanostructures is not only invalid by QM, but also gives unphysical results, e.g., thermal conductivity of thin films depends on thickness, heating nanocars does not cause observed motion, and so forth.

Lacking heat capacity, heat transfer in discrete nanostructures proceeds by the conservation of absorbed EM energy by the creation of non-thermal QED induced EM radiation that charges the discrete nanostructures by Einstein's photoelectric effect, or is emitted to the surroundings. EM stands for electromagnetic and QED for quantum electrodynamics.

MD by QM requires procedures that convert absorbed EM energy of the nanostructure into EM radiation and charge instead of an increase in temperature. How to modify MD in heat transfer simulations is proposed to be a topic of discussion in Fundamental Problems of Molecular Dynamics at MOLEC 2012.