Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Objectivity in Classical Molecular Dynamics: Objective Velocity, Temperature and Virial Stress ZIDONG YANG, JAMES LEE, AZIM ESKANDARIAN, The George Washington University — In classical mechanics, axiom of objectivity requires that all balance laws and all constitutive equations must be form-invariant with respect to rigid motions of the spatial frame of reference. Any tensorial quantity is said to be objective if it is independent of the motion of the observer. Quantities such as temperature and stress should be objective. In Molecular Dynamics(MD), objectivity was rarely discussed. This paper addresses the objectivity of the governing equation and constitutive equations in MD. It can be shown that the interatomic potential and force are objective because they are based on relative position vectors of atoms, which are objective. Also, the governing equation in MD can be shown to satisfy objectivity too. On the other hand, velocity and relative velocity are not objective. Consequently, quantities such as temperature and Virial stress that are based on velocities of atoms are not objective. This becomes an issue if the simulation is conducted in a non-inertial reference frame. To resolve this deficiency, this paper adopts the formulation of thermal velocity that is proved to be objective. Thus the application of axiom of objectivity on MD will provide more credibility to the simulations of complex systems.

Zidong Yang
The George Washington University

Date submitted: 15 Nov 2013 Electronic form version 1.4