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Objectivity in molecular dynamics

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ABSTRACT

In classical Continuum Mechanics, Principle of Objectivity requires that balance laws and 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 obeys the appropriate tensor transformation law. Quantities such as temperature and stress tensor are known to be objective. In Molecular Dynamics (MD) simulation, which is a prevalent numerical method in nanoscience on atomistic basis, Principle of Objectivity was rarely discussed. This research explores the objectivity issue in the classical MD by examining the governing equation and constitutive equation. It can be shown that the interatomic potential and the corresponding interatomic force are objective because they are determined by relative atomic positions, which are objective. On the other hand, velocity and relative velocity are not objective. As a consequence, quantities such as temperature and Virial stress that are calculated based on apparent atomic velocities are not objective. Therefore, multiphysics body forces generated by these nonobjective quantities are not objective either. This becomes problematic when the system or subsystem is described in a noninertial reference frame, i.e., the reference frame undergoes acceleration or rotation. To resolve this deficiency, this research proposes the theory of Objectivity Incorporated MD. With the adoption of an objective form of velocity, the objectivity of temperature and Virial stress are restored. The theory also requires all kinds of body forces to be objective so that the constitutive equation well satisfies the Principle of Objectivity. The theory further supplements the governing equation with fictitious force, which accounts for the motion of reference frame, so that MD simulation can be extended to noninertial reference frame. It is considered that the application of Principle of Objectivity on MD will provide more power and credibility to the simulations of complex systems.