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Design Sensitivity Analysis of Molecular Dynamics Considering NVT Ensemble

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Abstract

Due to the rapid development of nanotechnologies, there is an increase in the necessity of nanoscale analysis in both analysis and design problems. Molecular dynamic (MD) simulation is often utilized in many applications such as solid fracture, surface friction, and plasticity since these include the microscopic behavior which cannot be captured in the continuum sense. Moreover, the need for design optimization at the atomic level is naturally increasing for the development of new materials and to overcome the limitations in continuum-based analysis of modern engineering problems. However, a huge amount of computation is usually required for the MD simulations since they are typical transient dynamic problems. Furthermore, for the design sensitivity analysis (DSA) of MD systems that have many design variables, the required cost is very expensive.

From the engineering and practical point of view, thermal effects are very important for atomic level simulations. To make it realistic, we need to consider the ensemble concept to deal with macroscopic behaviors due to the variations of microscopic variables. In this research, we proposed an efficient DSA method of MD simulation considering NVT ensemble. Nose- Hoover thermostat is utilized for the MD system within a heat bath of desired temperature. The design sensitivities of general performance measure for Nose-Hoover thermostat are obtained by using direct differentiation method (DDM) and adjoint variable method (AVM). For the AVM terminal value problems, time reversibility of original MD system is investigated. The accuracy and efficiency of developed methodology are demonstrated through some numerical examples.