Molecular Dynamics Simulation of a Lenard-Jones Interacting Molecule for Obtaining Macroscopic Static Physical Properties

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Abstract

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I. Introduction

In this paper we intend to derive experimental macroscopic properties of a material from a microscopic description of the molecular interactions. In statistical physics many macroscopic quantities of many-particle systems can be found as an ensemble average over the possible microscopic states. Any practical macroscopic system consists of so many possible microscopic states that it is infeasible to average over all of the possible states computationally. But given a large subset of the possible states, we may assume that physical quantities averaged over the subset are close to the ensemble average. In molecular dynamics (MD) we initialize a specific state determined by some system parameters and let it evolve in time, traversing along its physical trajectory in the phase space as determined by the equations of motion. We therefore generate a large subset of possible states which are correlated in time. Using appropriate averaging over time we can obtain estimates of the ensemble average and therefore the relevant physical quantities.

We restrict ourselves to studying static physical properties of the system at equilibrium, although MD could also be used to study dynamical properties of a system. We carry out simulations for Argon, which is studied extensively in the literature and is modeled easily using the Lenard-Jones interaction potential. First we compute the heat capacity and compare it to theoretical results in the case of a hot and dilute gas or a cold and dense solid to verify the result. Next we compute the pressure as a function of the density at different temperatures and compare this with experimental results. Finally we compute the pair correlation function and comment on its qualitative behavior.

II. Methods

II.I. Molecular Dynamics and the interaction potential for Argon

Relevant topics in order are:

1. Interaction potential
2. Equation of motion
3. Discretization: Verlet algorithm
4. Boundary conditions
5. Initial conditions

II.II. Computation of physical quantities

1. Computation of the heat capacity
2. Computation of the pressure
3. Computation of the pair correlation function

III. Results and Discussion

III.I. Results

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IV. Conclusions

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