

Homework Assignment Number One

The Lennard Jones Fluid has been extensively studied via molecular simulation. These simulation results has also been used to parameterize an equation of state. Consider the following article:

Title: The Lennard-Jones Equation of State Revisited

Authors: Johnson, JK; Zollweg, JA; Gubbins, KE

Journal: Molecular Physics

Volume: 78 Issue: 3 Pages: 591-618 Published: FEB 20 1993

A pdf file containing this article has been uploaded to the password protected blackboard course website.

There are two tasks in this homework.

Task 1. Verify that your simulations are reasonable in terms of

- the number of atoms
- the size of the time step
- the duration of the simulation

Task 2. Reproduce three data points over a range of densities and temperatures from Table 2 of this article. Report

- density
- temperature
- pressure
- internal energy
- number of time steps
- size of time step

For the thermodynamic properties report not only the mean value but the standard error (not standard deviation) as well. Compare and discuss your results with those in the reference.

Append your three LAMMPS input files to your homework.

There is no need to attach lengthy output.

Submit the homework as a pdf file electronically through the CANVAS system.

Please do not submit a paper copy of this homework.