

Computational Physics II

Homework 9

Submission: January 21, 2020

Simulation at constant temperature with dissipative particle dynamics thermostat

Write a program to implement the DPD thermostat for MD simulation for Lenard-Jones (known form) particles in canonical ensemble. Use the integration scheme mentioned in table 1 (self consistent DPD-VV) of the attached paper of DPD thermostat.

1. Plot the kinetic energy (temperature) for 2-3 different choices of δt .
2. Fix δt to a particular value (say, $\delta t = 0.001$) and fix the temperature to 3 different values. Plot temperature vs. time for them.
3. compare the total energy for the above mentioned values of δt in (1).