CHE622A Assignment 5

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Q1a

Solution provided in file Q1a.py

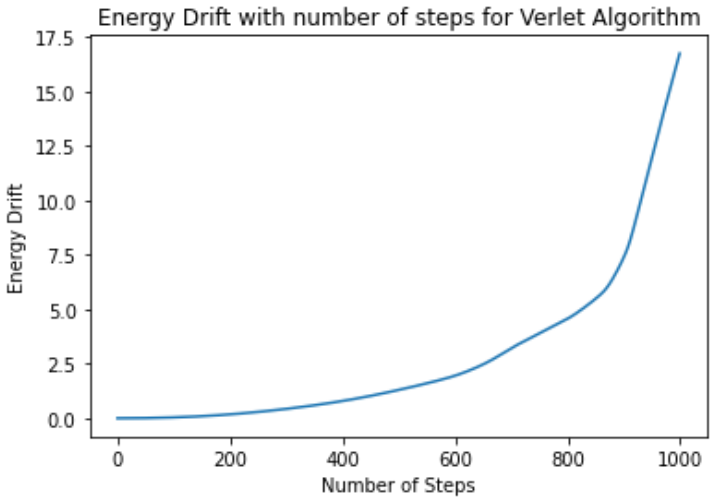
For values of time step > 0.0001 the energy and forces diverge and the simulation values go to nan

Sufficiently small time step should be given for simulation

Q1b

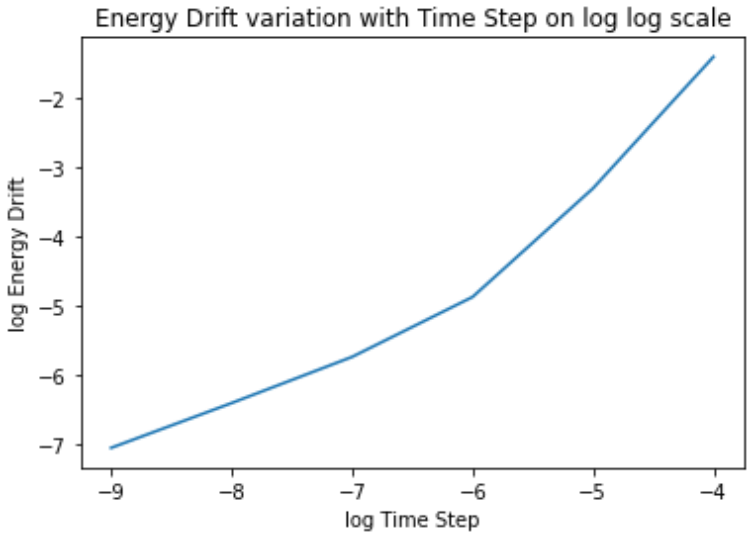
Solution provided in file Q1b.py

Plot for energy drift with time step made for Temperature = 1, density = 1 and time step = 0.0001

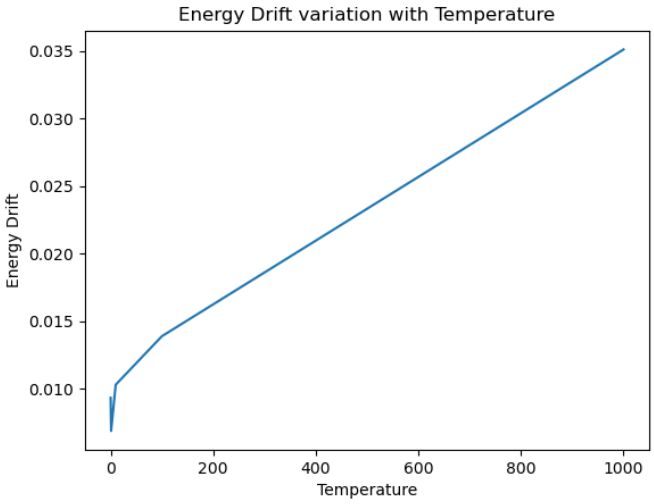


Now to study the dependence of time step with temperature and density for constant energy drift, we first study dependence of energy drift and time step, temperature and pressure.

Below is plot of dependence of energy drift on temperature which shows that Energy drift increases as time step size increases

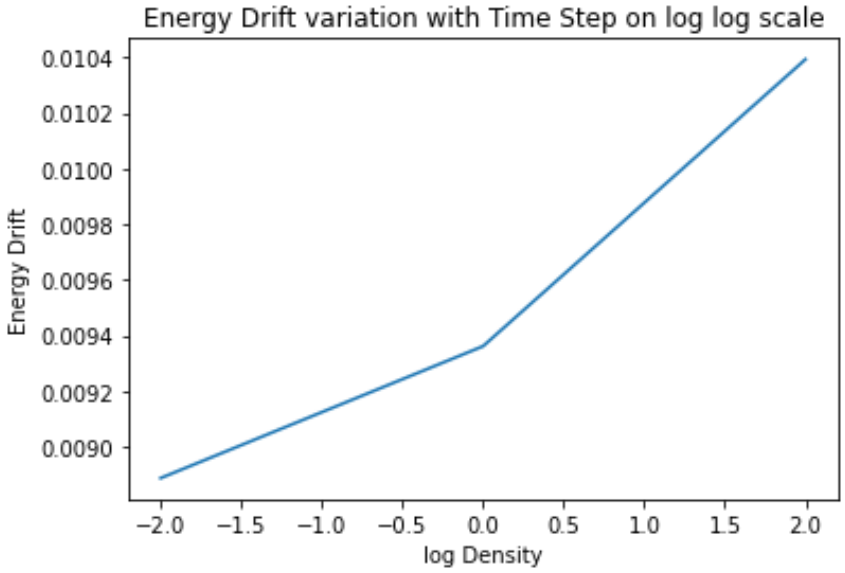


Below is a plot showing the dependence of temperature on energy drift



This shows that energy drift increases with temperature

Below is a plot showing the dependence of density on energy drift



This shows that energy drift increases with density

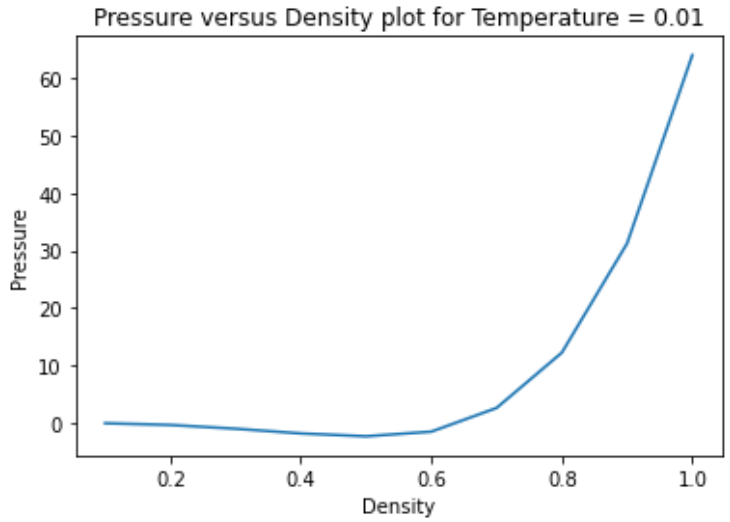
From the simulations we see that energy drift increases with time step size, temperature and density.

Hence, for constant energy drift when we increase time step we have to decrease density and temperature and when we decrease time step we have to increase density and temperature i.e. time step is inversely proportional to temperature and pressure

1c

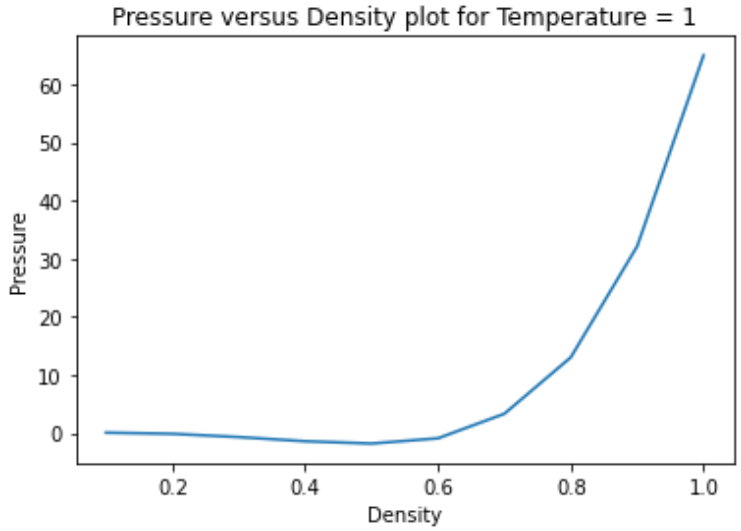
The modified code which can calculate pressure is present in file Q1c.py

Below is the Pressure vs density plot for T = 0.01 or small temperature

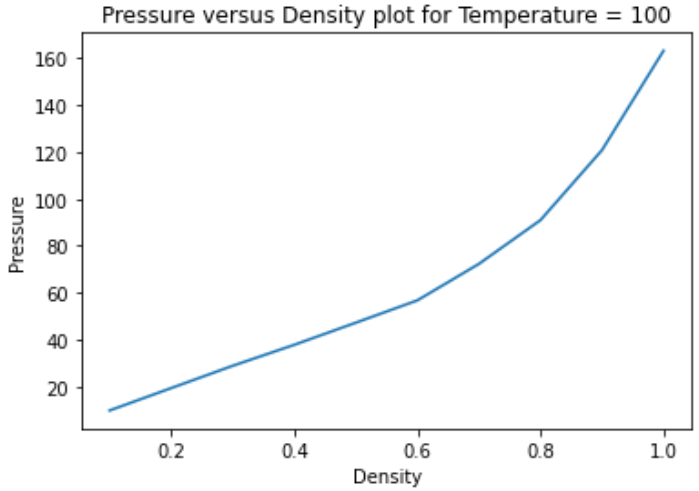


Pressure becomes negative because the system is in supercritical state for low temperature

Below is the Pressure vs density plot for T = 1

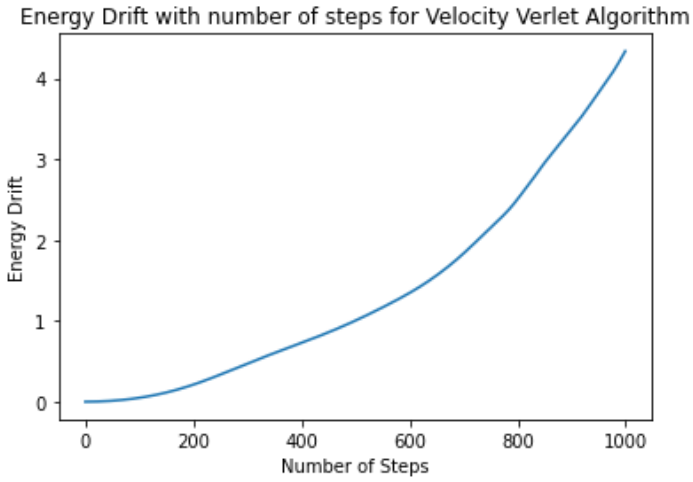


The Pressure versus density for T = 100 or high temperatures



1d

The code for this problem is given in file Q1d.py



The above plot is that of Energy Drift with number of steps made for Temperature = 1, density = 1 and time step = 0.0001

Comparing this to the plot in 1b we see that the energy drift for velocity verlet is lesser than drift in verlet algorithm.

The final energy drift for 1000 time steps for velocity verlet is 4.336 compared to 16.756 for verlet. This means that velocity verlet retains energy conservation for more time steps that verlet algorithm.