PHY453: Assignment 08

Molecular Dynamics

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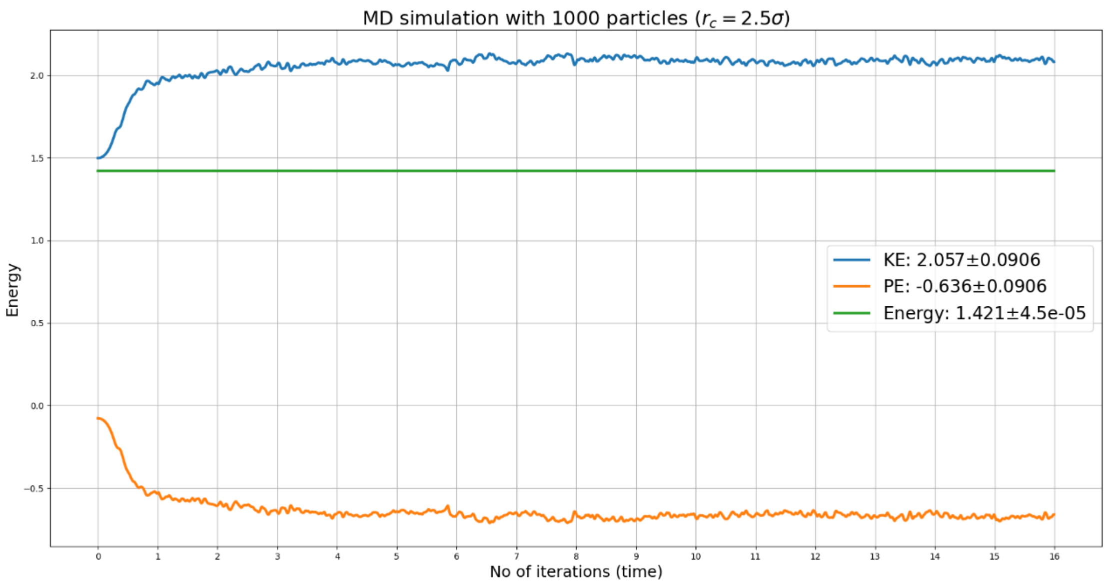
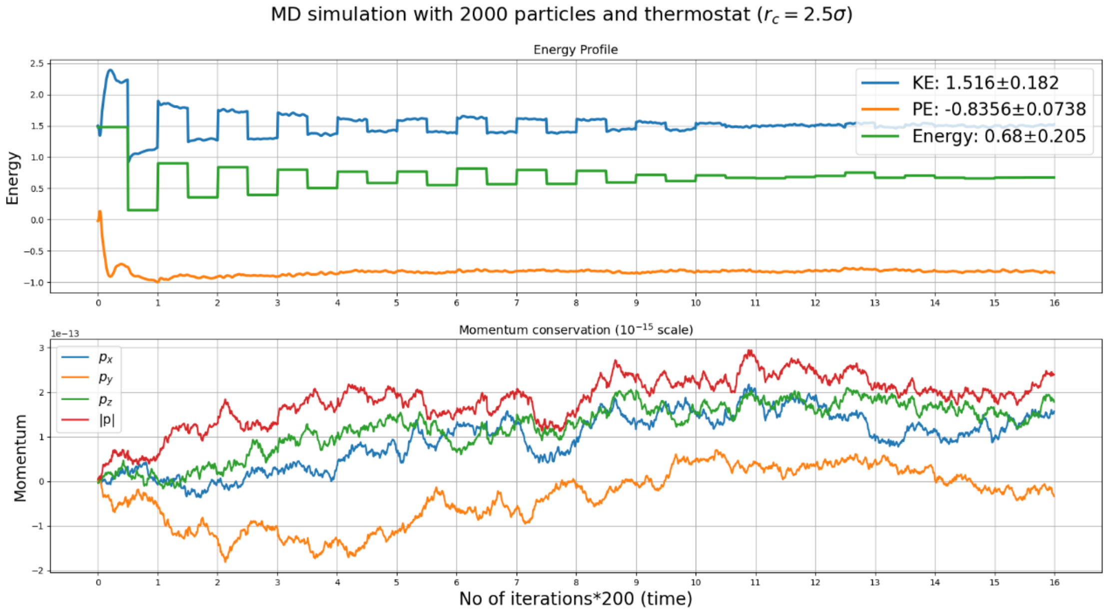
Q1. The code for this section is available at `MDQ1.f90`. The executable will read the lattice created by `lattice.f90` and thereby read the file `cubic.txt`. It then performs MD calculations, integrations, and the output is written to `data1.dat`. We use `plot1.py` to read and plot the data files.

Momentum per particle will be conserved to 10^(-15), whereas energy will conserved to about 1.42 units.



Q2. Here we increase the number of particles to 2000, and use a thermostat to regulate temperature. Energy is conserved for 100 MD steps, in between the two calls of thermostat. The momentum of the system is conserved and fluctuates between the 3 degrees of freedom in e-15 units.



Q3.

- Here, when we say unit of time (\tau), it is dimensional equivalent to \sqrt(Mass*Length^2/Energy). This means that numerically, time is equal to the iteration step size* the unit of time based on the units of length, mass and energy used.
- In other words, we can say that a free particle of mass M=1, energy KbT=1 will take T=1 unit of time to move a distance \sigma=1.
