

Module 6

Submitted by: Anirban Nath

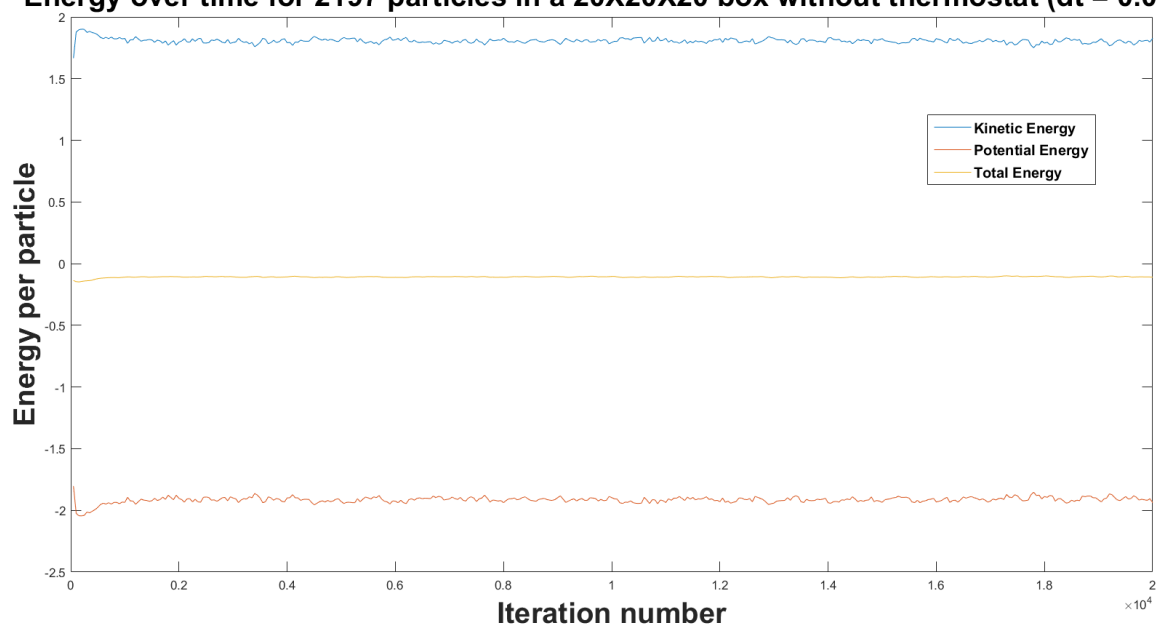
Register number: 20242019

Question 2.

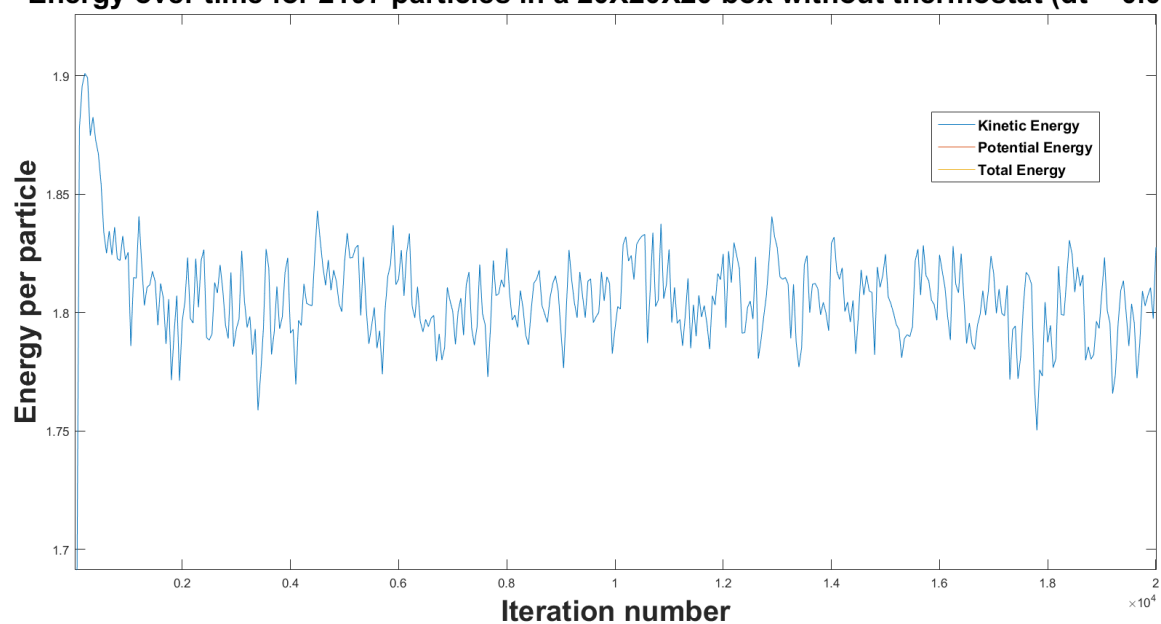
Parameters used: $\sigma = 1$, $\epsilon = 1$, $K_B T = 1$, $r_{\text{cutoff}} = 2.5 \sigma$, thermostat OFF, niter = 20000, sampling rate = 50 itrns.

We see PE fluctuates around -1.92 and KE fluctuates around 1.8. TE fluctuates around -0.107.

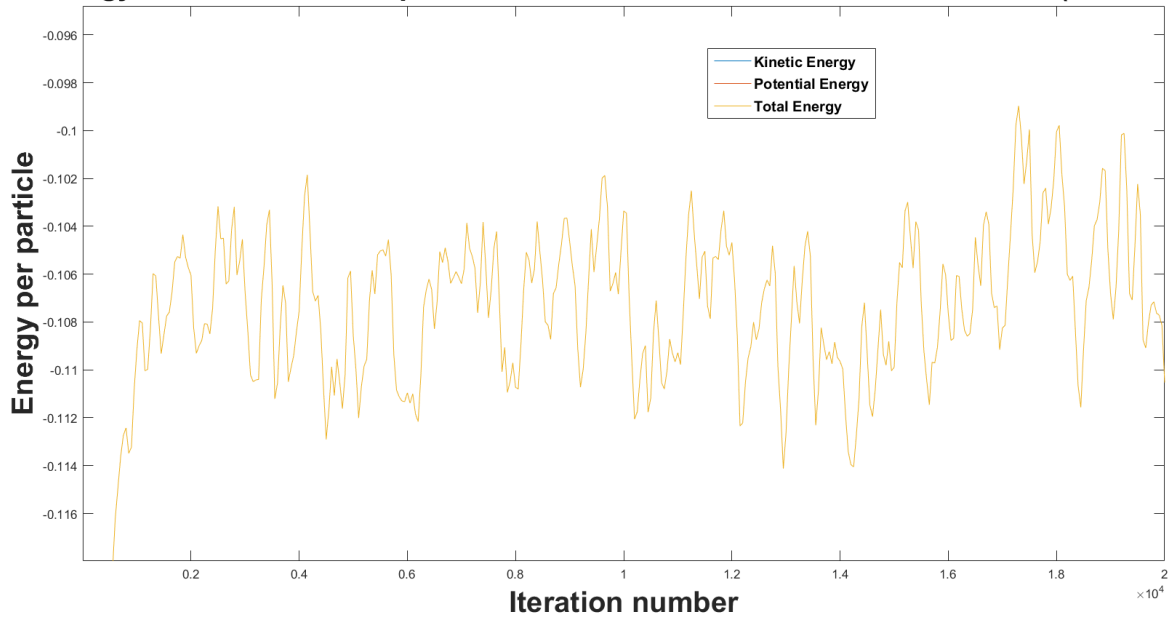
Energy over time for 2197 particles in a 20X20X20 box without thermostat (dt = 0.005)



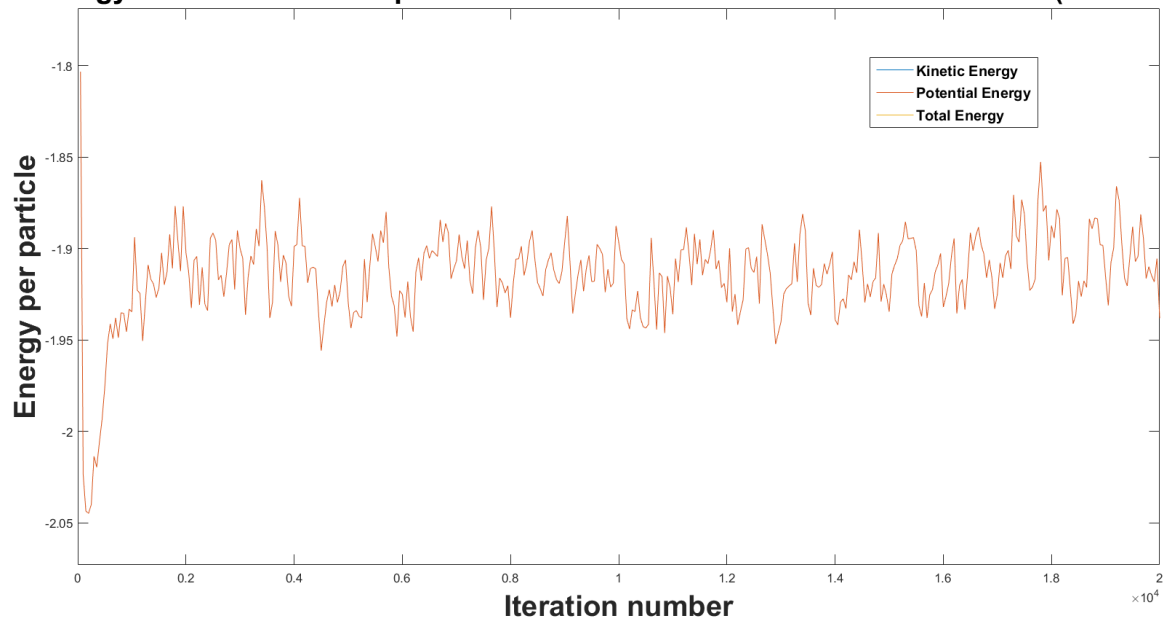
Energy over time for 2197 particles in a 20X20X20 box without thermostat (dt = 0.005)

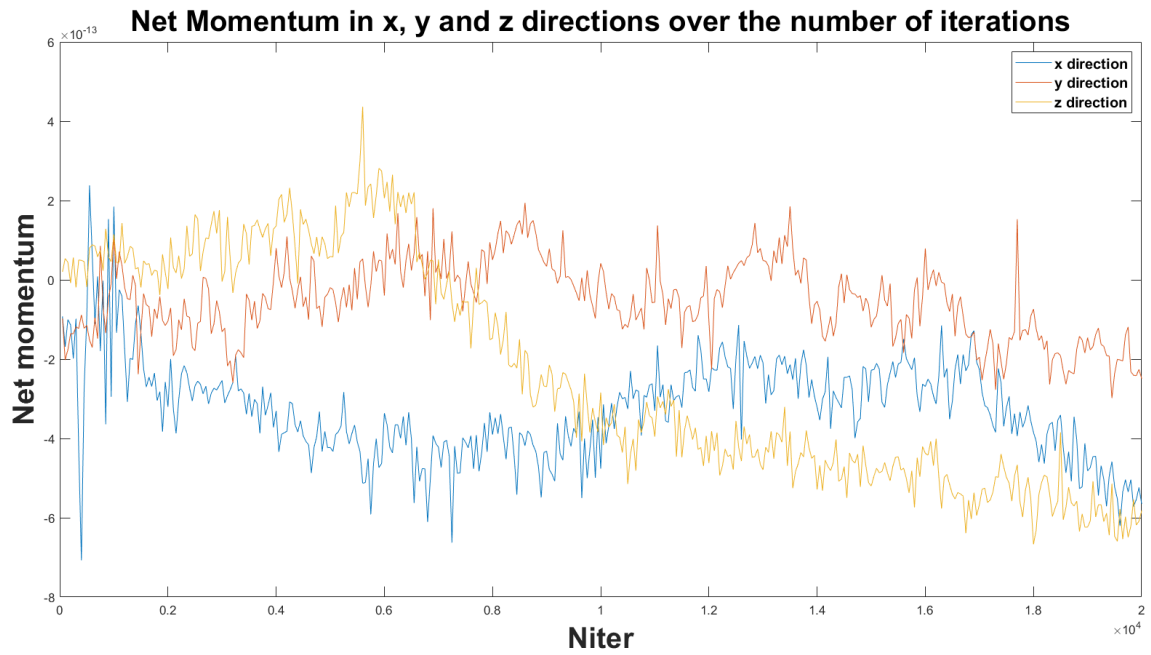


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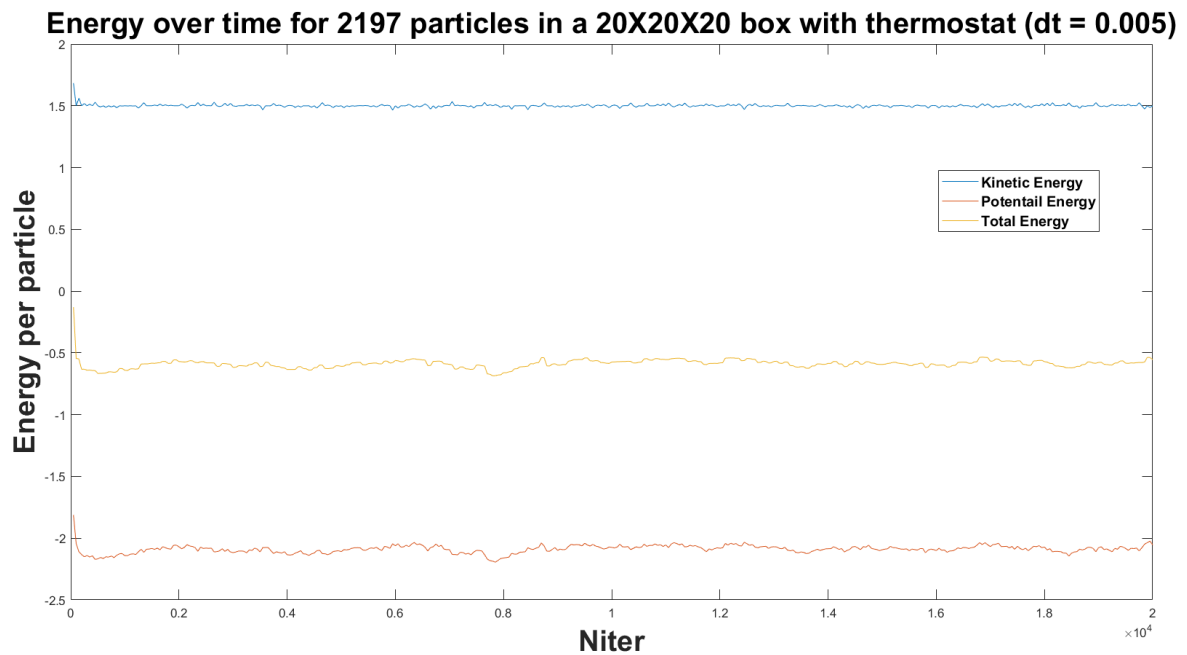




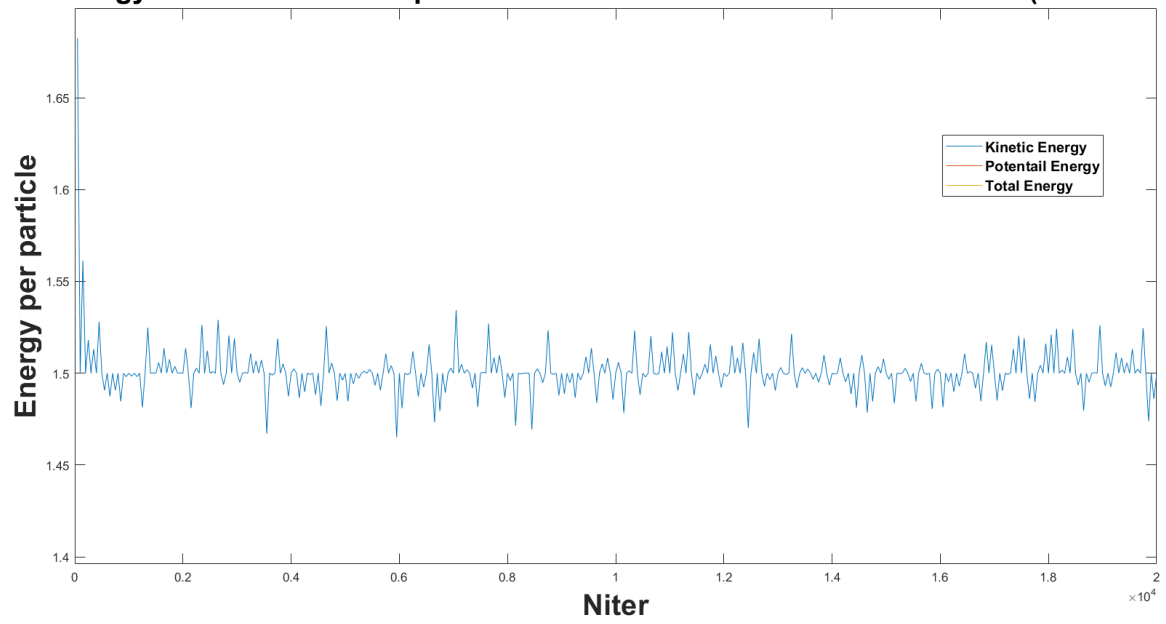
Question 3.

Parameters used: $\sigma = 1$, $\epsilon = 1$, $K_B T = 1$, $r_{\text{cutoff}} = 2.5 \sigma$, thermostat ON, niter = 250000, sampling rate = 50 itrns.

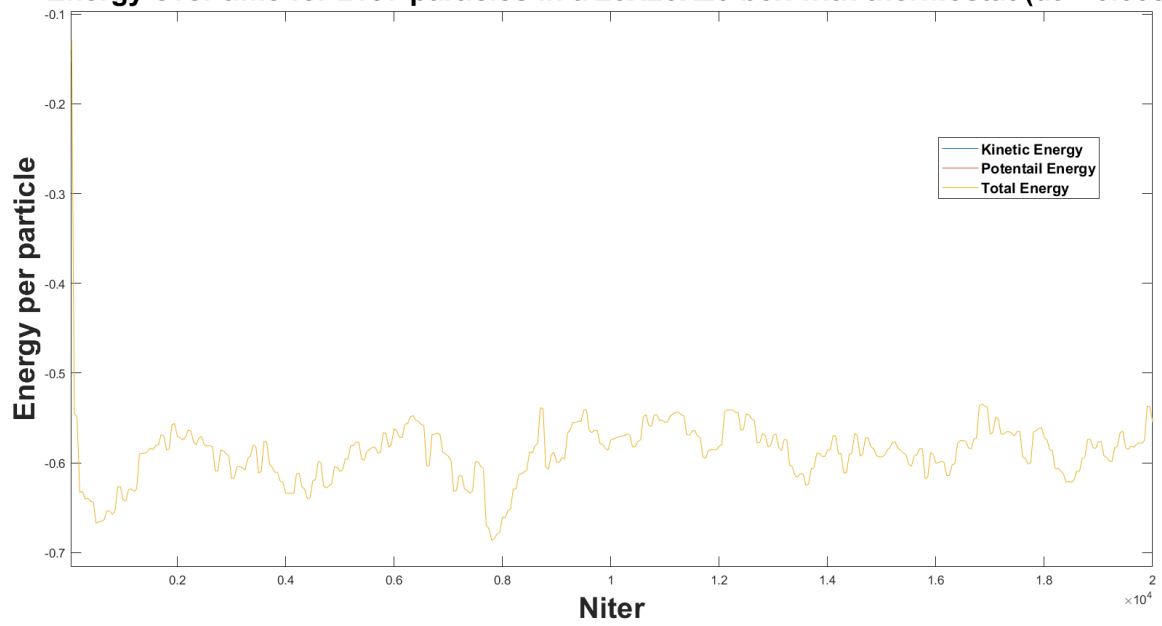
We see PE fluctuates around -2.1 and KE fluctuates around 1.5. TE fluctuates around -0.6.



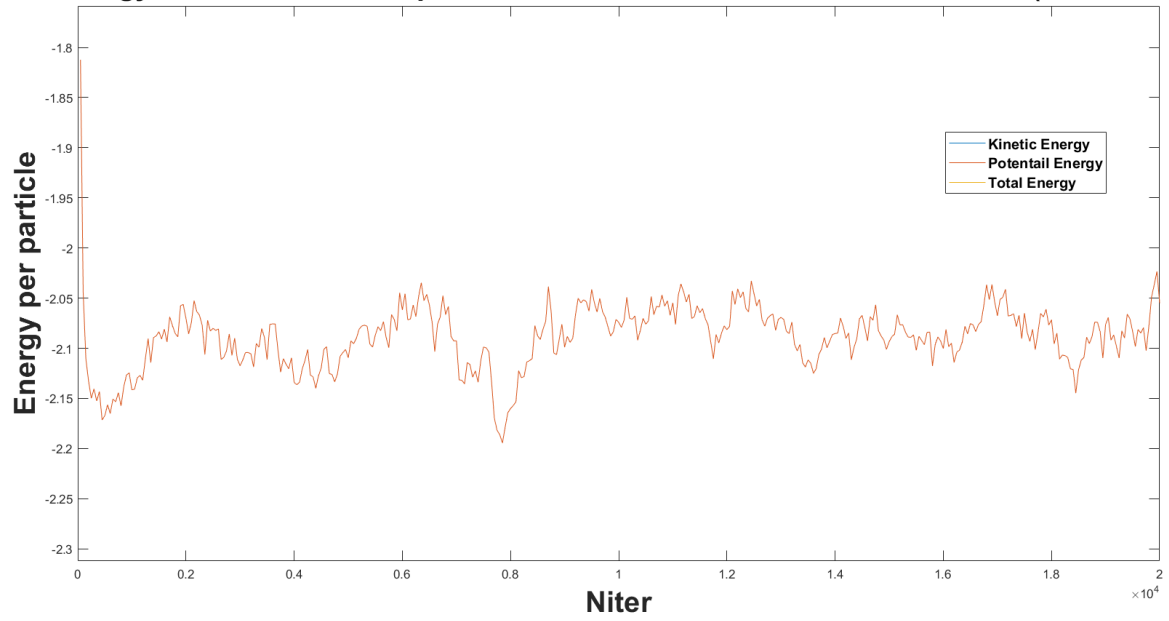
Energy over time for 2197 particles in a 20X20X20 box with thermostat (dt = 0.005)



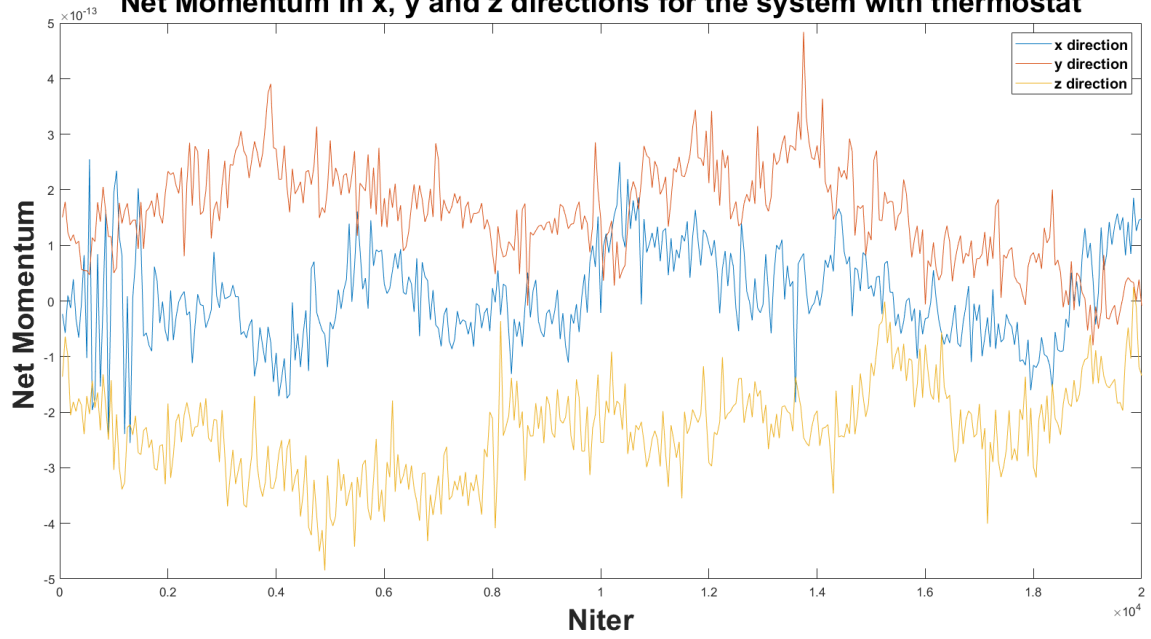
Energy over time for 2197 particles in a 20X20X20 box with thermostat (dt = 0.005)



Energy over time for 2197 particles in a 20X20X20 box with thermostat (dt = 0.005)



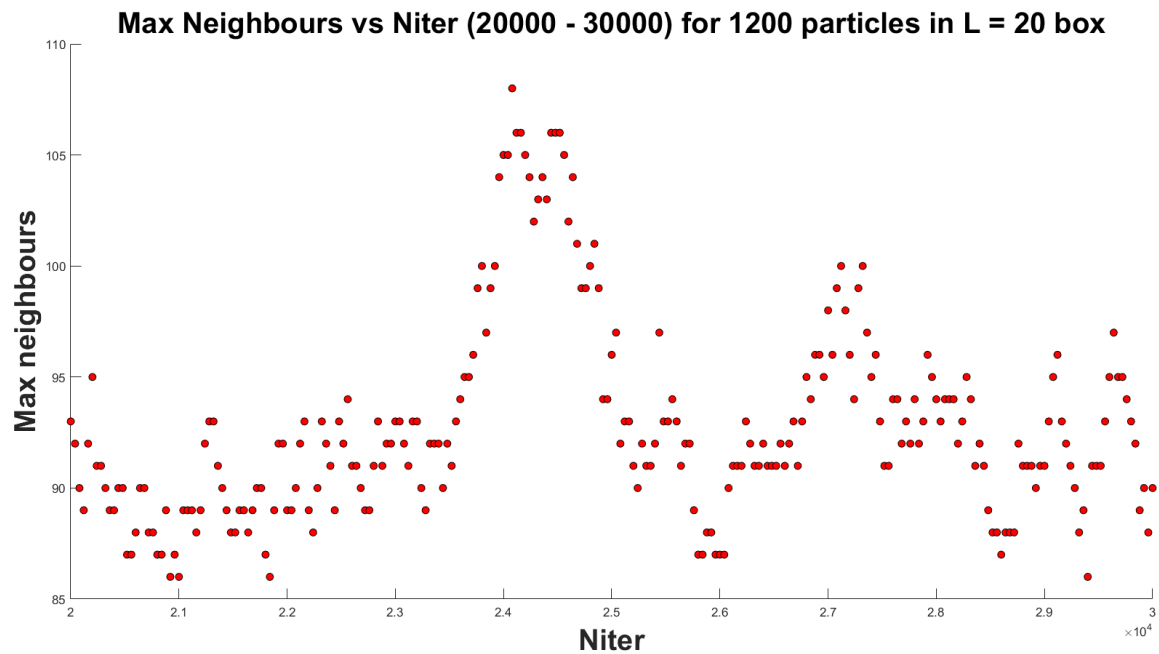
Net Momentum in x, y and z directions for the system with thermostat



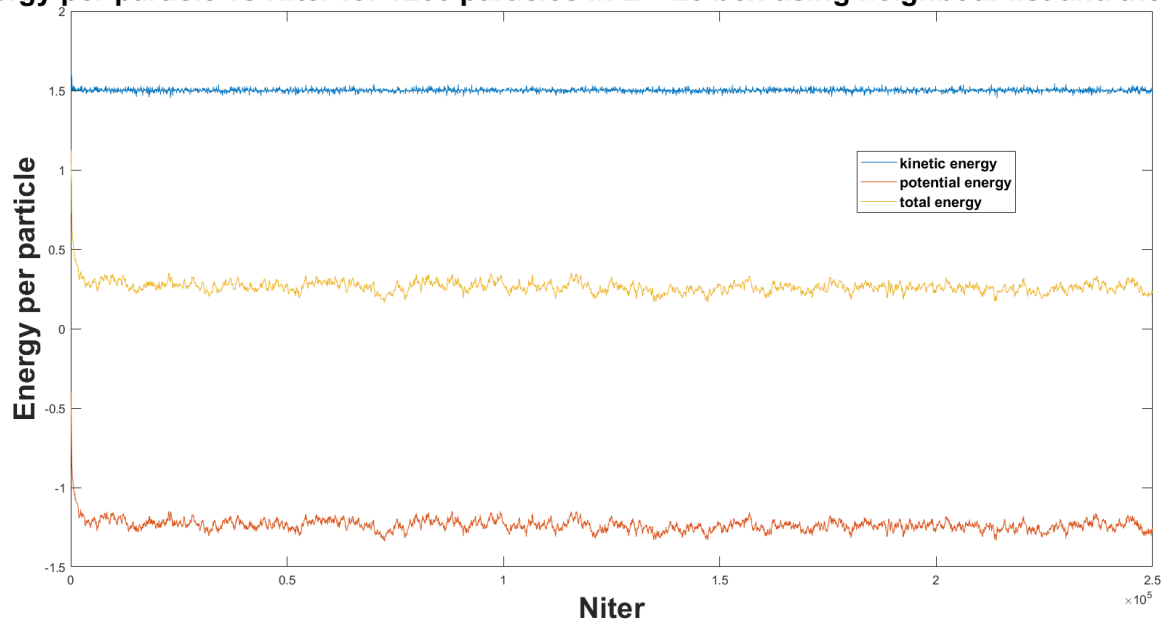
Question 4.

Parameters used: $\sigma = 1$, $\epsilon = 1$, $K_B T = 1$, $r_{\text{cutoff}} = 2.5 \sigma$, $r_{\text{nearby}} = 4.5 \sigma$, thermostat ON, neighbour list updated every 40 iters. Sampling rate = 50 iters.

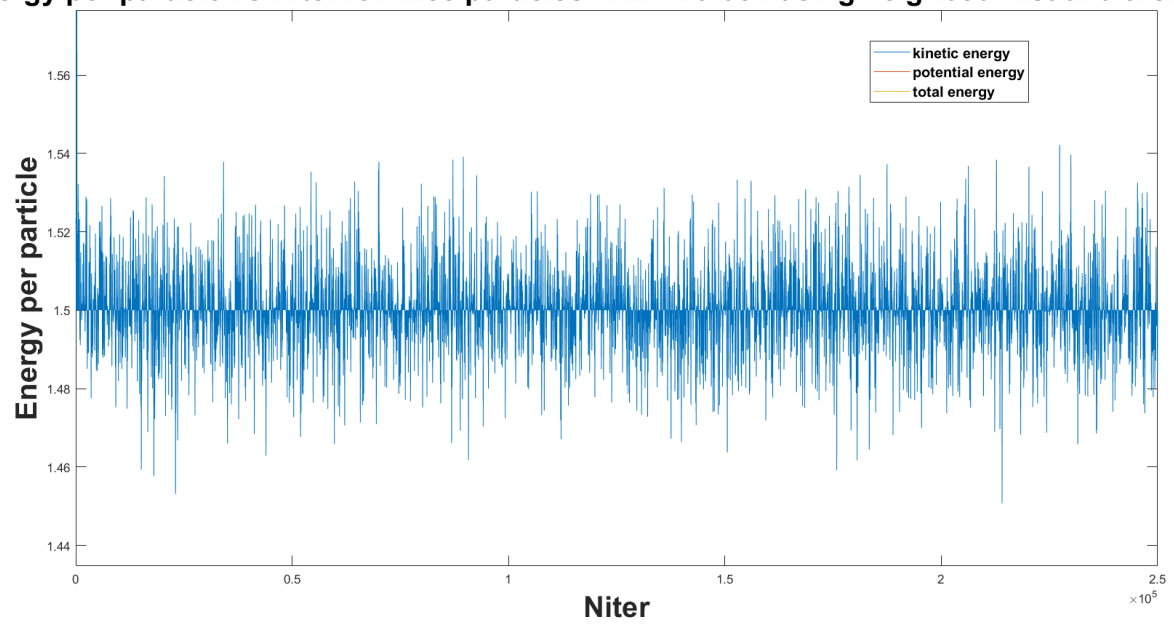
We see max number of neighbours lie between 86 and 103.



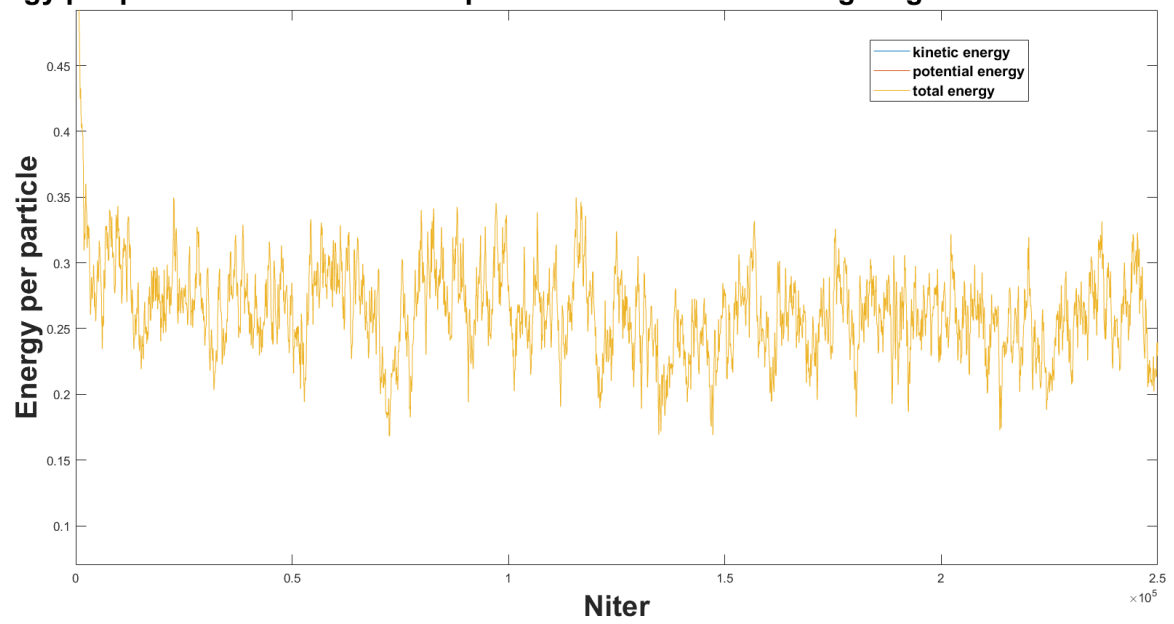
Energy per particle vs Niter for 1200 particles in L = 20 box using neighbour list and thermostat



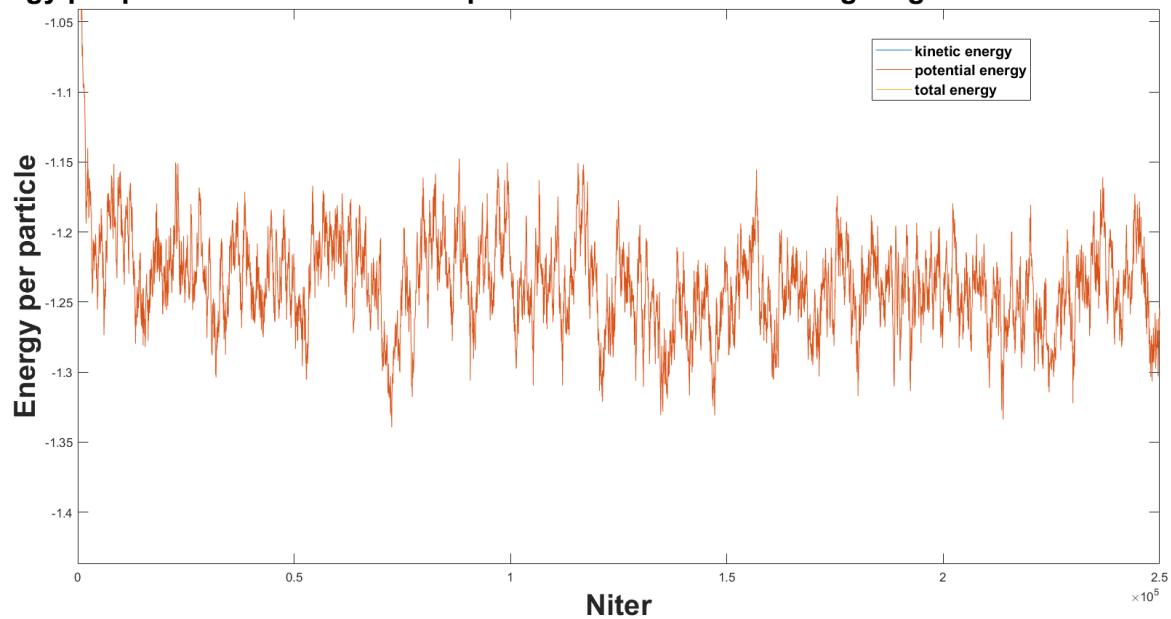
Energy per particle vs Niter for 1200 particles in L = 20 box using neighbour list and thermostat



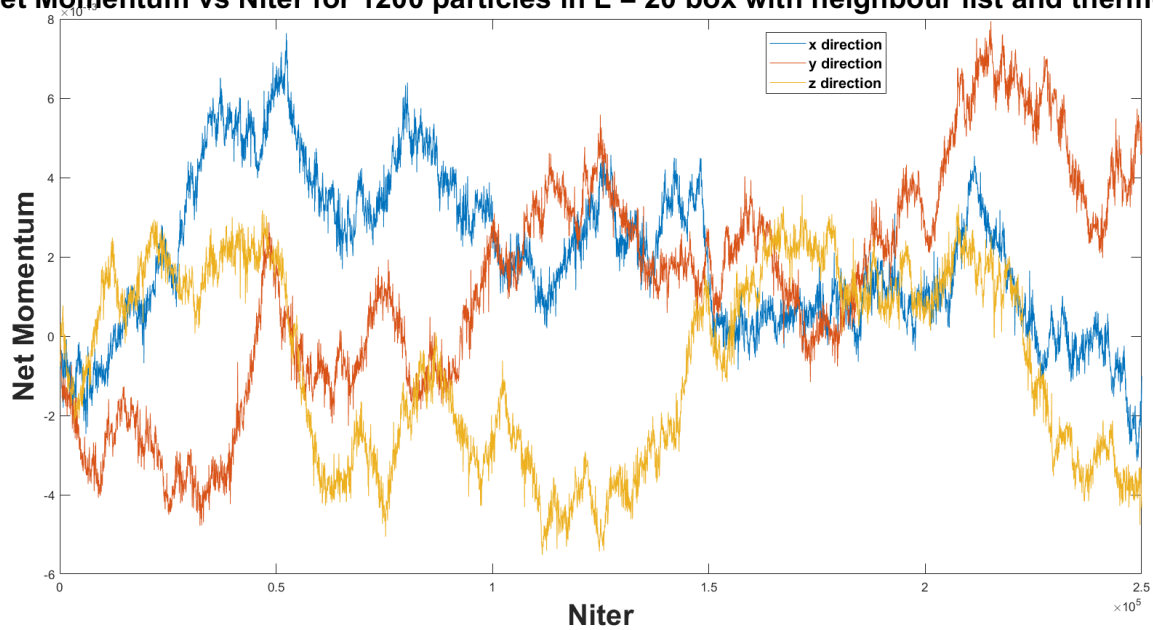
Energy per particle vs Niter for 1200 particles in L = 20 box using neighbour list and thermostat



Energy per particle vs Niter for 1200 particles in L = 20 box using neighbour list and thermostat



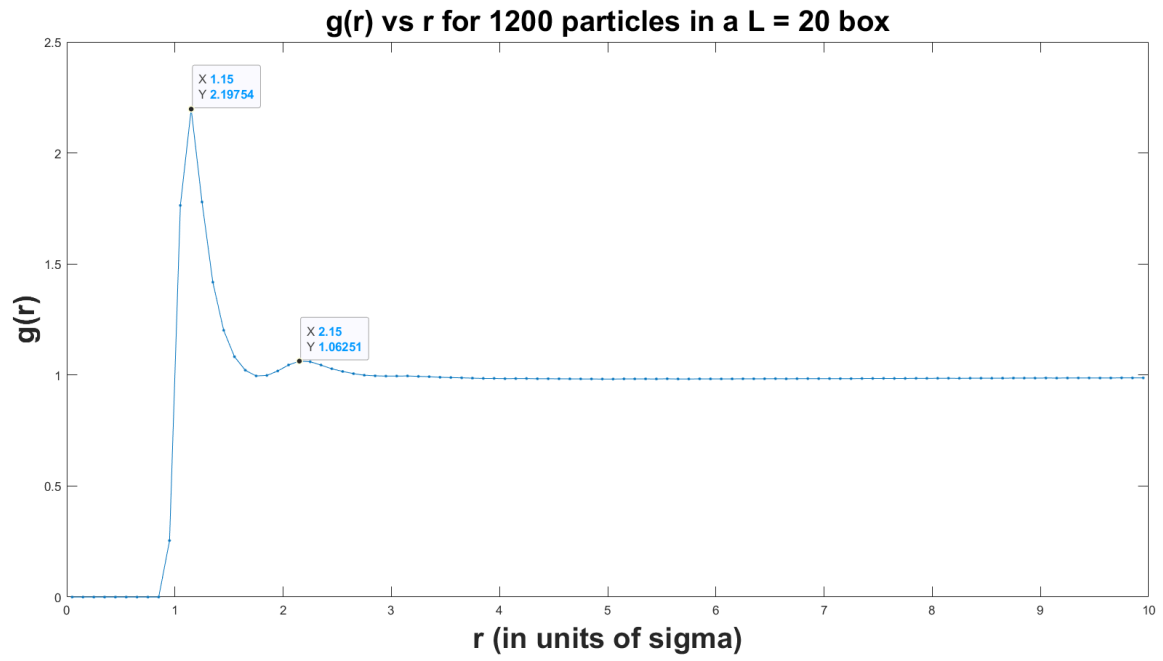
Net Momentum vs Niter for 1200 particles in L = 20 box with neighbour list and thermostat



Question 5.

Parameters used: $\sigma = 1$, $\epsilon = 1$, $K_B T = 1$, $r_{\text{cutoff}} = 2.5 \sigma$, $r_{\text{nearby}} = 4.5 \sigma$, thermostat ON, neighbour list updated every 40 iters. Sampling rate = 50 iters.

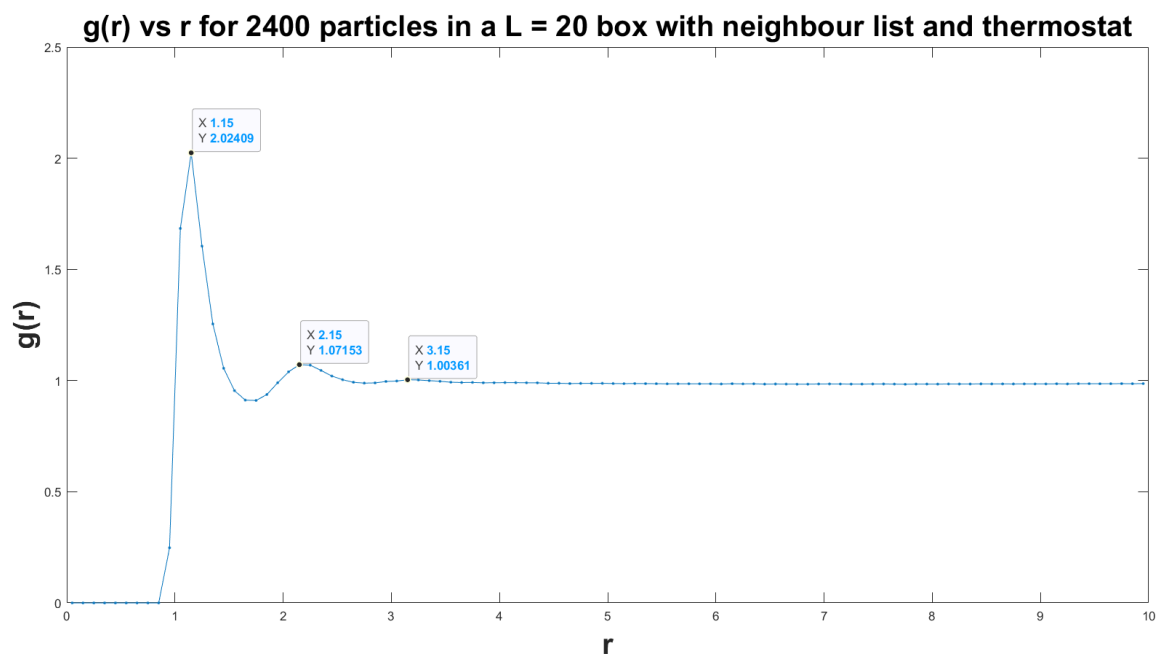
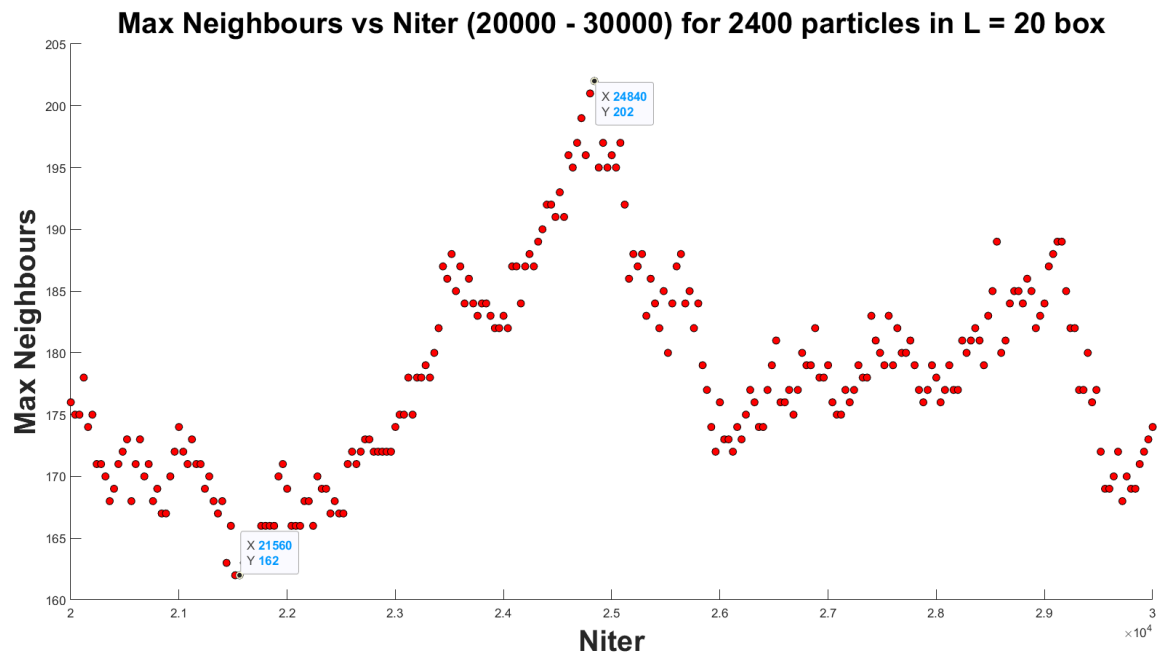
Max correlation happens at $r = 1.15$ and next highest at 2.15.



Question 6.

Parameters used: $\sigma = 1$, $\epsilon = 1$, $K_B T = 1$, $r_{\text{cutoff}} = 2.5 \sigma$, $r_{\text{nearby}} = 4.5 \sigma$, thermostat ON, $n_{\text{iter}} = 50000$, neighbour list updated every 40 iters. Sampling rate = 100 iters.

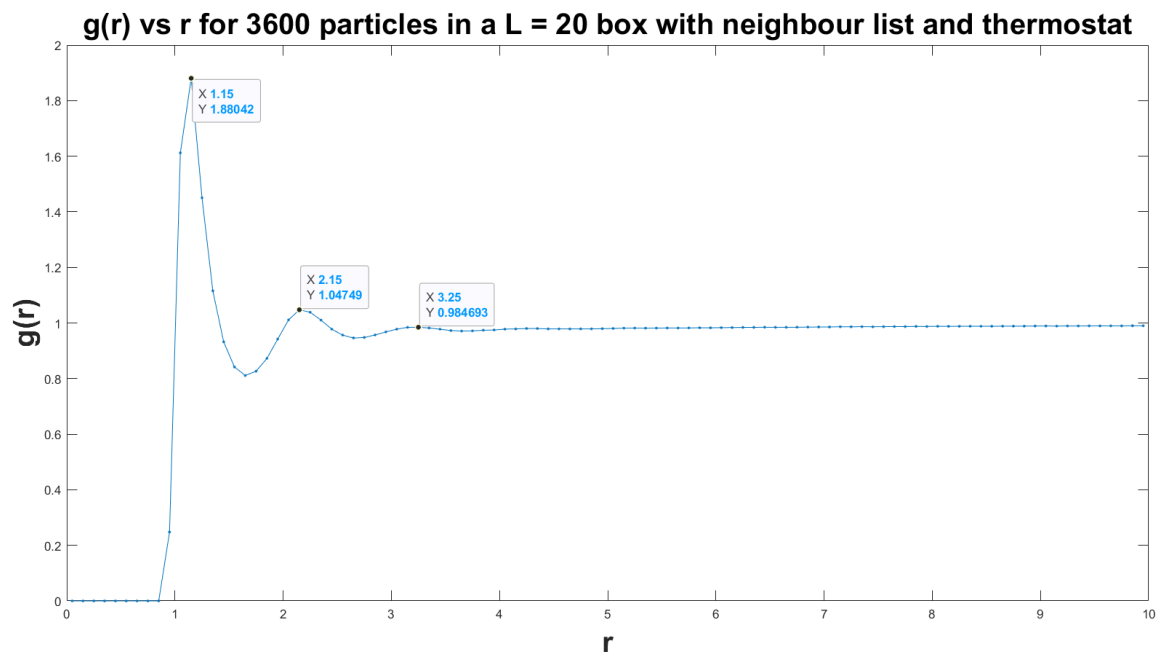
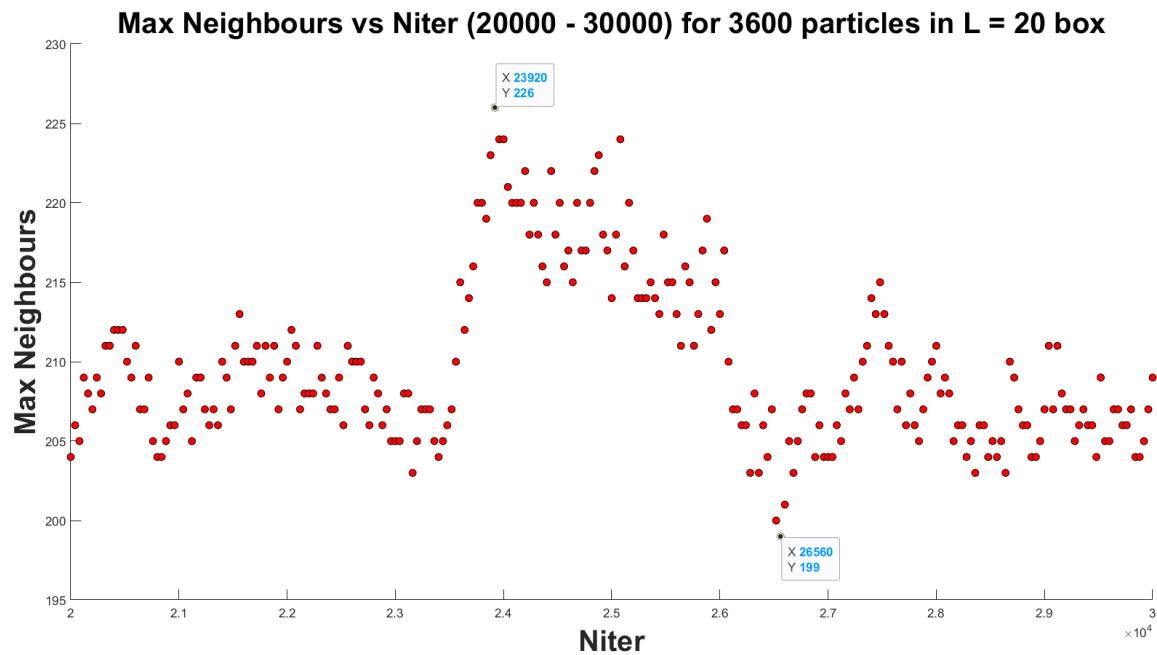
We see max number of neighbours lie between 162 and 202. Max correlation happens at $r = 1.15$ and next highest at 2.15 and the next one at 3.15.



Question 7.

Parameters used: $\sigma = 1$, $\epsilon = 1$, $K_B T = 1$, $r_{\text{cutoff}} = 2.5 \sigma$, $r_{\text{nearby}} = 4.5 \sigma$, thermostat ON, $n_{\text{iter}} = 50000$, neighbour list updated every 40 iters. Sampling rate = 100 iters.

We see max number of neighbours lie between 199 and 226. Max correlation happens at $r = 1.15$ and next highest at 2.15 and the next one at 3.25.

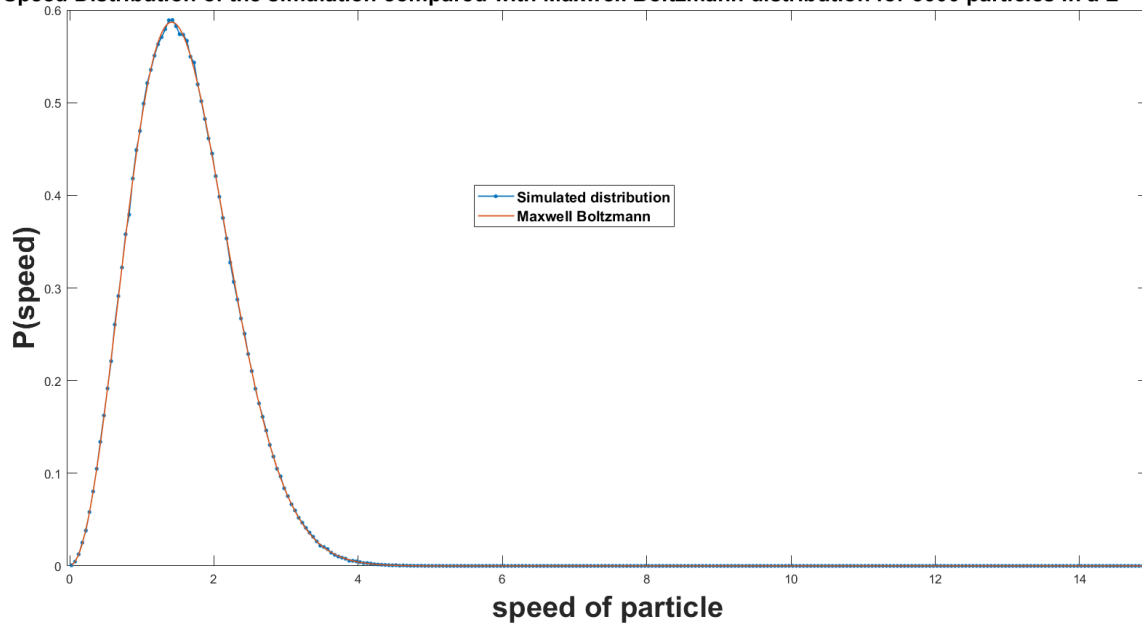


Question 8.

Parameters used: $\sigma = 1$, $\epsilon = 1$, $K_B T = 1$, $r_{\text{cutoff}} = 2.5 \sigma$, $r_{\text{nearby}} = 4.5 \sigma$, thermostat ON, $n_{\text{iter}} = 50000$, neighbour list updated every 40 iters. Sampling rate = 100 iters.

We see the Maxwell Boltzmann speed distribution curve obtained from the simulation is in agreement with the theoretical curve.

Speed Distribution of the simulation compared with Maxwell Boltzmann distribution for 3600 particles in a $L = 20$ box



Speed Distribution of the simulation compared with Maxwell Boltzmann distribution for 3600 particles in a $L = 20$ box

