Assignment 6: Molecular dynamics:

Q1. The quantity llx=30. Practice for PBC

x=modulo(27.05d0,llx) y=modulo(30.05d0,llx) z=modulo(-0 .03d0,llx)

Q2. Do a molecular dynamics simulation with 2197 (=13*13*13) particles in a 20*20*20 box with dt=0.005 with Lennard Jones particles. Epsilon=1, r_c =2.5d0. r_c is the distance at which potential is cutoff.

CHECK FOR ENERGY MOMENTUM CONSERVATION.

Run the simulation for 20000 iterations **without thermostat**. The potential energy (PE) and the kinetic energy (KE) fluctuates around the values ??

Q3. Do a molecular dynamics simulation with 2197 particles in a 20*20*20 box with dt=0.005.

Run the simulation for 20000 iterations **with thermostat k_BT =1**. The rest of parameters are same as in the previous question. The potential energy (PE) and total energy (TE) a fluctuates around the values.

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Q4. Do a molecular dynamics simulation with 1200 particles in a 20*20*20 box with dt=0.0025 with Lennard Jones particles of diameter sigma. Epsilon=1, r_c =2.5d0. r_c is the distance at which potential is cutoff. Implement neighbour list: update neighbour list every 40 iterations. r_s = r_c + 2.0 =4.5 sigma. Equilibrate the system for 50000 iterattions with thermostat.

After the first 50K iterations are over, start collecting data over the next 2,50,000 iterations to calculate g(r): the pair correlation function. The bin size for calculating g(r) is dr=0.1 sigma. Data to calculate g(r) is collected every 100 iterations.

The initial configuration of particles in the can be random OR arrange the particles in a lattice such that box is uniformly filled (i.e. there are no large voids in the box).

(a). In the first 20,000-30000 iterations, the most number of neighbours (i.e. within distance r_s) that a particle could have lies in the range:

Q5. The height of the first peak of the pair correlation function g(r) is:

Q6. The number of particles in the (20)^3 box is changed to 2400. Everything else remains the same as above. The height of the second peak of g(r) is "**h**" and the position of the peak is at "**r1**" sigma. The values of **h** and **r1** are

Q7. The number of particles in the (20)^3 box is 3600. Everything else remains the same as above. The position of the (weak) third peak is at "**r1**" sigma. The values of **r1** in units of sigma are:

Q8. Check that you are getting the correct Maxwell Boltzmann speed distribution of the particles and check that it MATCHES EXACTLY with the theoretical distribution.