Assignment 08: Molecular Dynamics Simulations

Due: December 10, 2021

Q1.

Write A molecular dynamics code interacting with each other with LJ interaction, with 1000 particles in 20*2*020 box with PBC, and show explicity that energy and momentum is conserved. Use the velocity Verlet Algorithm. dt =0.005 τ. Cutoff for potential r_c =2.5 σ.

Momentum per particle will be conserved to 10^(-15), whereas energy will conserved to – ??

Remember to put Center of mass vel=0, at the beginning of simulation.

Q2.

If increase number of particles to 2000, and you also incorporate a thermostat called every 100 iterations, show momentum is still conserved and energy is fluctuating about mean values. Energy should be conserved for 100 MD steps, in between the two calls of thermostat.

Q3. What is the meaning of unit of time, τ in the simulations ? How will you make sense of "τ" beyond the formula ?