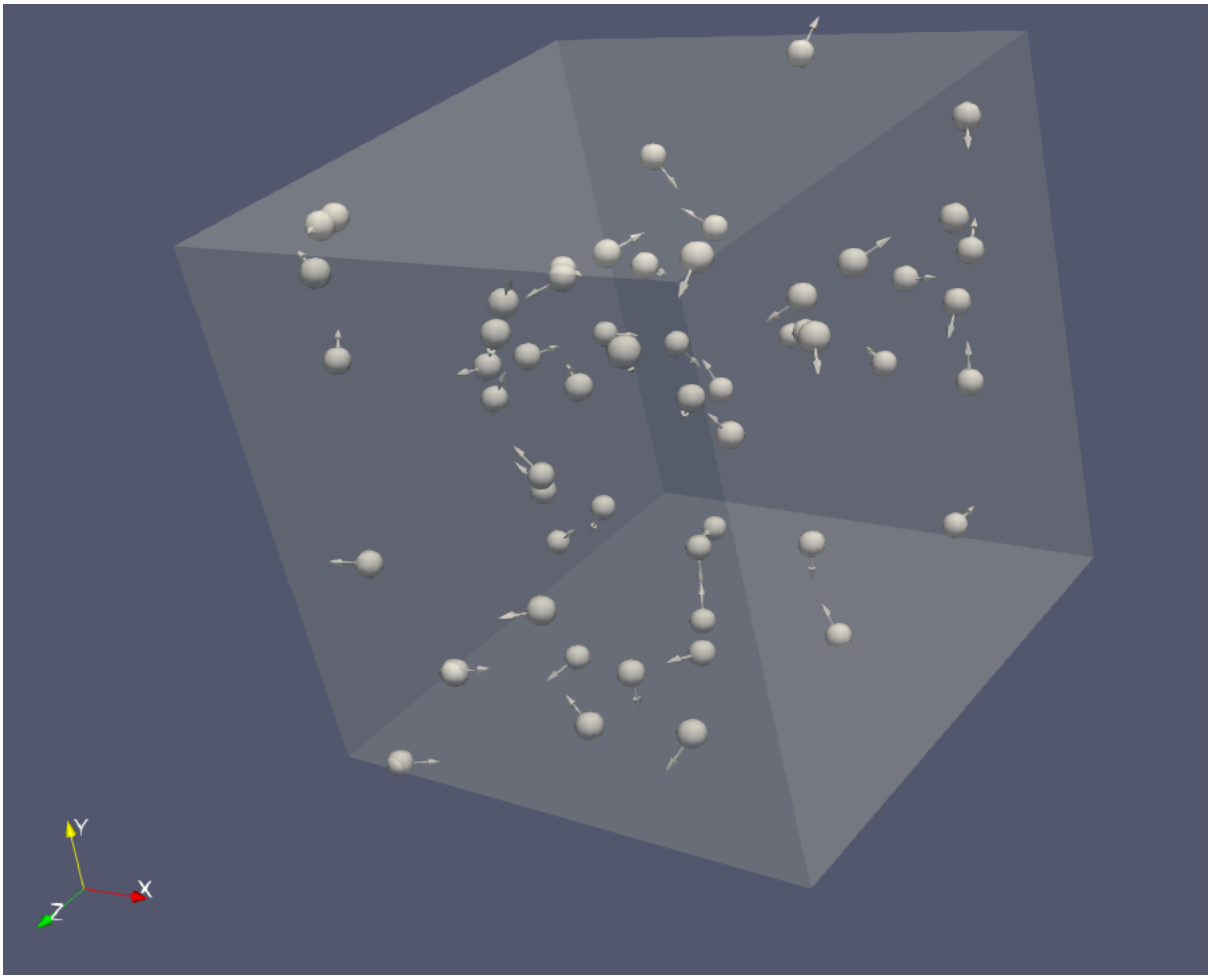
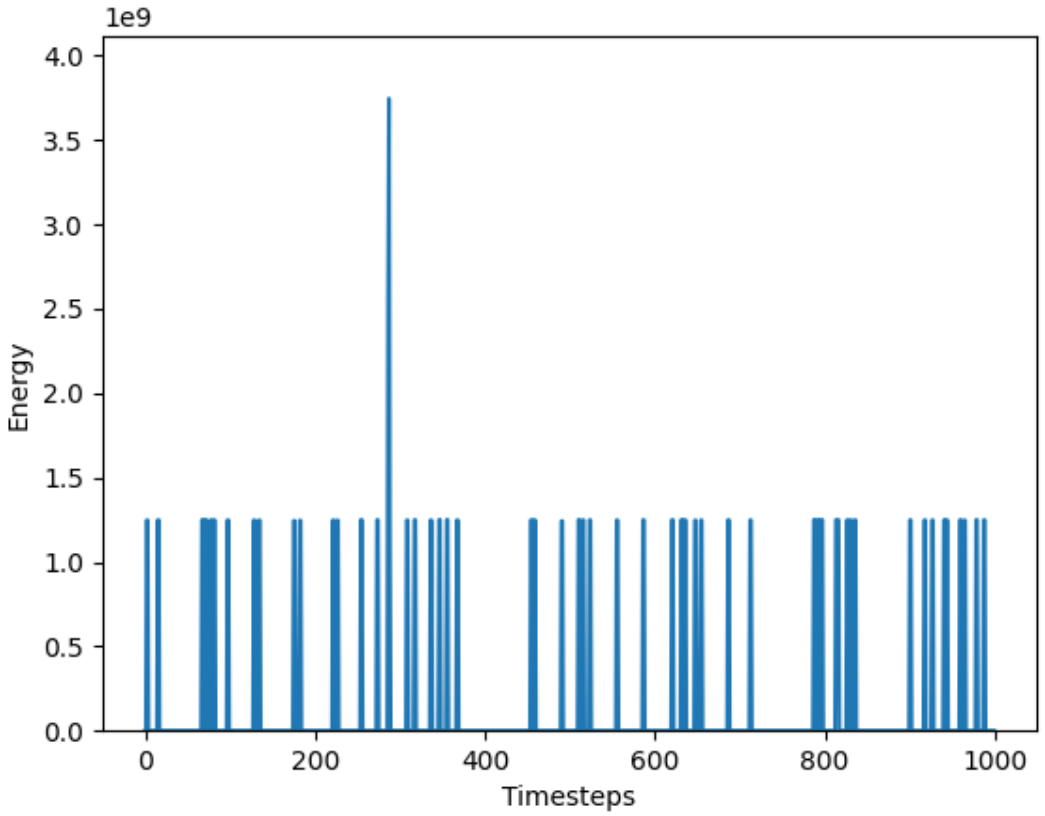
CSEP Ex07

How to run: “python3 md_verlet_basic.py”

Task1: Looking at paraview’s movie, the simulation looks right and how the particles behave.



Task2: Energy stays pretty constant, except those really big spikes which I don’t know why they happen. Maybe some of you can explain this? Using a normal distribution with var=1 was exactly right for the system total energy. The MD simulation pretty much stays at this total energy (hence energy conserved), except those outliers (spikes). In the normal case, the system should go to an equilibrium state. I think if we would run the simulation for very long, we would lose energy and go to zero, due to rounding error and the cutoff.



Task3: The smaller the time step the more accurate our measurements over smaller time steps are. We measure things more specific than if we would use a bigger timestep.