Exercise 1: MD simulations of LJ-Ag

In all simulations model Ag interatomic interactions using the LJ potential ($\varepsilon = 0.345\ eV$ and $\sigma = 2.644$ Å) with the cutoff radius at $r_c = 4.5$ Å. Assume $t_{th} = 3\ ps$ as thermalization time and use the simulation cell of 256-atoms (file **`fcc100a256.txt`** on the elearning page) unless stated differently. From point 3,

1. Use a sharp-cutoff approach and find the optimal timestep to perform a simulation from an initial temperature $T_{ini} = 50\ K$. The optimal timestep is the maximum one such that $\delta E/|\langle E\rangle| < 10^{-5}$. Consider the range $[1, 25]\ fs$ and perform 5000 integration steps for each trial. Repeat the analysis for $T_{ini} = 500\ K$ and show that the criterion cannot be fulfilled however reducing the timestep.
2. Implement a 7-degree polynomial junction for $r_p < r < r_c$ with $r_p = 4.2$ Å. Use the coefficients **`A, B, ..., H`** for the 0th, 1st, ..., 7th degree term respectively, as provided in the file **`poly7.py`** on the elearning page. Adapt the definition of forces accordingly. Check that for $T_{ini} = 50\ K$ the simulation is consistent with the sharp-cutoff one and find the optimal timestep for $T_{ini} = 500\ K$, $1000\ K$ and $2000\ K$.

For the following points, implement a steepest-descent procedure to start the simulation from a minimum energy configuration (use **`C`**$= 0.005$ Å$/eV$ and stop when the maximum force falls below $0.001\ eV$/Å).

3. Using the optimal timesteps found in point 2, perform $10\ ps$ long simulations for $T_{ini} = 50\ K$, $500K$, $1000\ K$ and $2000\ K$. Plot $\langle T\rangle$ as a function of T_{ini}, check if the condition $\langle T\rangle = T_{ini}/2$ is fulfilled and explain the result. Visualize the atomic trajectories of the atoms at the center of the cluster and at the cube vertices for both the lowest and highest temperature and comment on their difference.
4. Consider an infinite crystal slab ($L_x = L_y = 16.6416$ Å) with free-surfaces in the z direction. Add one adatom at the center of the upper surface, with z coordinate set 2.4 Å above the maximum z coordinate of the atoms in the cell. Perform a $300\ ps$ long simulation starting from the minimized configuration. Set T_{ini} such to achieve an equilibrium temperature $T = 850 \pm 30\ K$ and use an appropriate timestep. Trace the trajectory of the adatom over time.
5. Repeat the analysis of point 4 using a (111)-oriented cell from the file **`fcc111a336+1.txt`** on the elearning page with $L_x = L_y = 20.3817$ Å and compare the results for the two orientations. Is the adatom diffusion likely to happen at room temperature on one or both surfaces on the same time interval?