Molecular dynamics projects

Exploring 6ll1 model

Intro

6ii1 is 4 chain structure haemoglobin from cattle (Bos taurus).

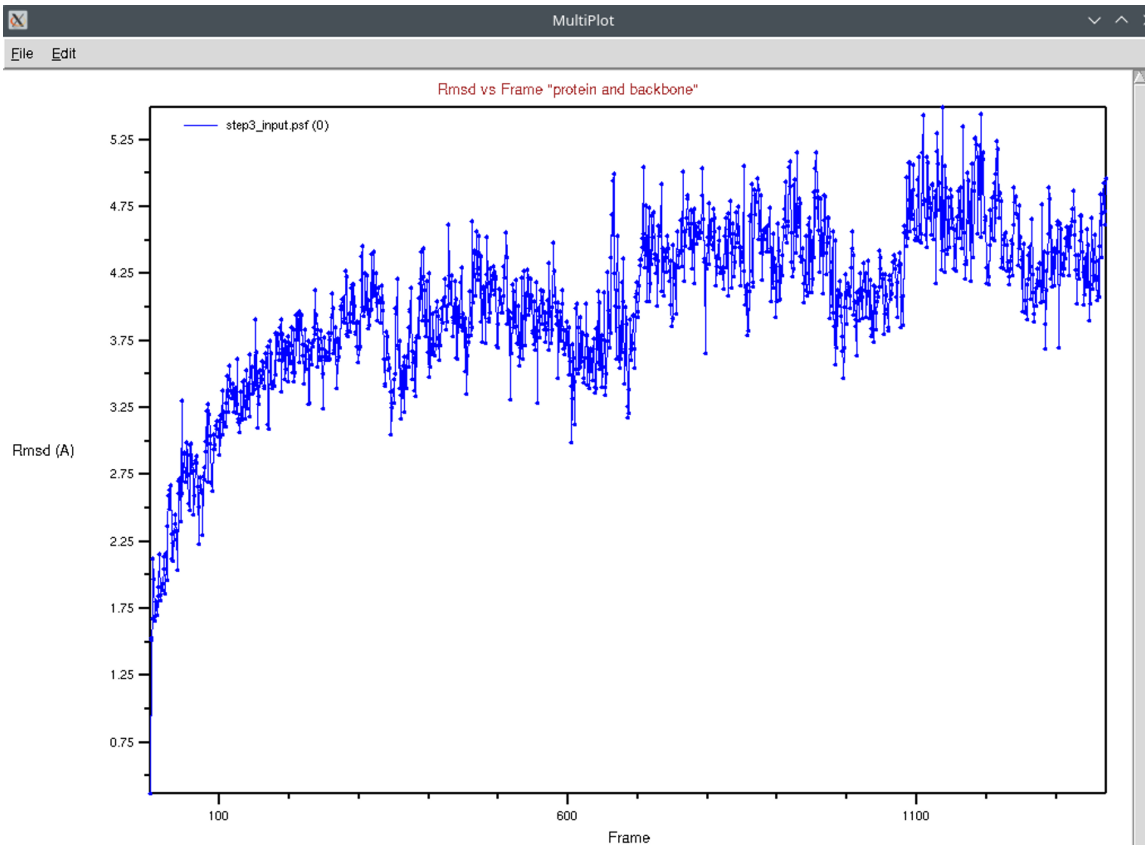
The task was to explore the haemoglobin structure using different techniques from VMD, tcl programming language and Gromacs, while familiaring ourselves the basics of biological modelling

Methods and results

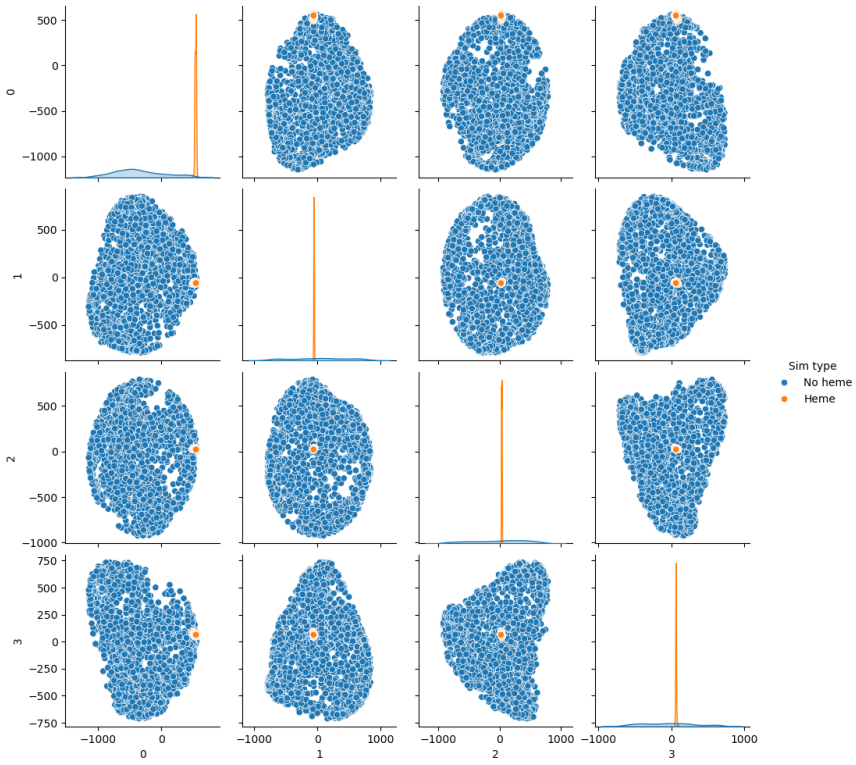
Using AlphaFold structure database and CHARMM-GUI structure bank to we get haemoglobin PDB structures.

List of VMD analyses perfromed

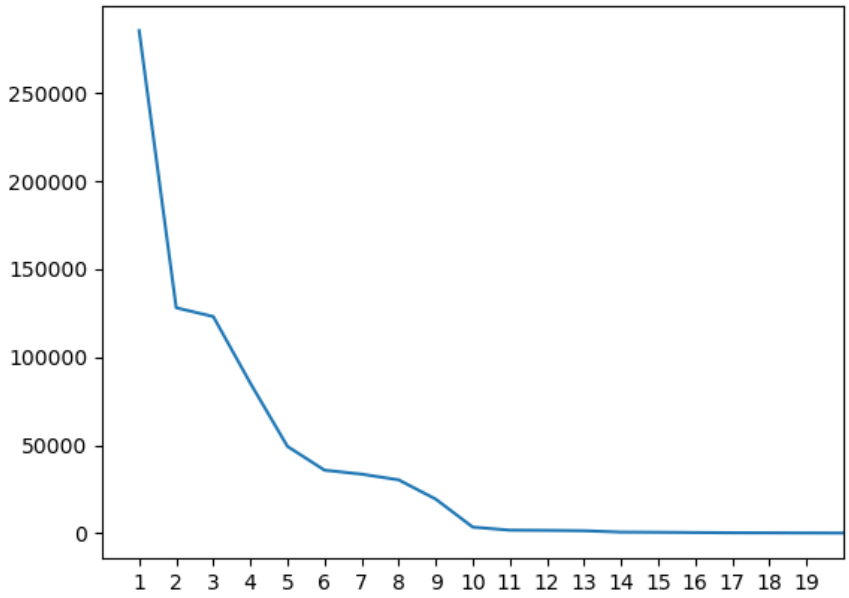
- Comparing the structure differences: using MultiSeq and Stamp Structural Alignment -tool
- Root-Mean-Squared-Deviation analysis on haemoglobin backbone structure



  - Ramachandran plot
  - Salt Bridge analyses
- Get basic molecular data (TCL-programming with VMD)
- Comparison of energy minimization methods for energy minimization (Gromacs)
- Principal componen analyses (Python)

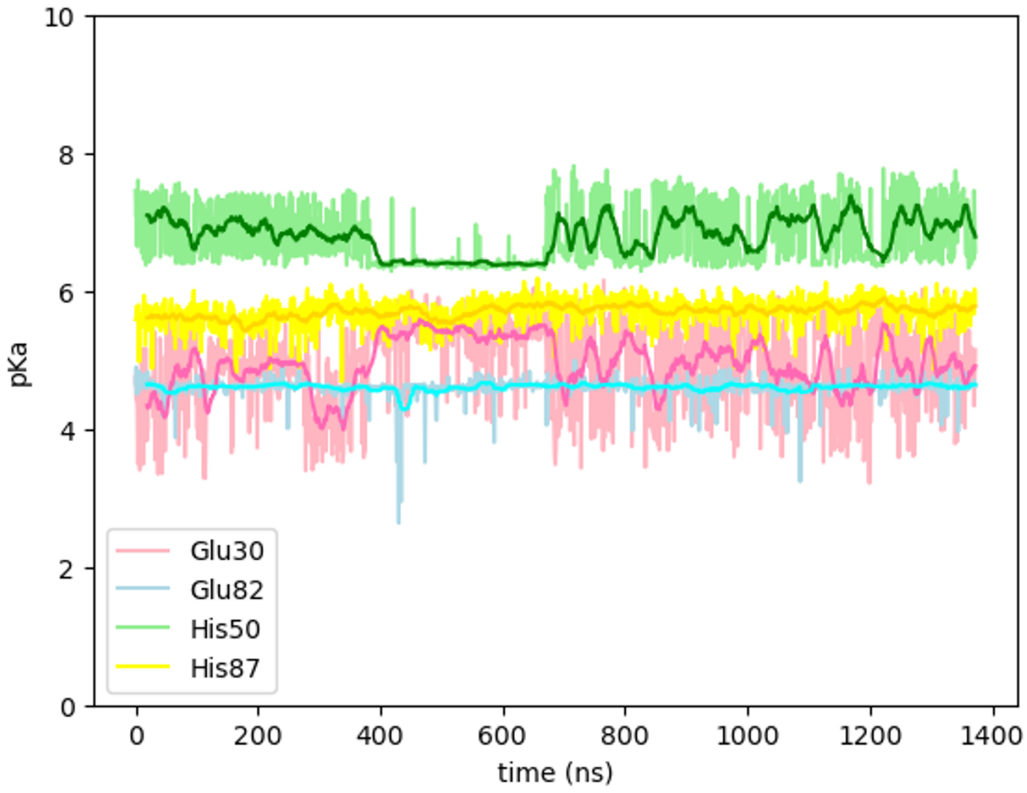


Pairplots of haemoglobin, using its backbone structure, and trajectories from heme-bound haemoglbin



PCA-analyses, eigenvalues of principal component plotting.

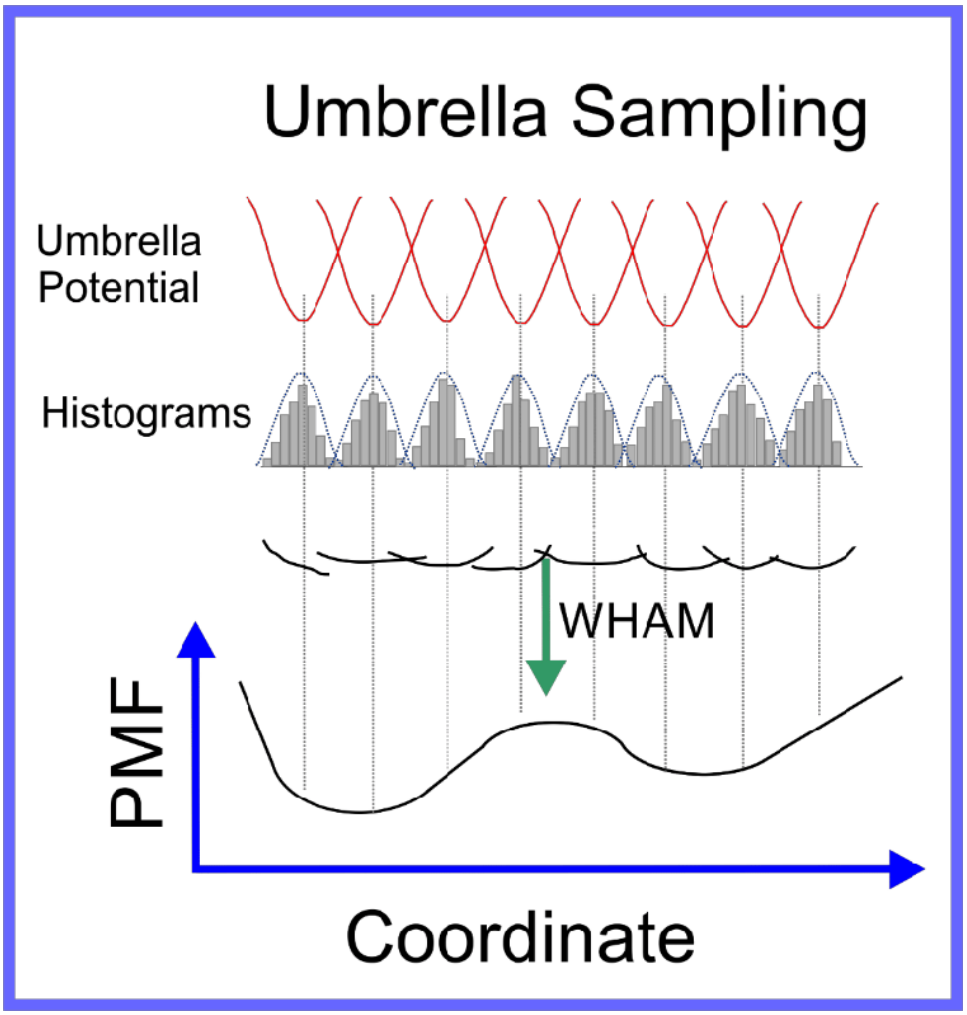
- pKa-value analyses on selected residues of haemoglobin:



Umbrella analysis with water dimer

Intro

Umbrella analysis is an effective method to get the energy profile between two conformations of a molecule or similar systems.

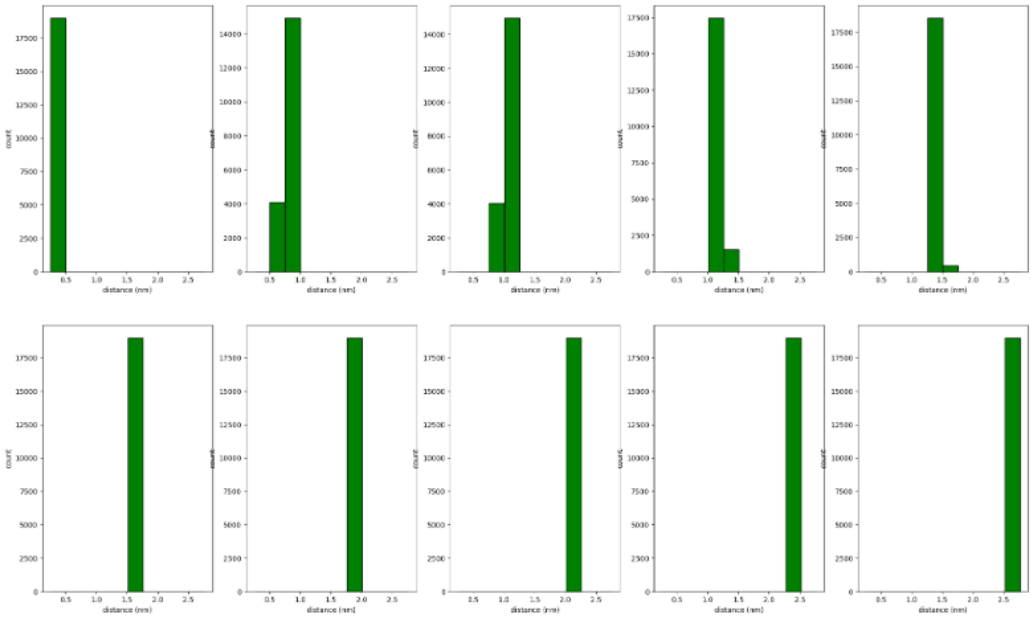


Simple figure from the lecture note of Molecular dynamics simulations -Course

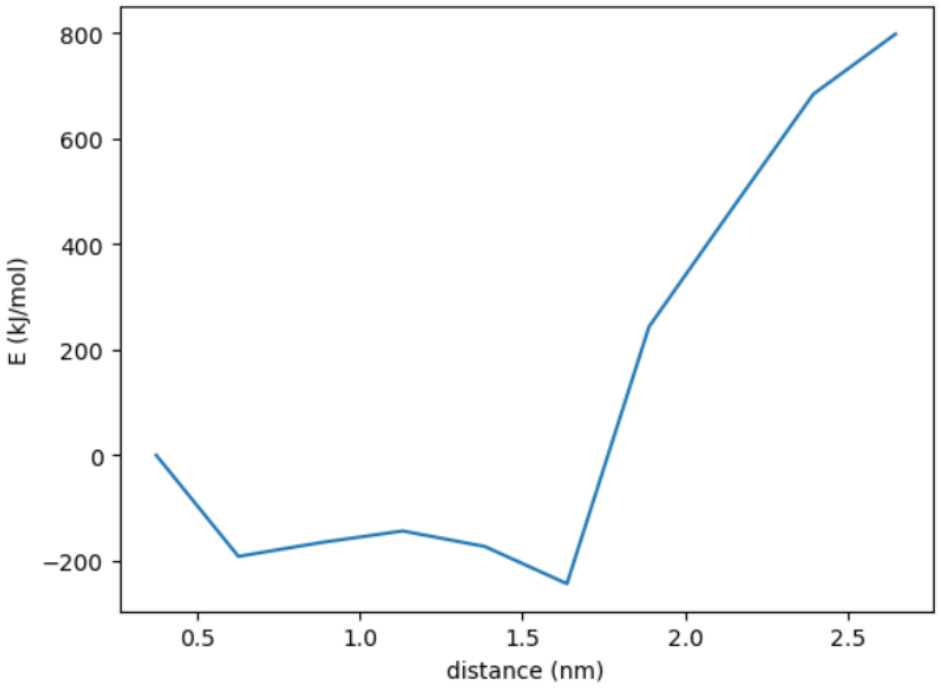
The task of this exercise is investigating energy profile of water dimers, produced by the different range of center of mass (COM) distances.

methods and results

I edited the readily made scripts provided by the course reponsibles and made umbrella sampling in Gromacs. I created a Python script for creating different runs, each run corresponding to different COM distances of the two water dimer, and creating .sh files for executing each runs. Using parallel computing system of Puhti I got the results:



Histograms for each COM distance



Energy profile of water dimer

From the histogram, we see there is only slight overlapping of different COM distances. If we could better the umbrella sampling, we should choose smaller distance differences between consecutive distances.

Nucleation of Argon gas

Intro

The nucleation of argon gas was investigated using LAMMPS, using the simplified Lennard-Jones potential. Under supersaturated conditions, two forms of phase transition are possible, nucleation and spinodal decomposition. In spinodal decomposition, a single thermodynamic phase spontaneously separates into two phases, effectively manifesting as nucleation occurring everywhere at the same time.

In this exercise, we simulated N=8192 Ar atoms with independent NVT-ensemble runs, each corresponding to differing box sizes, and calculated the approximate crossover point between the two forms of phase transition occurs.

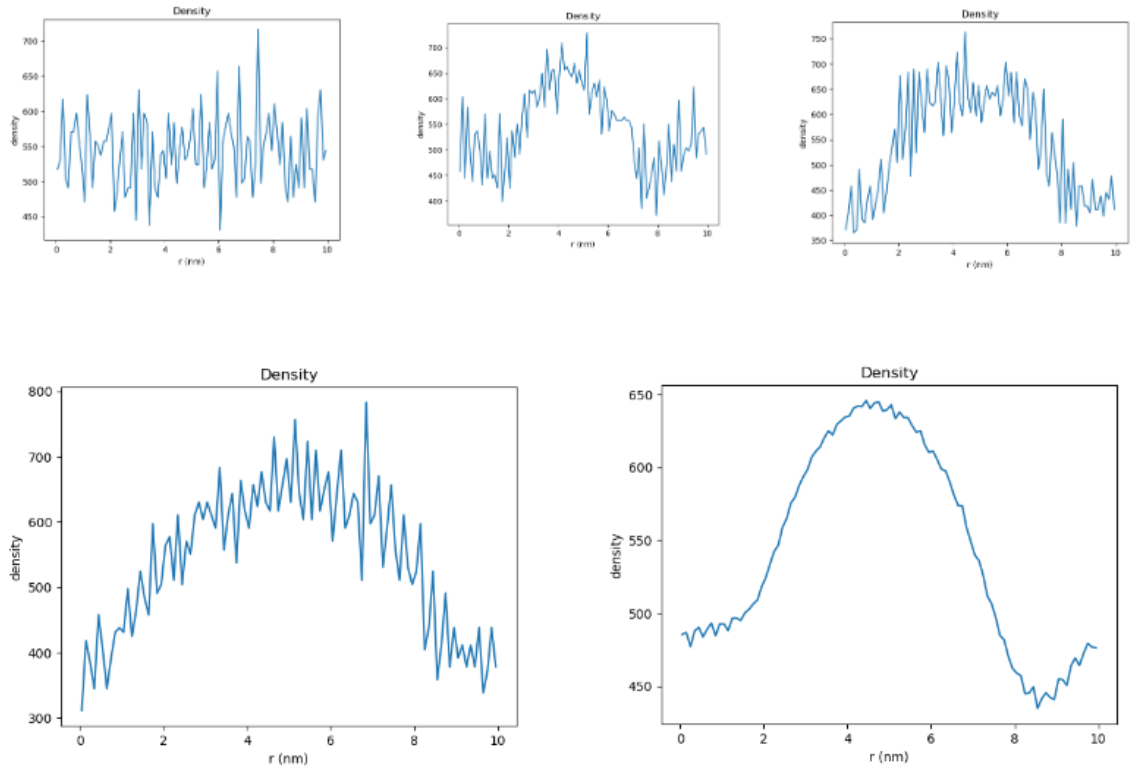
Methods

We used Packmol to prepare the systems for each independent NVT run, the length of one side in cubic box in the range of 10.5 nm–15 nm, with 0.5nm intervals . Then I created the scripts for energy minimization and equilibration for the Gromacs. These are all done in Python.

The output trajectories are then first visually inspected and analyzed using Cluster Analysis tool in Ovito, to determine whether the spinodal decomposition occurred or if it is just simple nucleation.

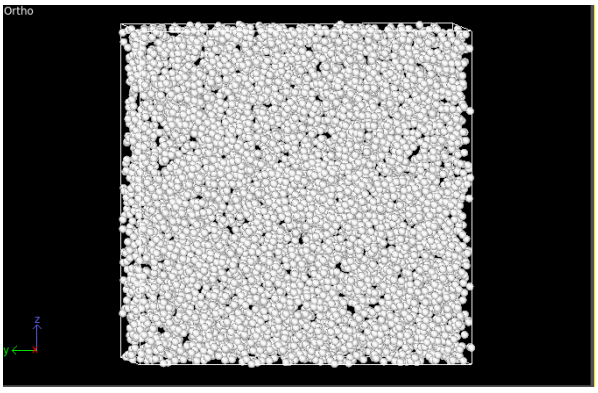
Results

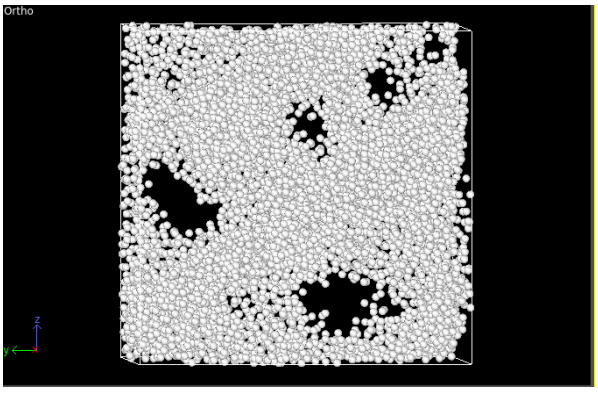
At 10 nm, I detected the spinodal decomposition forming.

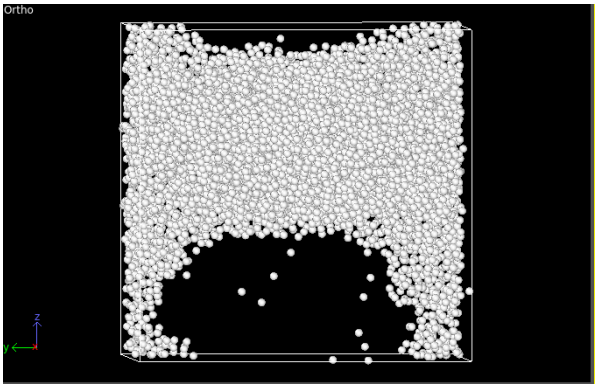


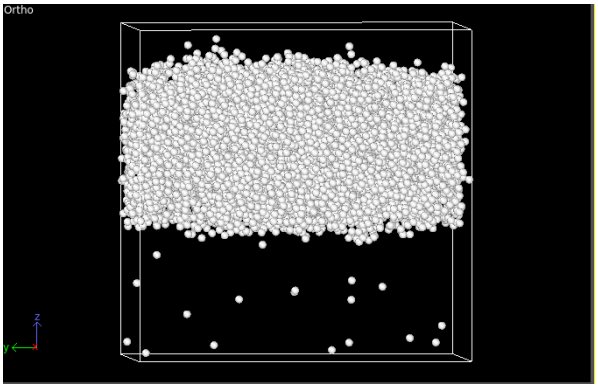
Time evolution of local density plots at 10nm box size. In the final frame, the expected sinusoidal curve is fully formed.

Below we see the time evolution of the spinodal decomposition. In the final stage, we get a slab of continuous phase of liquid argon, from which we computed the surface tension $\gamma = 116.84 nm \cdot bar$









Based on different NVT runs, we determined the supersaturation density at which the crossover happens is somewhere between:

$$4.194304nm^{-3} < x < 2.985423nm^{-3}$$

Molecular dynamics of seeded ice crystal growth on AgI surface

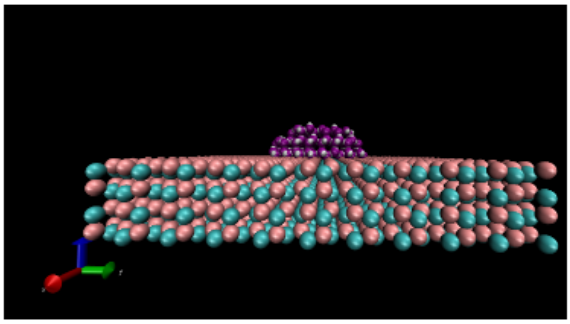
Intro

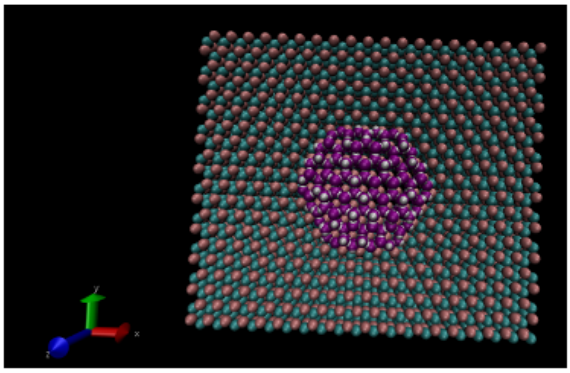
Silver Iodide (AgI) is a commonly used salt for cloud seeding. In this exercise, I investigated seeded ice crystal growth by placing the ice hemisphere on AgI crystalline surface. Some relevant quantities are calculated.

We are provided with pre-made ice crystal hemisphere structure file, AgI crystalline structure file and a script for solvating the system. Our task was then placing the ice crystal hemisphere on the AgI hemisphere, and then run the script to solvate the system. And finally by determining the resulting contact angle and the critical radius of the ice crystal hemisphere, ie. the minimum radius at which it is thermodynamically stable, we can determine the nucleation rate.

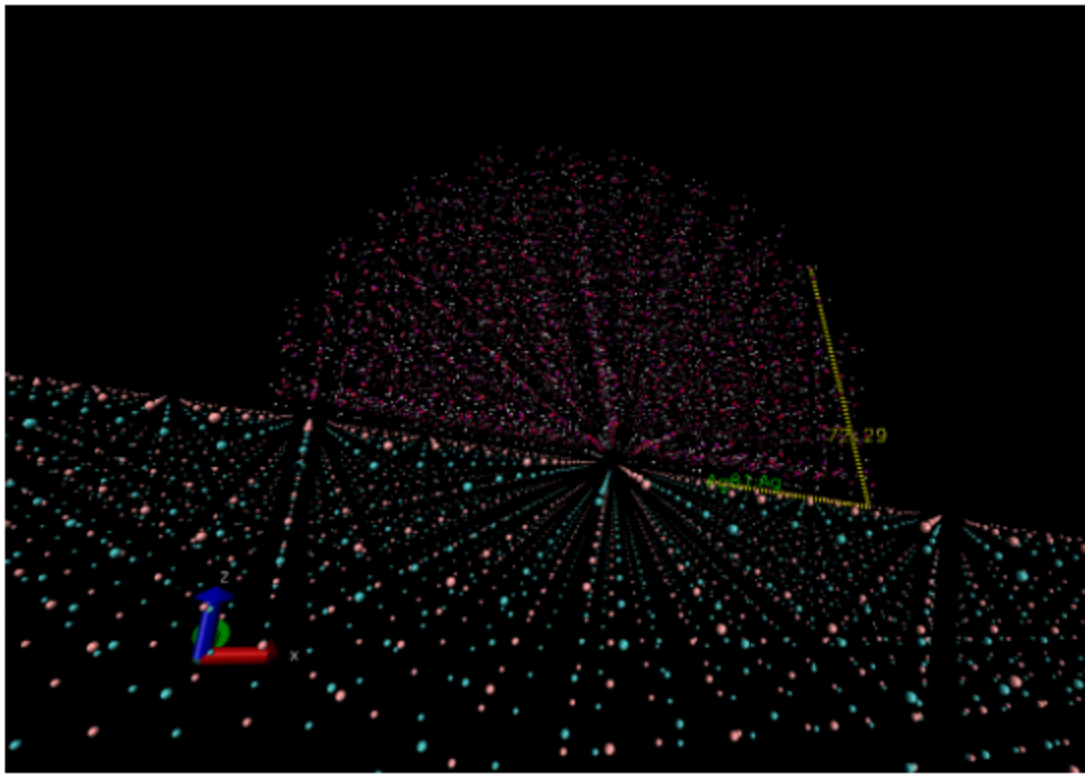
Method and Results

VMD was used to place the ice crystal on top of the AgI crystal:





Contact angle was also determined using VMD Angle-tool, about 72.29 degrees.



Heterogeneous nucleation rate formula:

$$\mathcal{J} = \mathcal{J}_0 \exp(-\frac{\Delta G_{het}}{k_B T}) = \mathcal{J}_0 \exp(-\frac{\Delta G^*_N f(\theta)}{k_B T})$$

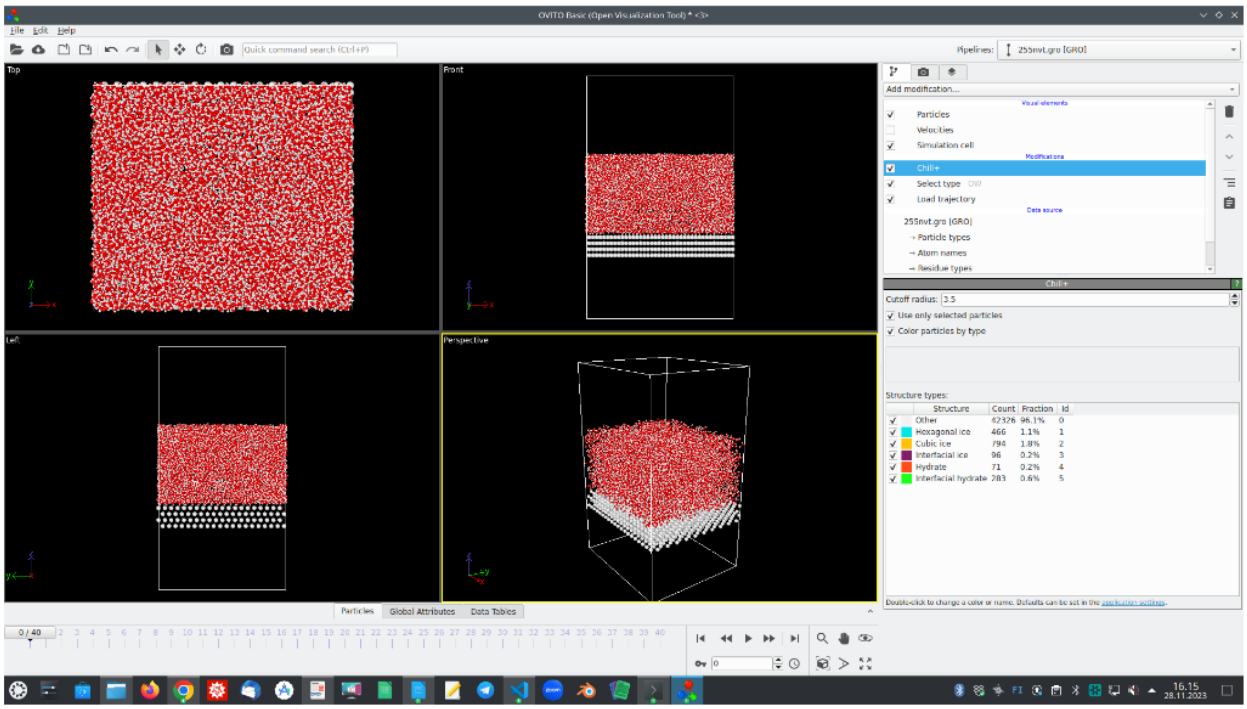
$$\Delta G^*_{\mathcal{N}} = \frac{16\pi}{3} \frac{{\gamma_S}^3}{{\Delta\mu_{\mathcal{V}}}^2}$$

γ_S: surface free energy

$\Delta\mu_V$: chemical potential energy, per volume per molecule of ice (single ice molecule's volume)

So we need to know surface free energy (aka. surface tension) and the temperature at which the critical radius occur.

To determine the temperature at which the hemisphere is of the size of its critical radius, I runned multiple NVT-ensemble runs on Puhti computing system, with differing temperature. Then I used CHILL+-algorithm in Ovito to determine whether the ice crystal hemisphere is growing, shrinking or just stabilizing.



T=255K, a sample procedure of applying CHILL+-algorithm to determine the critical radius of the ice crystal hemisphere. By comparing different time frames, and noticing whether the portion of hexagonal ice is changing, we can know whether the critical radius occurred at this temperature.

Surface tension can be computed knowing the contact angle, determined previously.

Using provided script, I got the nucleation rate of

$$J = 2.74579 \cdot 10^{-14} \frac{1}{s \cdot m^3},$$

where we omitted the constant factor in the nucleation rate, and assumed it does not affect the magnitude of the result value significantly. Comparing to the literature nucleation rate for homogeneous ice nucleation rate of

$$J = 10^{-83} s^{-1} m^{-3}$$

, which is smaller than our value. The result is reasonable, since heterogeneous nucleation (our case) should be easier than homogeneous nucleation, and thus in theory too, AgI can be used effectively for cloud seeding.