report.pdf

Filesystem

- Exercise2_executed_*: separate executions using different set of random seeds to initiate configurations
  - analysis/: contains analyses
    - cluster_analysis/: for problem 2 and 3
    - analysis.ipynb: here I made all the analyses for the final report
  - ***nm/:** for each box sizes
    - run.sh: execute this folder and run the MD
    - ar8192.inp: input file for packmol
      - using python random number generator to generate unique seeds for each box size.
  - set_differing_box_sizes.ipynb:
    - for preparing files related to different box sizes.
  - execute_run.sh: execute run.sh in each ***nm/**
  - execute_packmol_locally.sh:
    - execute packmol and generate starting configurations for each box sizes
    - **should be executed locally**, since Puhti does not have some modules for executing Packmol.

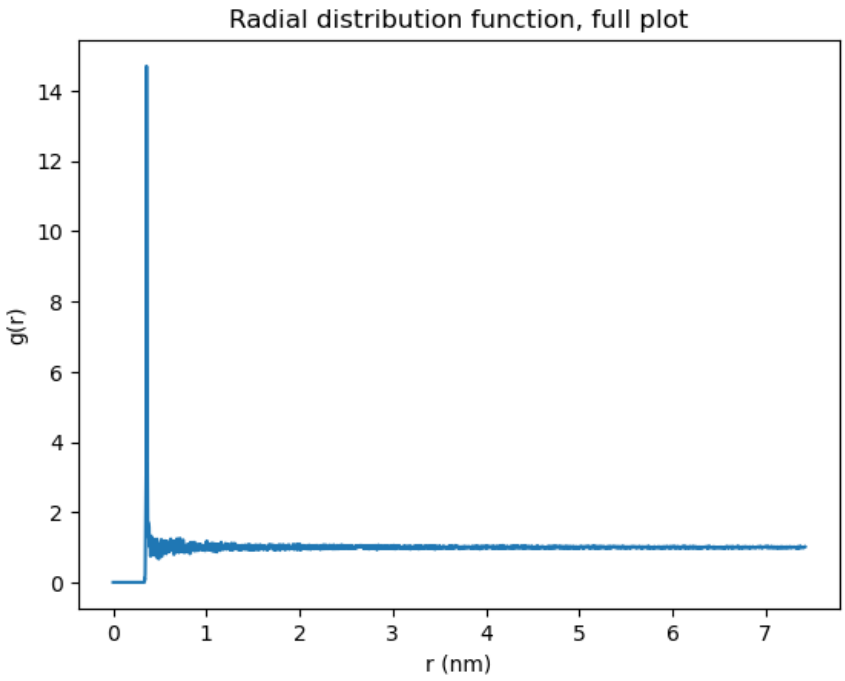
- **Note:** the following folders/files were deleted in the submission folder, due to too large resulting zip-folder sizes, causing unreturnable Moodle submission (50MB limit)
  - Exercise2_executed_1
  - .xtc files
  - Full zip-folder can be found in the following Github link: https://github.com/Absolute7070/exercise_returns

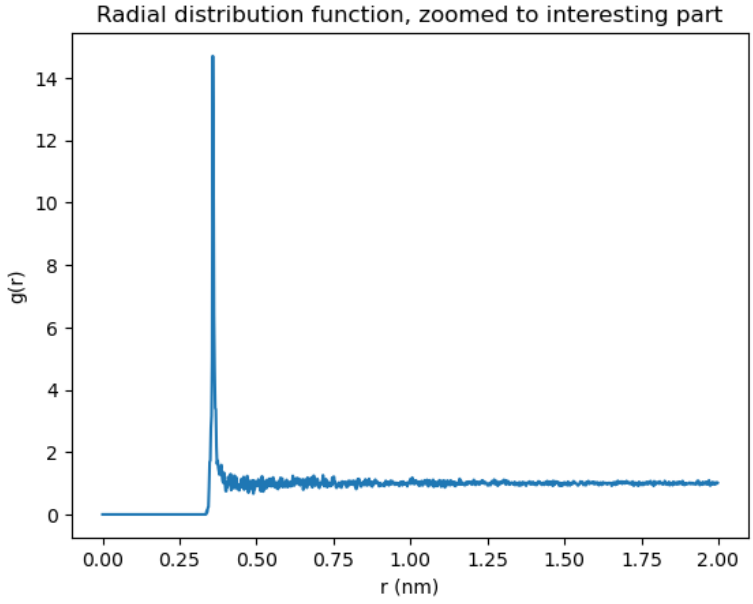
problem 1

- steep.mdp:
  - used `emtol=100`

We calculated radial distribution function using `gmx rdf` and plotted as shown below.

- Radial distribution function plot:



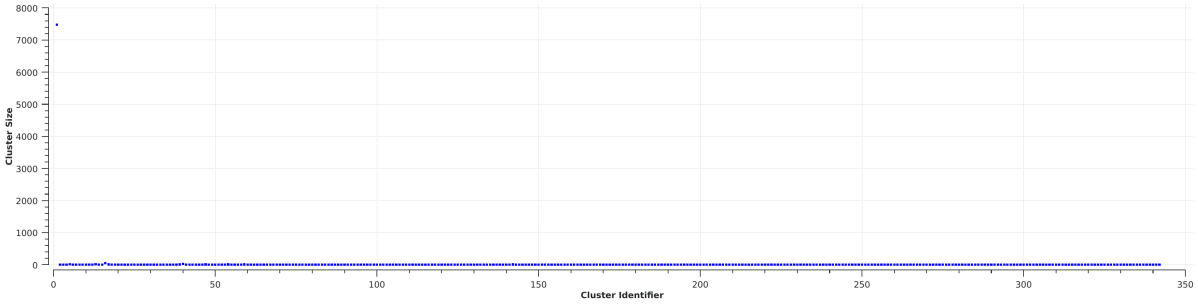


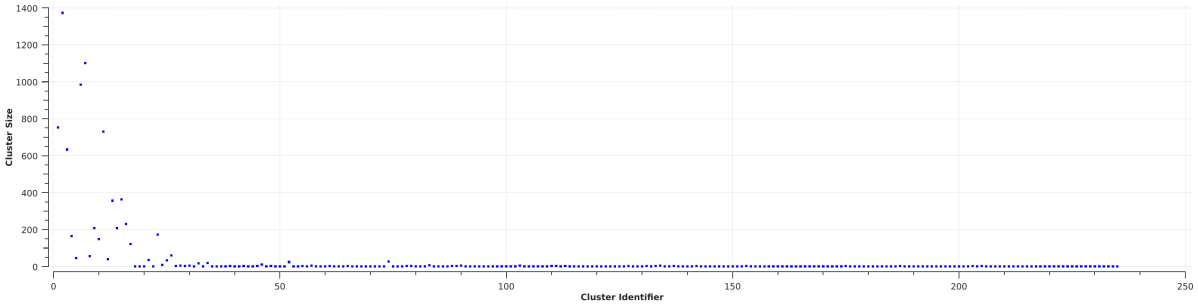
problem 2

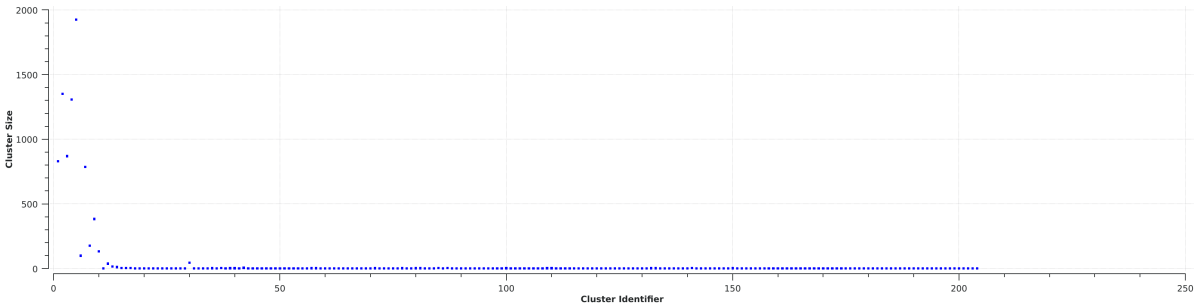
- NVT.mdp:
  - **Cut-off** from the paper: $r_{VdW}, r_{Coulomb} = 6.78\sigma_{LJ} = 2.30859nm$, where $\sigma_{LJ} = 0.3405nm$

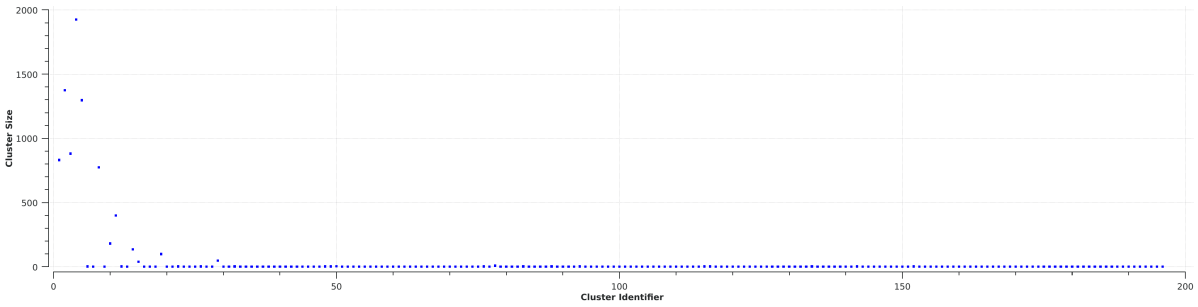
- Cluster analysis plots from Ovito:

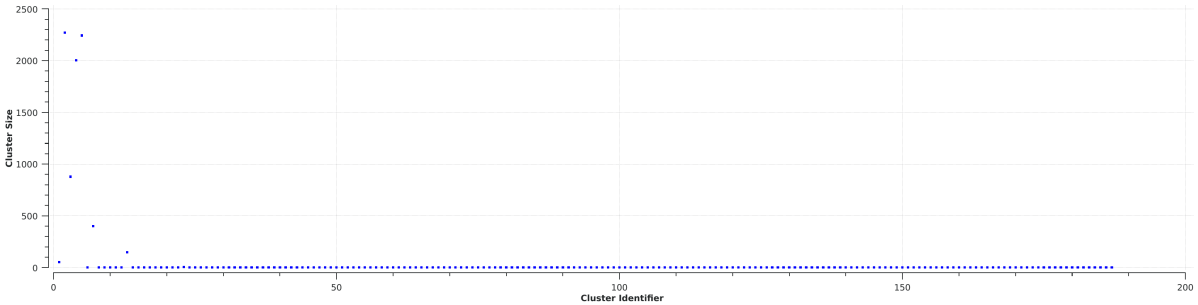
  Frames: 0–2500, every 500 frame

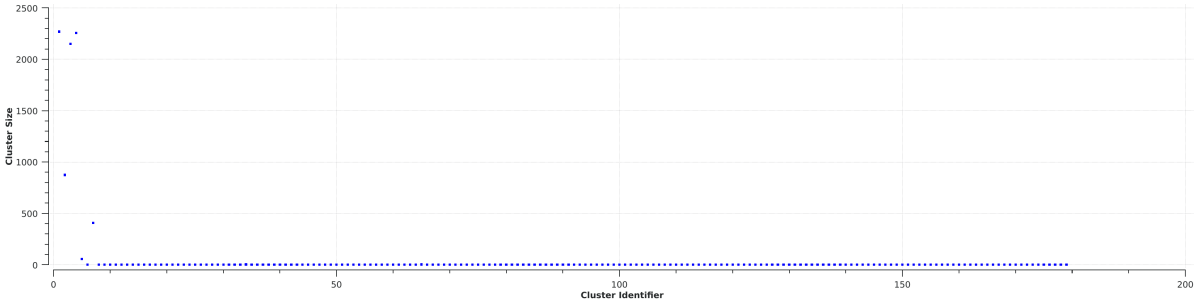










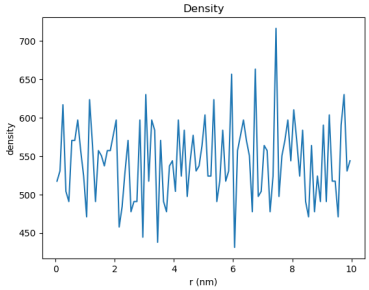


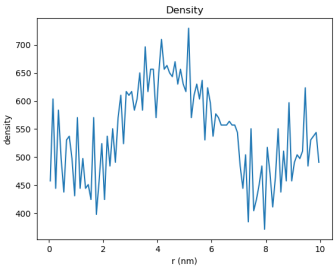
We see that N~900 is stable, not growing and not shrinking. It is also our critical nucleus. Bigger than N~1300 tends to grow, and smaler than N~800 tends to shrink.

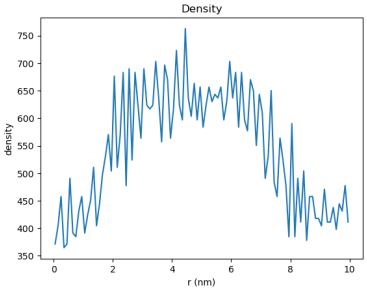
Critical nucleus has the minimum particle size from which an aggregate is thermodynamically stable. So in our case the number of atoms in the critical nucleus is N~900.

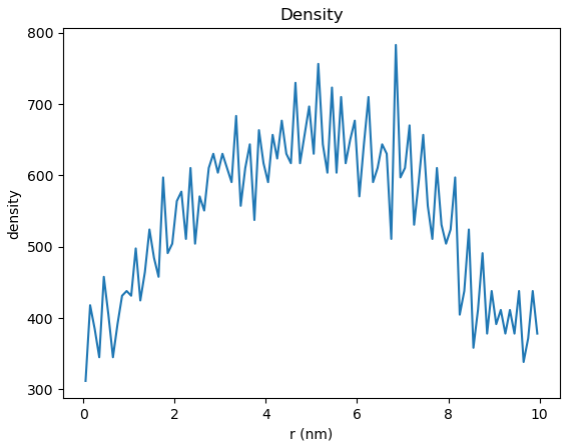
Problem 3

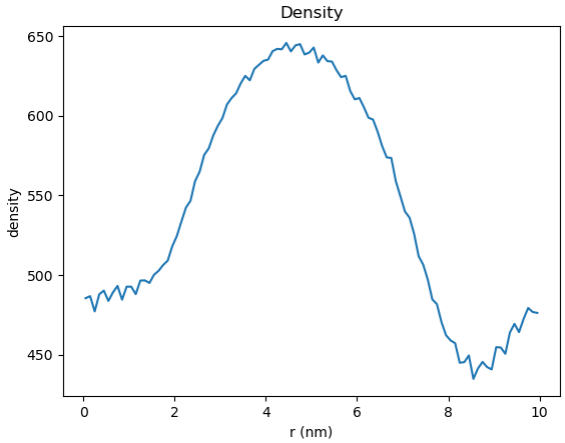
Local density fluctuates sinusoidally, when ignoring smaller background fluctuations. Below see plots for time evolution of density (frame 3, 100, 300, 400, 500, subfinal, in respective order)







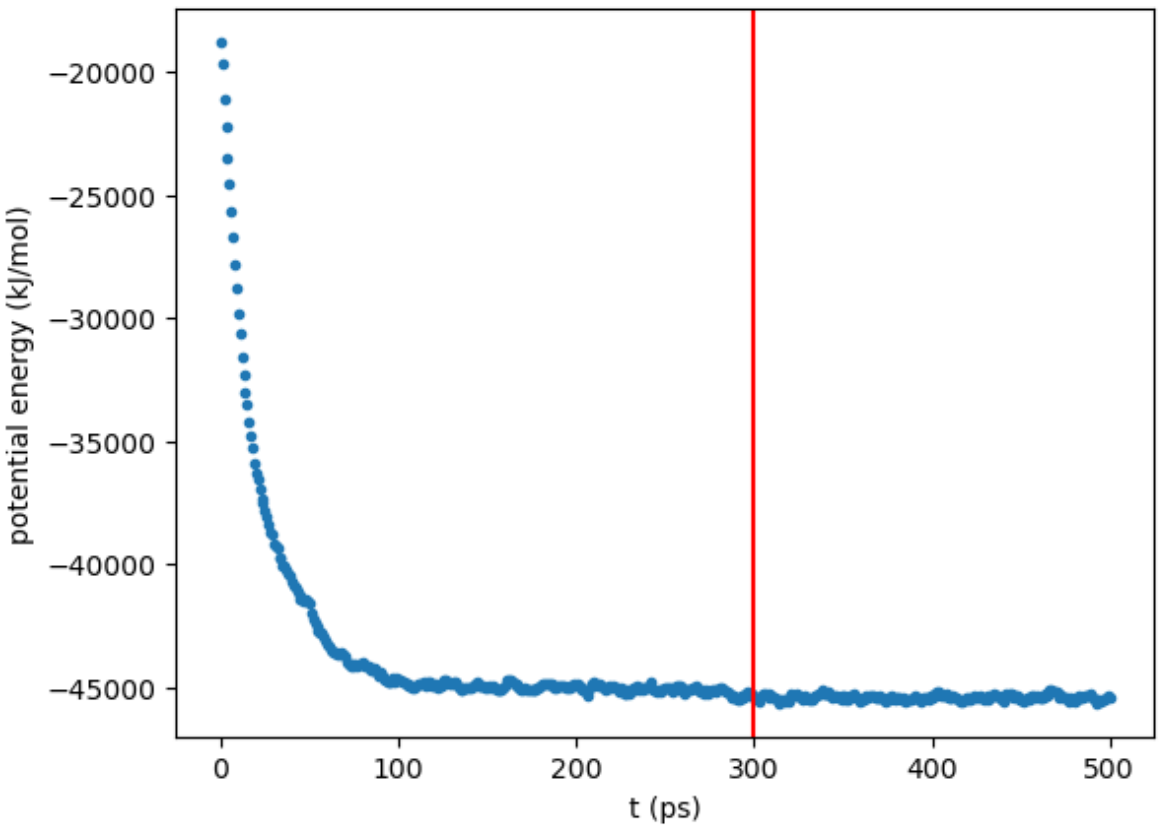




We then checked, using Ovito, that the slab of Argon is formed on xz-plane. We used surface tension formula:

$$\gamma = \frac{L_z}{2}(P_{yy} - \frac{P_{zz} + P_{xx}}{2})$$

We computed surface tension values after equilibrium, which happened arround t>300ps:



Surface tension values are then averaged and we got the following:

Last instantaneous surface tension value: 116.5872325 (nm bar)
Mean surface tension during equilibrium: 116.83625415422885 (nm bar)

Problem 4

We created differing box lengths from 10nm to 15nm with 0.5nm intervals, using NVT-ensemble.

- Running the script, the following line of each box sizes will not be executed, because we need to choose the atom group whose density we are trying to calculate. Need to execute afterward.

```
x=10.5
```

```
gmx density -f ${x}nm_8192.gro -s ${x}nm_8192.tpr -d Y -sl 100 -o density_afterNVT.xvg
```

We executed two times with different sets of random number seeds for packmol input files (and thus subsequent configuration files), and we got the following results, based on eye-balling the Ovito visualization:

1. Execution:
    - 13.0nm (spinodal) – 14.0 nm (nucleation)
2. Execution:
    - 12.5 nm (spinodal) – 13.0nm (nucleation)

We conclude, based on these executiong the box length limit is somewhere between 12.5nm < x < 14nm, i.e. the supersaturation density at which the crossover happens is somewhere between:

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

The precision can be achieved higher if we have more time for:

1. conducting separate executions with different set of random seeds
2. for each execution, the box length interval could be decreased from 0.5nm we used.