report.pdf

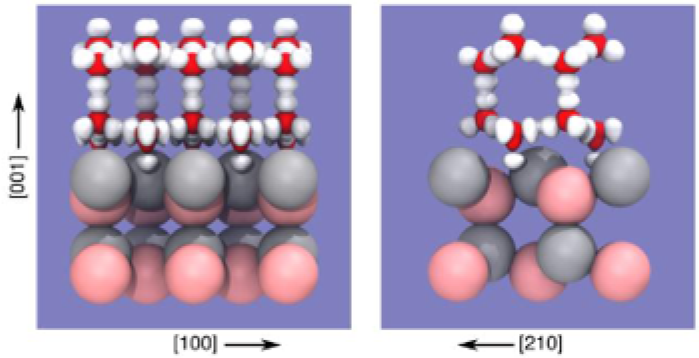
Files

- exercise3/: I have done the part of the first exercise using this
- updated_ex3_main/: later assistant/lecturer updated folder. The remaining part of the exercises done with this
  - `create_files.ipynb`: responsible for creating input files (.mdp) with different temperatures, .sh files for running the scripts.
  - `calculate_nucleation_rate.ipynb`: calculating nuclearion rate (problem 4)
- updated_ex3_executed*/: after preparing all .mdp files and .sh files in the previous step, we move the `updated_ex3_main/` to Puhti for execution. After each execution, we renamed it.
  - each execution differs by temperature ranges.

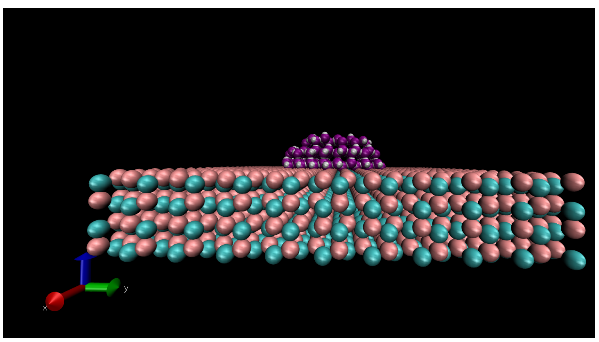
I removed all the .xtc files, otherwise it would result in very large .zip folder. Full files available via this link: https://github.com/Absolute7070/exercise_returns

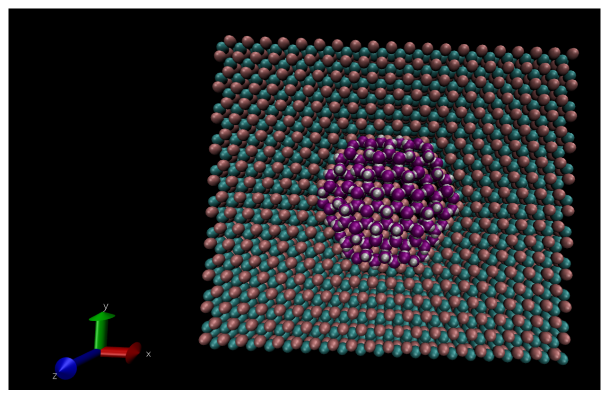
Problem 1

The hemisphere is approximately placed onto the surface according to lecture note, which supposedly is approximately negatively charged part of the hemisphere on top of positively charged part of the surface, and positively charged part on top of negatively charged part.

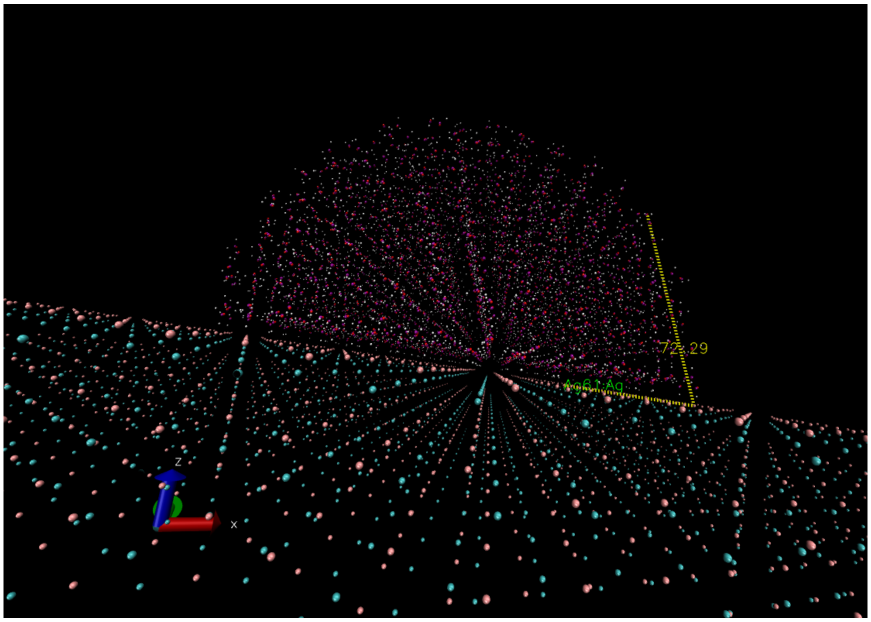


Snapshots:





- Contact angles using `updated_ex3`: 72.29 degrees = 1.2616985 rad



Problem 2

We used pre-made solvated configuration file and minimized the system with following:

```
gmx grompp -f minim.mdp -c 3nm_em.gro -p topol.top -n index.ndx -o minimized.tpr
gmx mdrun -v -deffnm minimized
```

problem 3

We used Chill+ algorithm of Ovito to identify the ice crystal. Using Chill+, we selected only oxygen atoms and cutoff distance of 3.5Å [https://www.ovito.org/manual_testing/reference/pipelines/modifiers/chill_plus.html] partially according to the advice by Golnaz (FMI) Roudsari.

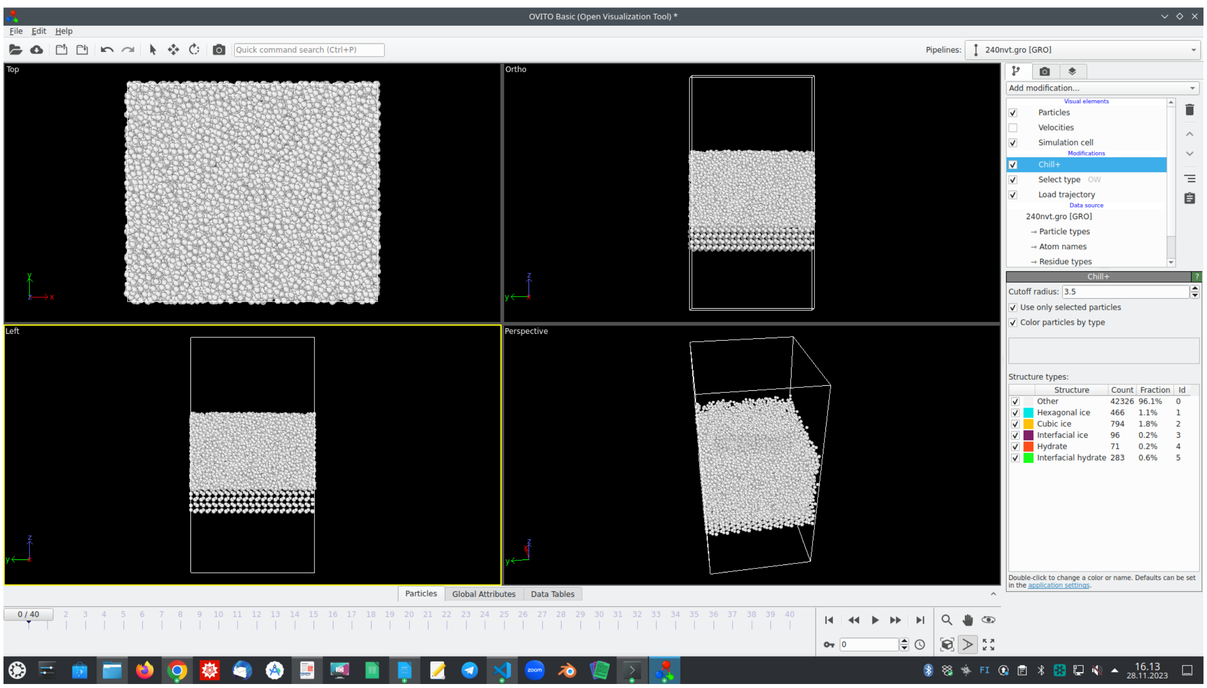
- Execution on Puhti:

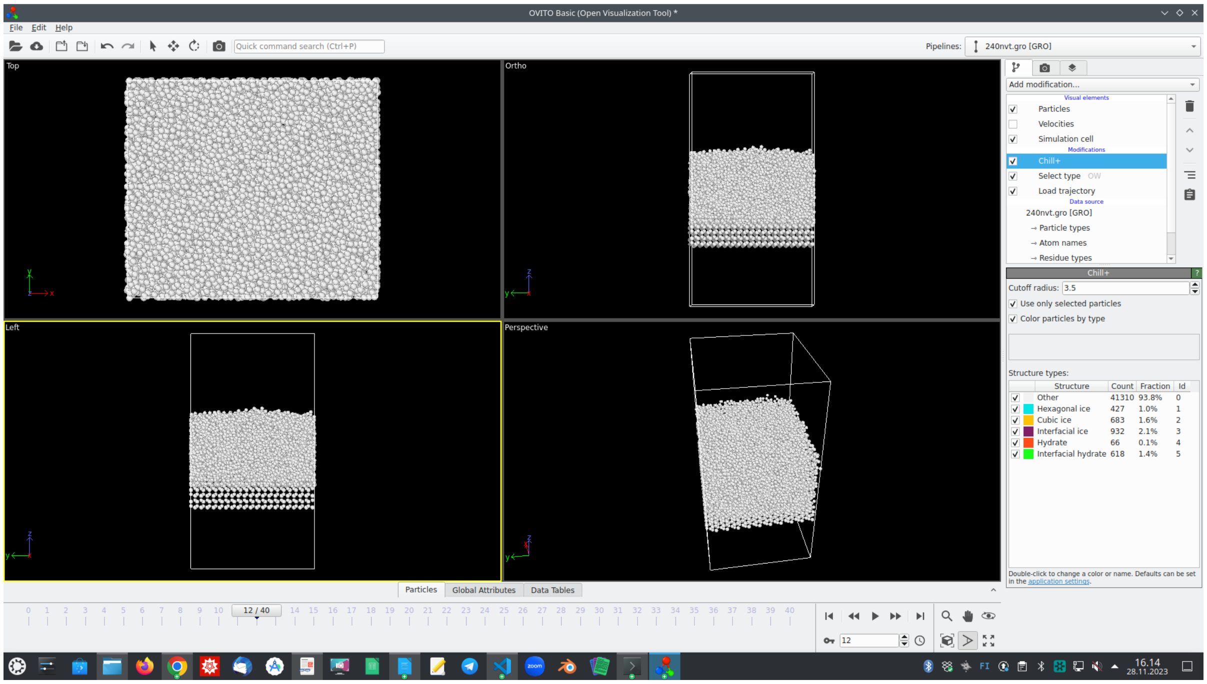
```
chmod -R u+rwx updated_ex3
```

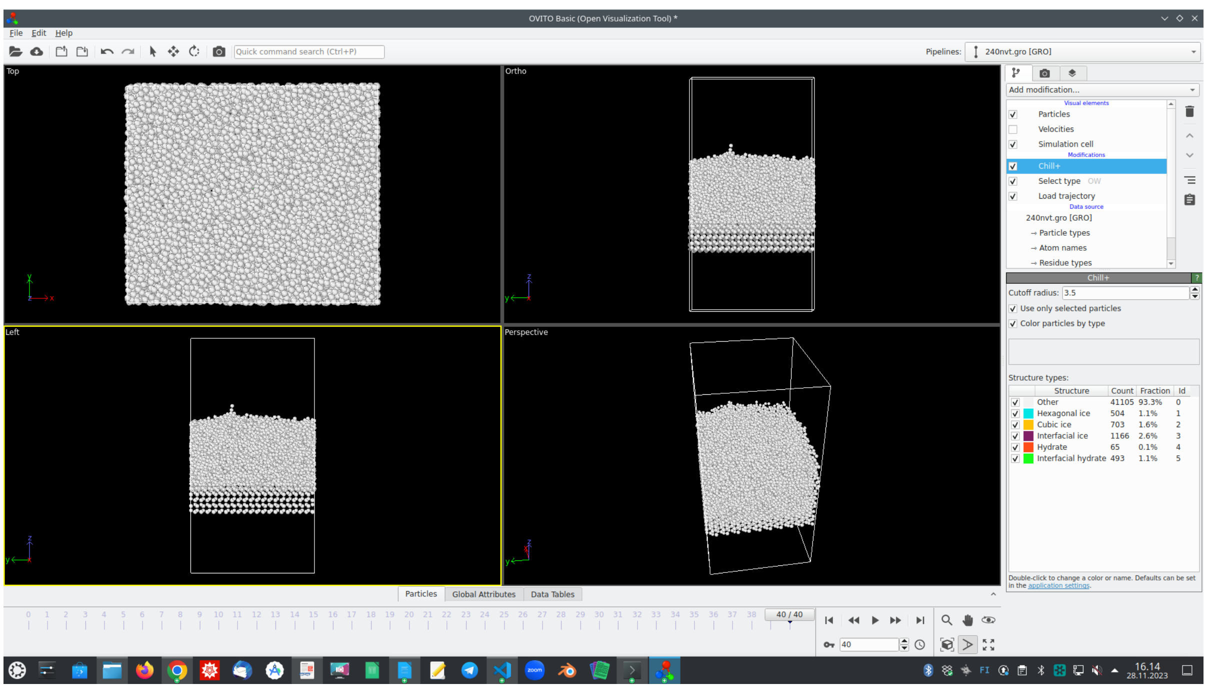
```
find ./ -name "run_*" -exec sbatch {} \;
```

We report 1. frame, a middle frame and the last frame:

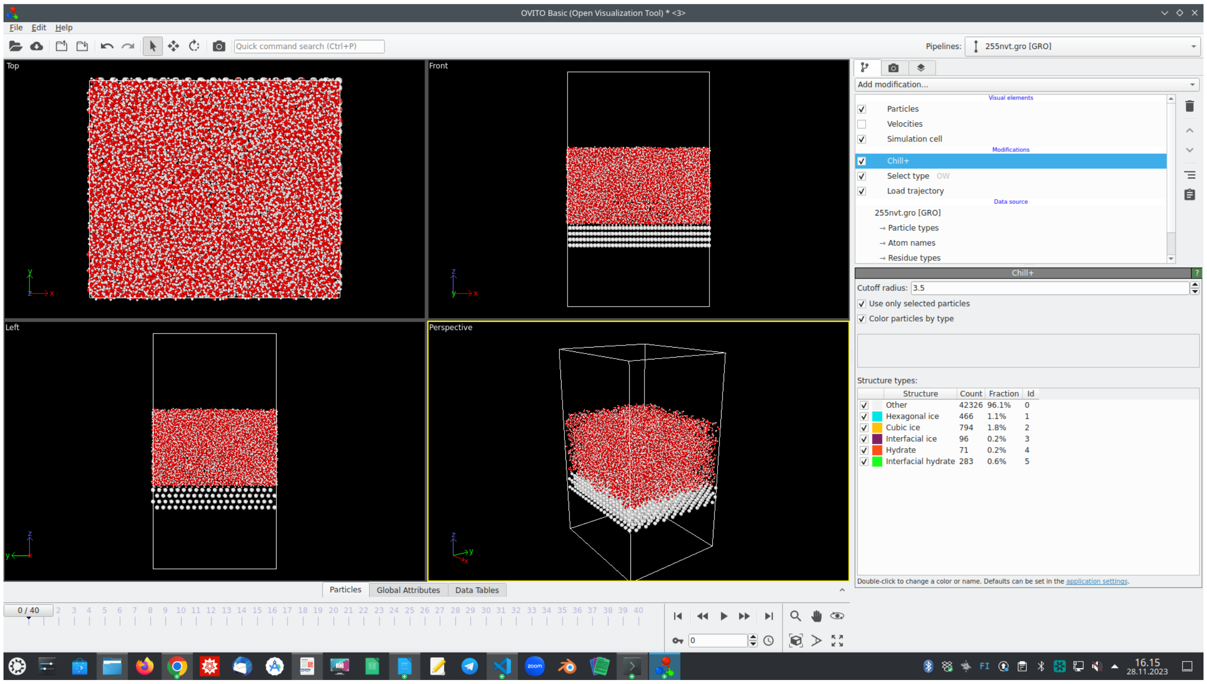
T=240:

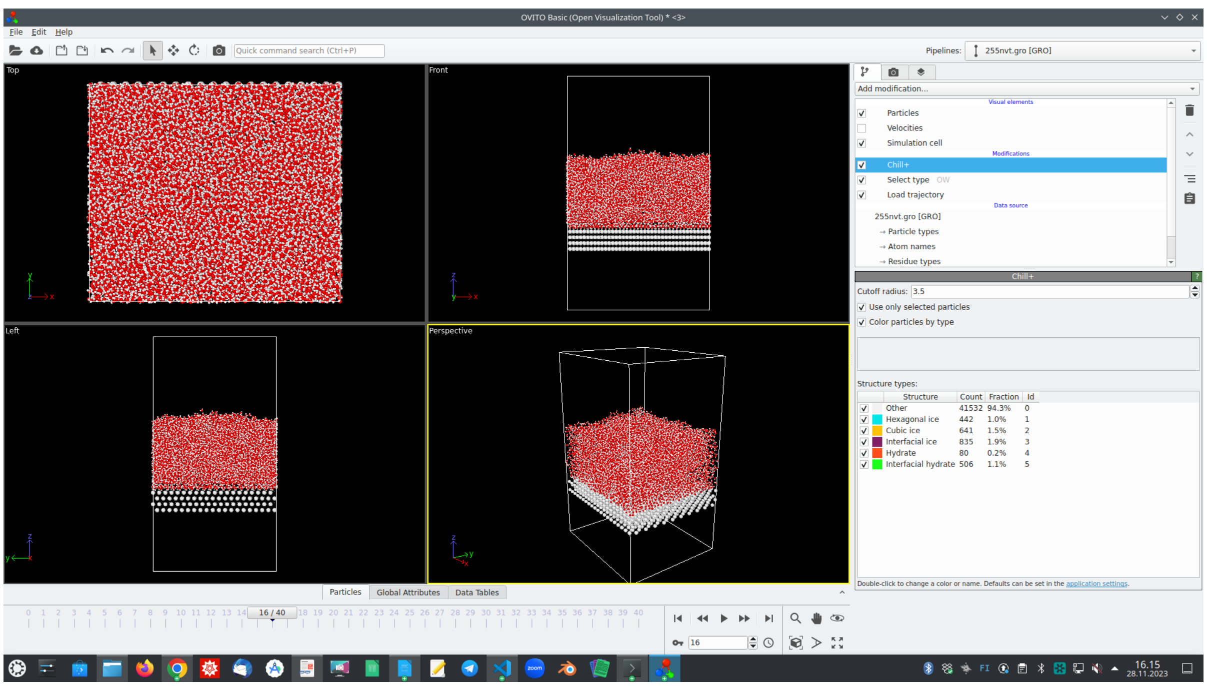


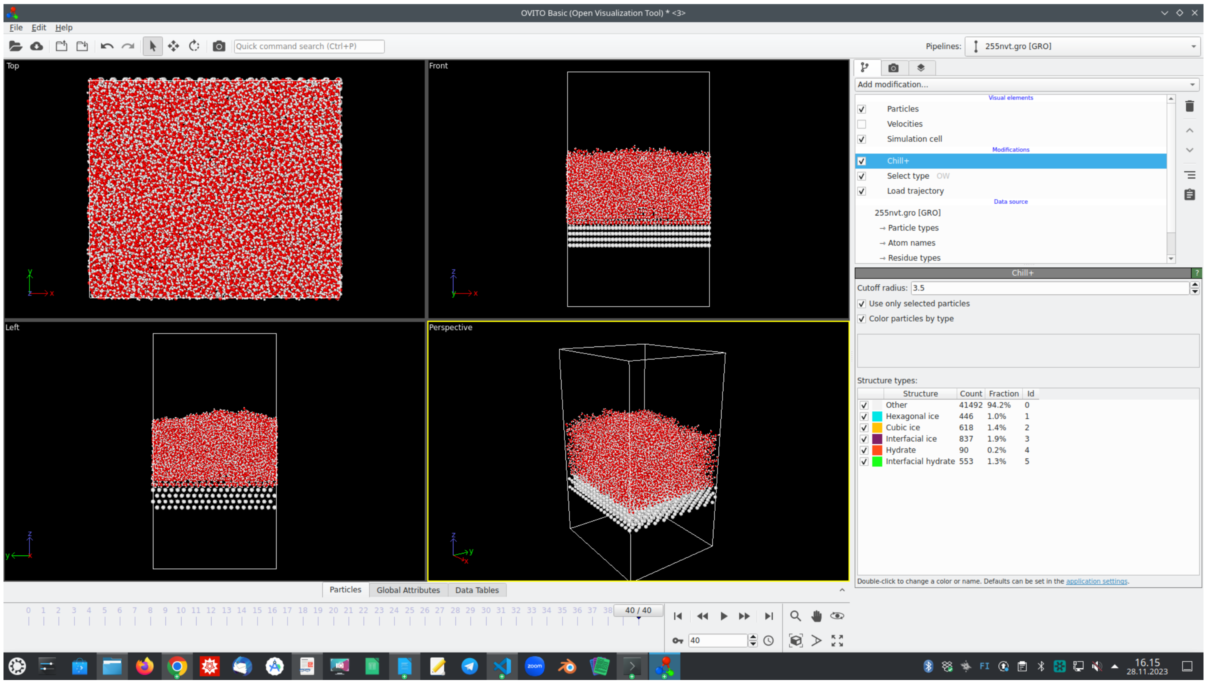

OVITO Basic (Open Visualization Tool) *
Pipelines: 240nvt.gro [GRO]
Top
Ortho
Left
Perspective
Particles
Velocities
Simulation cell
Chill+
Select type
Load trajectory
240nvt.gro [GRO]
Cutoff radius: 3.5
Use only selected particles
Color particles by type
Structure types:
Structure Count Fraction Id
Other 41310 93.8% 0
Hexagonal ice 427 1.0% 1
Cubic ice 683 1.6% 2
Interfacial ice 932 2.1% 3
Hydrate 66 0.1% 4
Interfacial hydrate 618 1.4% 5
12 / 40


OVITO Basic (Open Visualization Tool) *
Pipelines: 240nvt.gro [GRO]
Top
Ortho
Left
Perspective
Particles
Velocities
Simulation cell
Chill+
Select type
Load trajectory
240nvt.gro [GRO]
Cutoff radius: 3.5
Use only selected particles
Color particles by type
Structure types:
Structure Count Fraction Id
Other 41105 93.3% 0
Hexagonal ice 504 1.1% 1
Cubic ice 703 1.6% 2
Interfacial ice 1166 2.6% 3
Hydrate 65 0.1% 4
Interfacial hydrate 493 1.1% 5
40 / 40

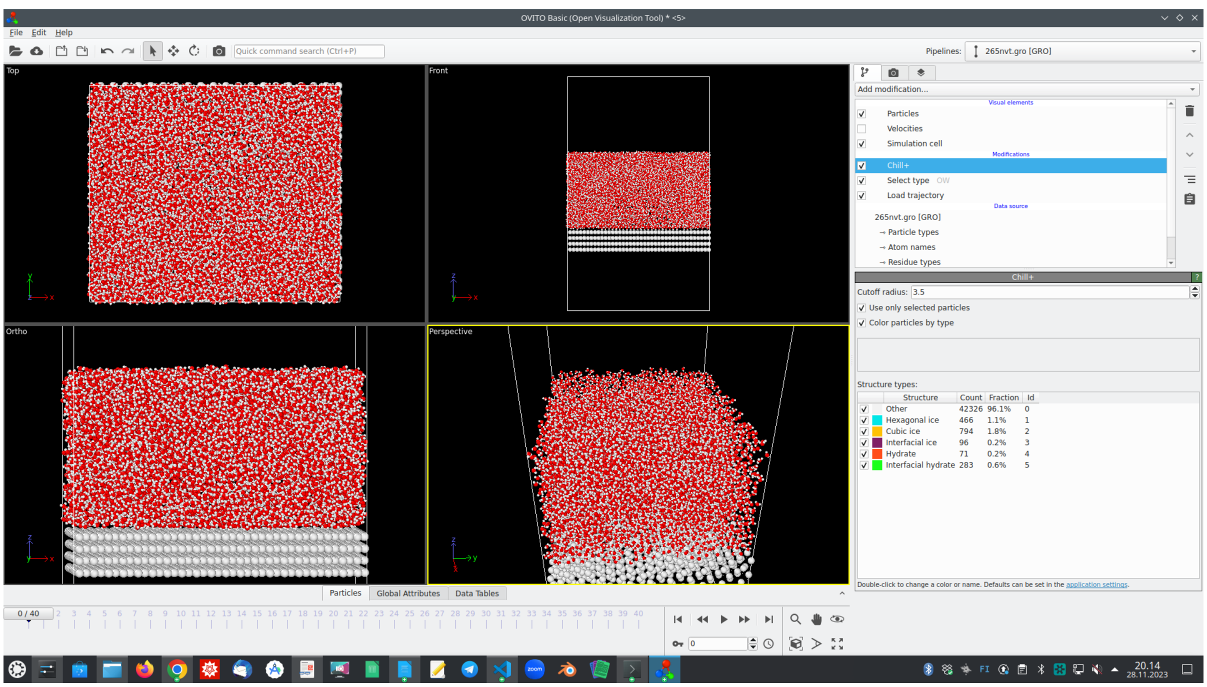
T=255:

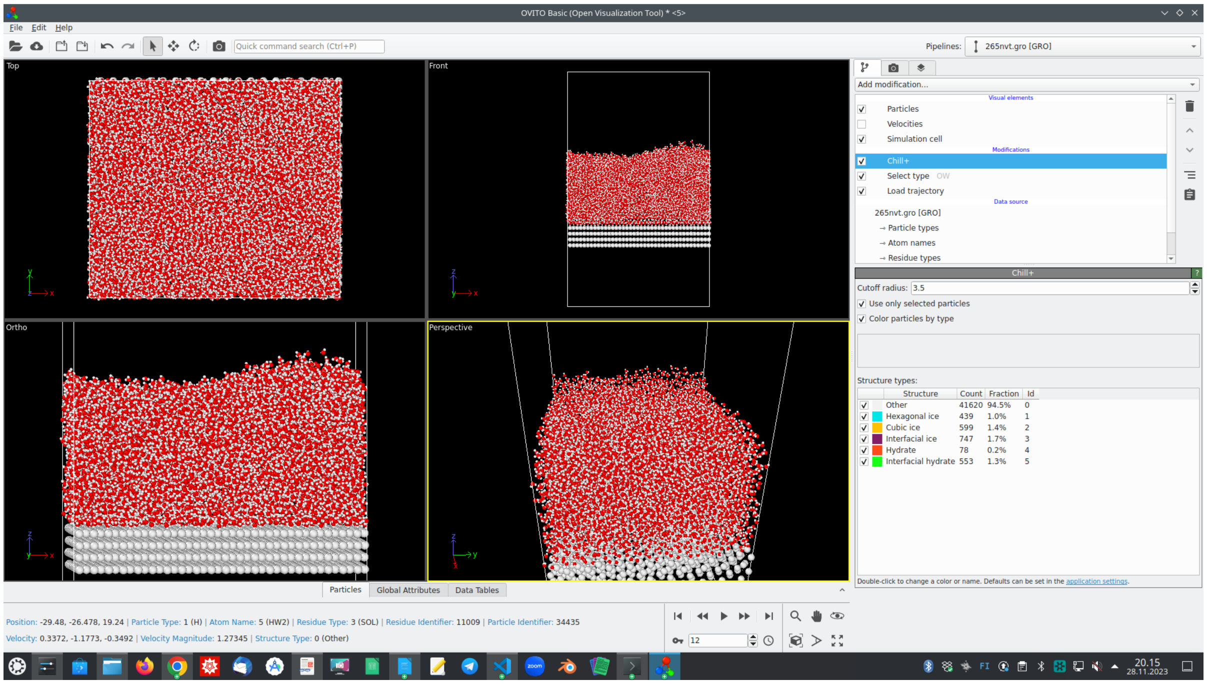

OVITO Basic (Open Visualization Tool) * <3>
File Edit Help
Quick command search (Ctrl+P)
Pipelines: 255nvt.gro [GRO]
Top
Front
Left
Perspective
Add modification...
Visual elements
Particles
Velocities
Simulation cell
Modifications
Chill+
Select type OW
Load trajectory
Data source
255nvt.gro [GRO]
→ Particle types
→ Atom names
→ Residue types
Chill+
Cutoff radius: 3.5
Use only selected particles
Color particles by type
Structure types:
Structure Count Fraction Id
Other 42326 96.1% 0
Hexagonal ice 466 1.1% 1
Cubic ice 794 1.8% 2
Interfacial ice 96 0.2% 3
Hydrate 71 0.2% 4
Interfacial hydrate 283 0.6% 5
Double-click to change a color or name. Defaults can be set in the application settings.
Particles
Global Attributes
Data Tables
0 / 40
16.15
28.11.2023

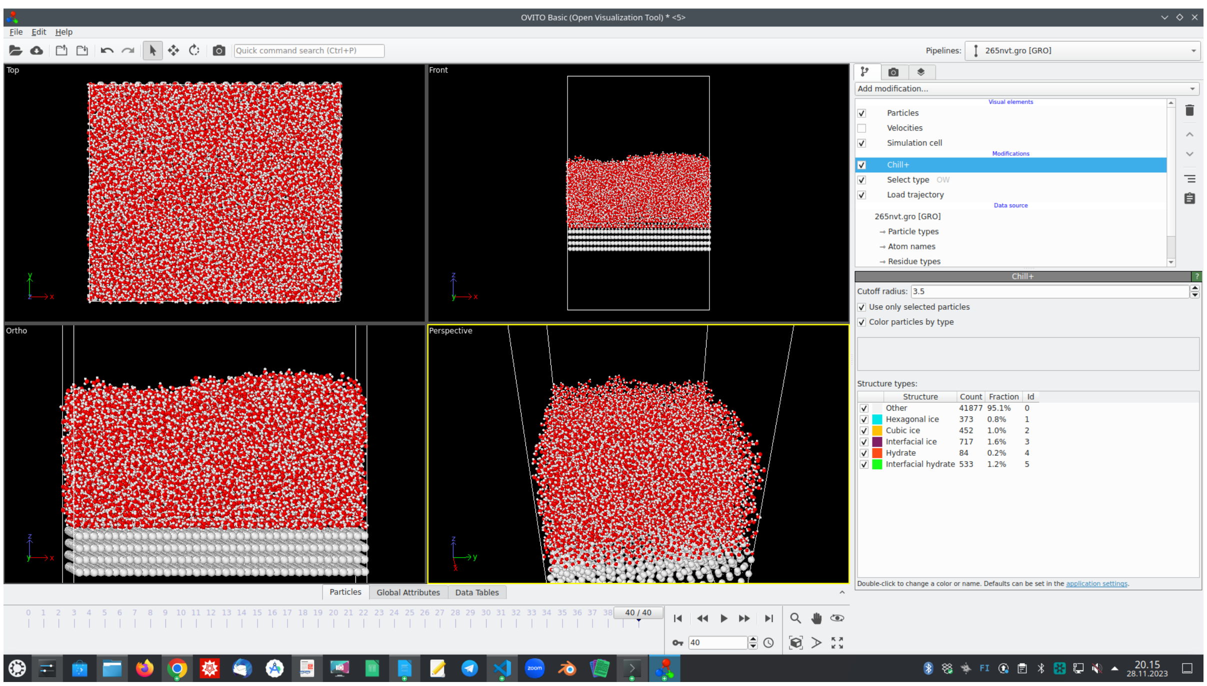

OVITO Basic (Open Visualization Tool) * <3>
File Edit Help
Quick command search (Ctrl+P)
Pipelines: 255nvt.gro [GRO]
Top
Front
Left
Perspective
Add modification...
Visual elements
Particles
Velocities
Simulation cell
Modifications
Chill+
Select type OW
Load trajectory
Data source
255nvt.gro [GRO]
→ Particle types
→ Atom names
→ Residue types
Chill+
Cutoff radius: 3.5
Use only selected particles
Color particles by type
Structure types:
Structure Count Fraction Id
Other 41532 94.3% 0
Hexagonal ice 442 1.0% 1
Cubic ice 641 1.5% 2
Interfacial ice 835 1.9% 3
Hydrate 80 0.2% 4
Interfacial hydrate 506 1.1% 5
Double-click to change a color or name. Defaults can be set in the application settings.
Particles
Global Attributes
Data Tables
16 / 40
16.15
28.11.2023



T=265







Now T=240 is a very good approximation of critical nucleus temperature. (We investigated other lower temperatures too)

We use the following values as inputs for calculating nucleation rate:

```
T = 240
theta = 1.2616985 #  72.29
```

Then nucleation rate (ignoring the constant factor) is 2.74579e-14. Comparing this to literature value for homogeneous ice nucleation rate of $J = 10^{-83} s^{-1} m^{-3}$ [https://arxiv.org/abs/1312.0822] with constant factor, we have much smaller nucleation rate, assuming our constant factor, if included, does not affect too much of the magnitude of our result. This is reasonable, since heterogeneous nucleation should be easier than homogeneous nucleation.