Indian Institute of Technology Bombay

MM 722, Autumn 2024-25

End-term Project Report

Solid-Liquid Phase Transition for a Nano-Confined Fluid

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MEMS

Acknowledgements

We would like to thank Prof. Ajay S. Panwar for guiding us throughout and making the subject matter interesting and rigorous. Moreover, we would also like to thank the TAs, Madhur Gupta and Debarna Bhattacharjee, for their continued support.

Harsh and Saransh

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1 Introduction

For our end-term project for MM 722, we aimed to replicate the results of an interesting paper that investigated the phase transition of confined fluid in slit by Lennard-Jones potential for fluids-fluids and walls-fluids interaction. [1]. While we were not able to replicate the exact results exhibited by the paper, we were able to qualitatively replicate the solid-liquid phase transition of confined Argon under the same settings. The effects of temperature, pressure, and distance between the two walls on the phase transition were investigated by using the molecular dynamics simulation and LAMMPS software. It was found that wall distances had a significant effect on phase transition. Although the molecules were spherical and the walls structureless, liquid-liquid phase transition was observed when wall distances were approximately

2 Methodology

2.1 Simulation Setup

- Box dimensions: x = 100σ, y = 100σ, z = 3σ
- Number of atoms: 12000
- Temperature Range: $0.6 - 1.8K$
- Pressure values (reduced units): $0.5, 0.8, 1.0$
- Pressure control in xy direction: Berendsen barostat
- Temperature control: Nose-Hover thermostat
- Timestep: 0.004
- Total steps: 50000

2.2 Code

The following LAMMPS script was used to conduct the experiment and collect the relevant data:

```
# Phase Transition Simulation of Argon Fluid with Wall Interactions
in LJ Units

units   lj
dimension  3
boundary  p p f
atom_style  atomic
```

```
# Create the simulation box and atoms
lattice  fcc 0.8442
region   box block 0 100 0 100 0 3.0
create_box  1 box

region  inner block 0 100 0 100 0.5 2.5
create_atoms  1 random 12000 13432 inner


mass  1 1.0

group  act region inner


# Set additional pair coefficients for wall-wall interactions (type 2 and type 2)
pair_style  lj/cut 3.0
pair_coeff  1 1 1.0 1.0 3.0

fix   wallhi all wall/lj126 zhi 3.0  1.0 1.0 3.0
fix   walllo all wall/lj126 zlo 0.0  1.0 1.0 3.0

# Apply Berendsen barostat for pressure control in x and y directions
fix    1 act press/berendsen x 1.0 1.0 5
fix        2 act press/berendsen y 1.0 1.0 5

# Apply Nose-Hoover thermostat for temperature control
fix        3 act nvt temp 0.6 0.6 0.5

timestep  0.004

# printing thermodynamics parameters
thermo  100
thermo_style    custom step temp ke press etotal density pzz enthalpy

compute         1 all rdf 100
fix             4 all ave/time 1 1 10000 c_1[*] file 4_1_1.8.rdf mode vector

# Dump atomic positions for visualization
dump   id all custom 100 dump.argon.lammpstrj id type x y z vx vy vz

minimize 1e-4 1e-6 100 1000
```

```
# Run the simulation
run   50000
```

3 Results and Discussion

3.1 DENSITY vs TEMPERATURE

- From Figure 1, we can infer that solid-liquid transition is occurring in the system. Moreover, as we increase the slit height, the phase transition varies as well, which results in a decrease in density.
- The transition appears to be gradual over a long temperature range. On the other hand, the authors of the original paper studied the transition happening over a relatively very short temperature range.

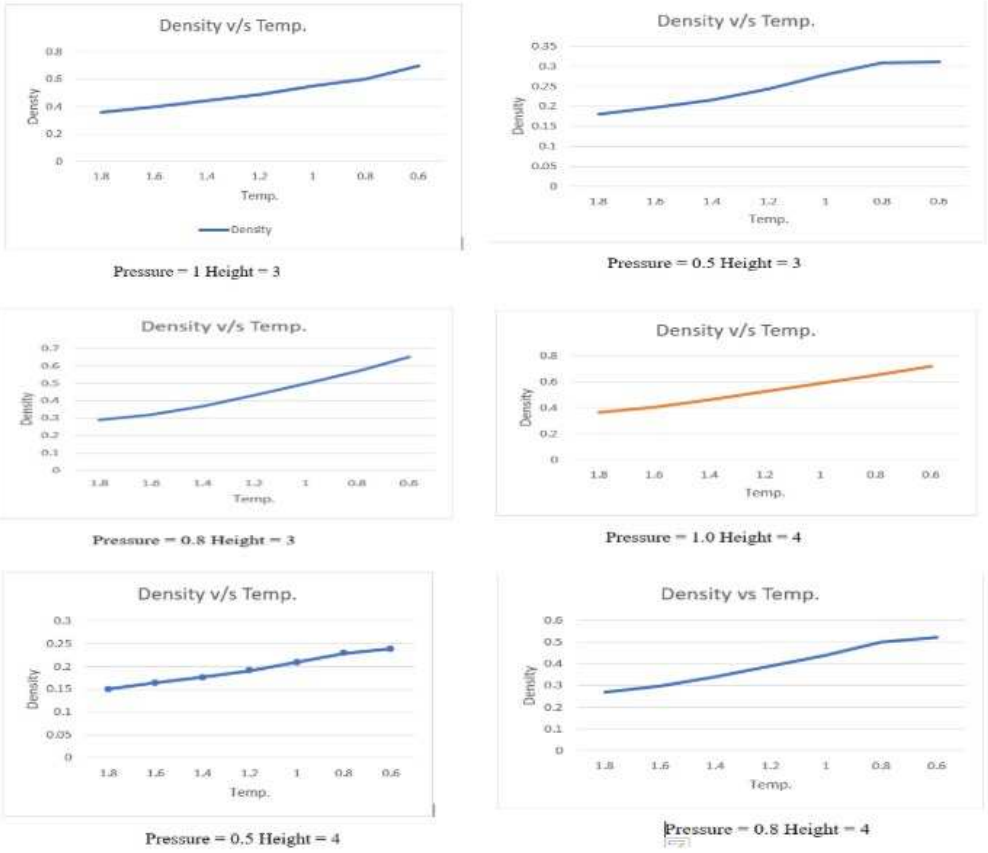
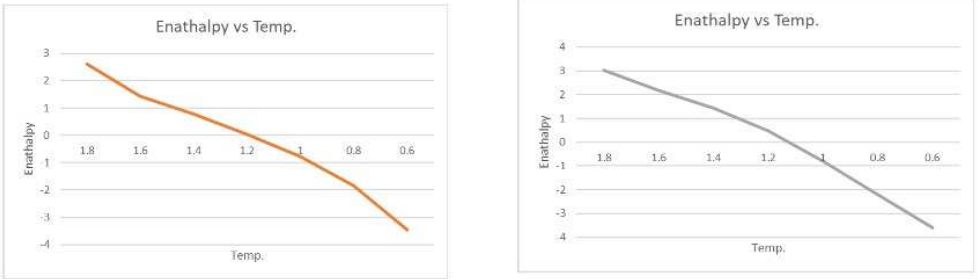


Figure 1: Density vs Temperature plots for different slit height and pressure configurations

3.2 ENTHALPY vs TEMPERATURE

As is evident from Figure 2, the variation of enthalpy with respect to temperature did not change as the slit height or the pressure changed.

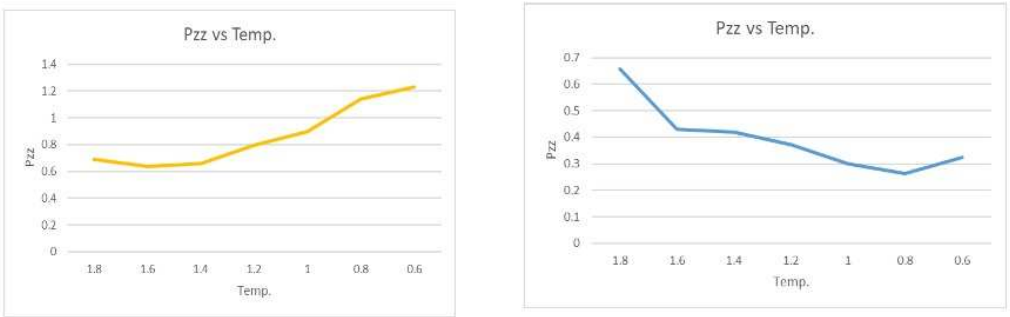


Height = 3, Pressure = 1 Height = 3,Pressure = 0.5

Figure 2: Variation of Enthalpy vs Temperature upon increasing the slit height

3.3 P_{zz} vs TEMPERATURE

Figure 3 tells us that as we increase the height of the slit, the pressure in the z-direction started to increase instead of decreasing. The original paper had this P_{zz} vs T decreasing relation preserved even after increasing the height. We were not able to understand why an inverted trend was emergent from our data.



Pressure = 0.8 Height=3 Pressure = 0.8 Height=4

Figure 3: Variation of P_{zz} with Temperature upon increasing the slit height

3.4 VISUALIZATION

We used VMD [2] to visualise the transition. As shown in Figure 4, the first image shows the confined Argon to be present in the liquid phase, while the next image shows it to be present in the solid phase.

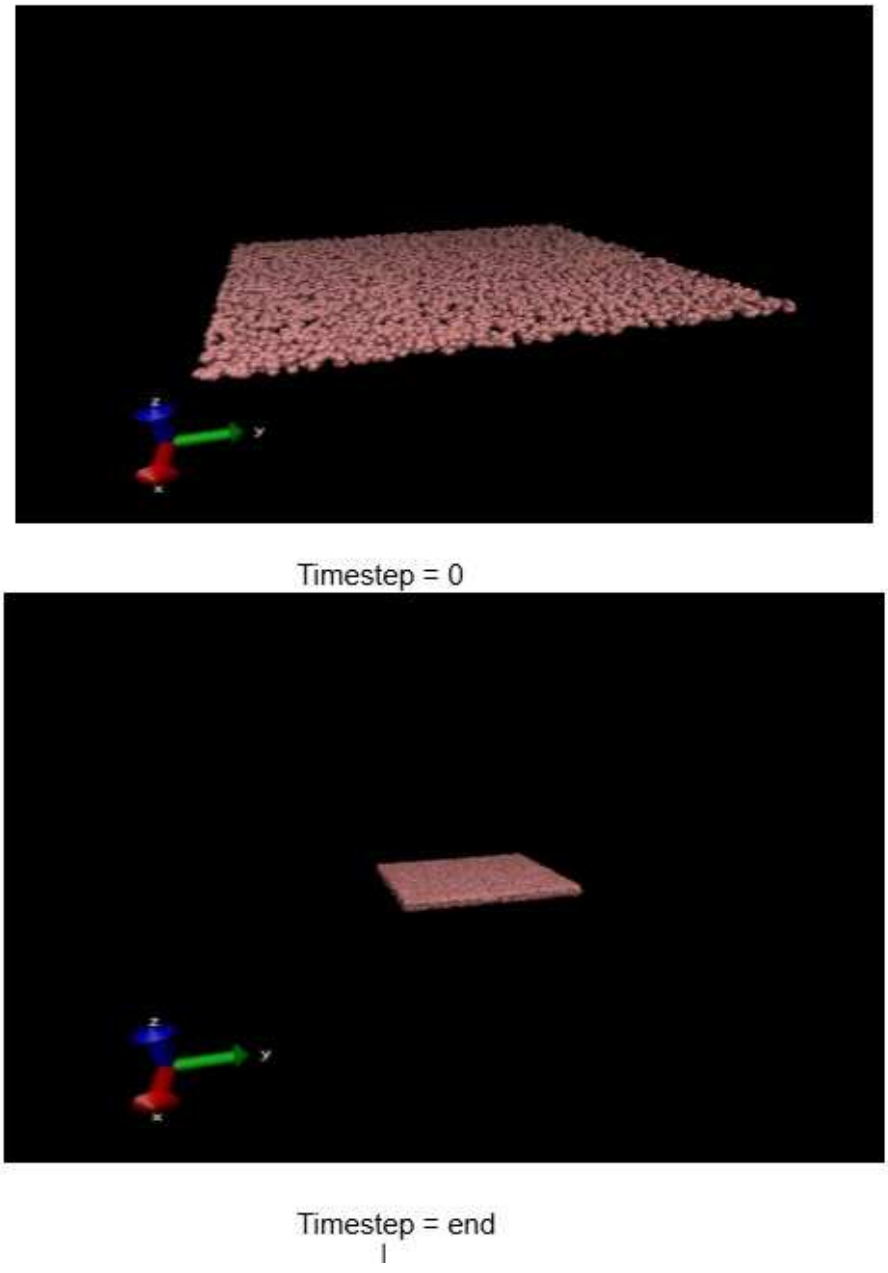


Figure 4: Visualizing the system at timestep = 0 and timestep = end

3.5 RADIAL DISTRIBUTION FUNCTION

From Figure 5, it is clear that phase transition is happening with temperature because the number of atoms near a particular atom is decreasing, which can be easily seen from the RDF plot. The phase transition is happening for both the height of slits.

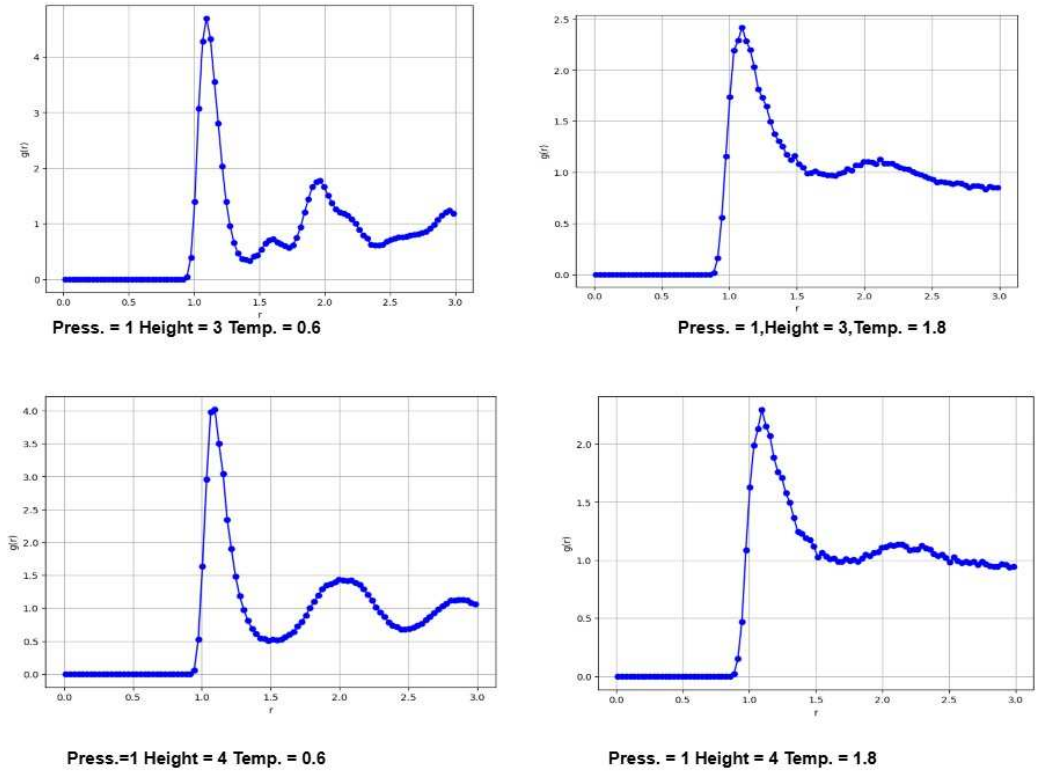


Figure 5: RDF comparisons for different slit height and temperature configurations

4 Conclusion

In this report for the end-term project in MM 722, we presented our findings in simulating the solid-liquid phase transition for a nano-confined fluid. While we were not able to replicate the original liquid-liquid phase transition, we were able to replicate most of the results as presented in the paper for a solid-liquid transition.

References

(1) Sheibani, N.; Kamalvand, M. *Fluid Phase Equilibria* **2020**, *510*, 112495.

(2) Humphrey, W.; Dalke, A.; Schulten, K. *Journal of Molecular Graphics* **1996**, *14*, 33–38.