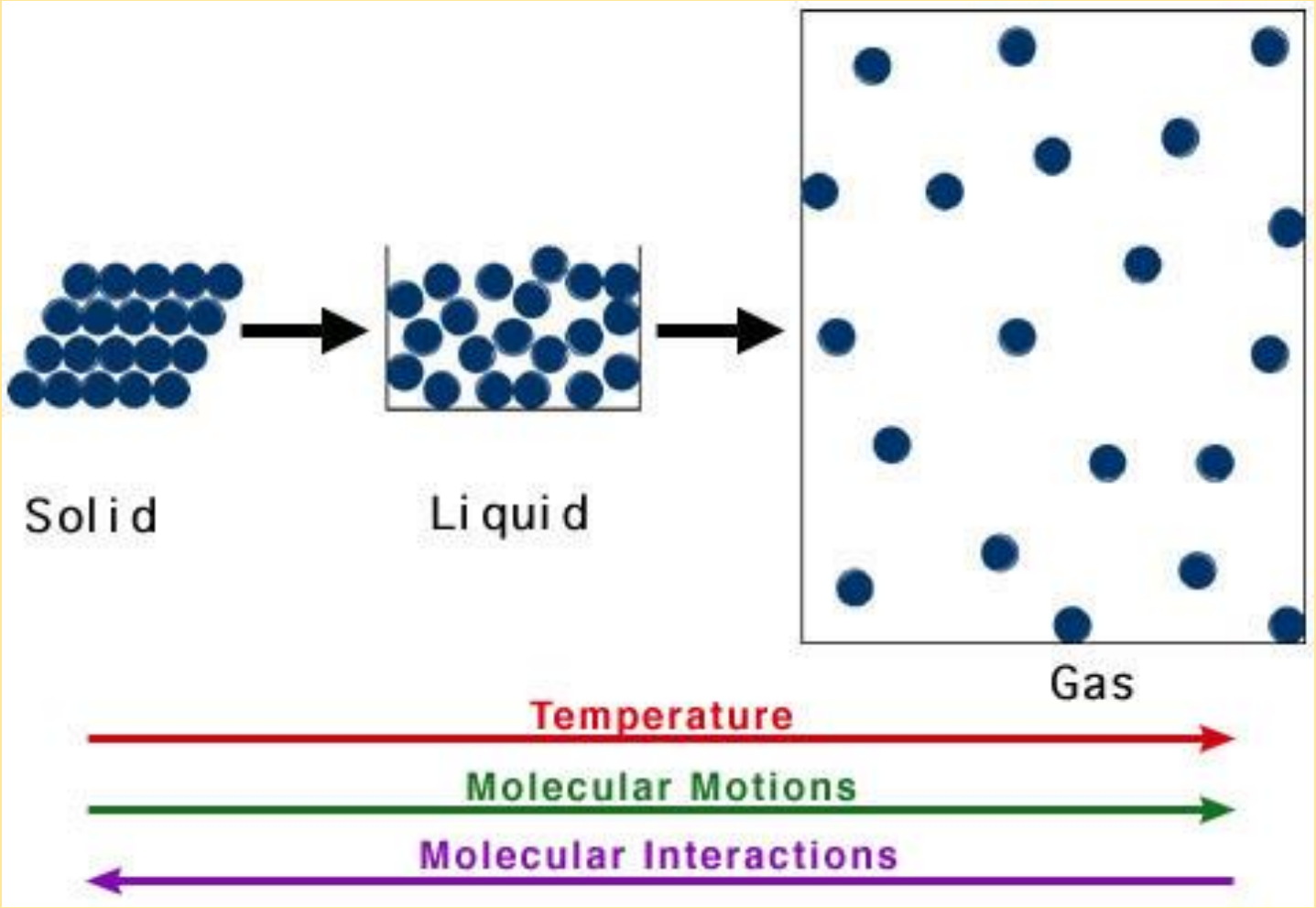
Phase Transitions of Argon

Argon Wikipedia

Core Concept

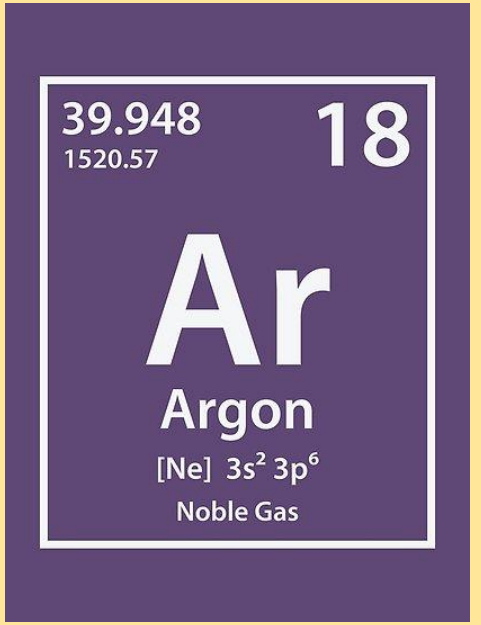
- Simulate phase transition of substance
- Observe changes in potential energy
- Learn basics in Gromacs and molecule visualization (VMD, pymol)

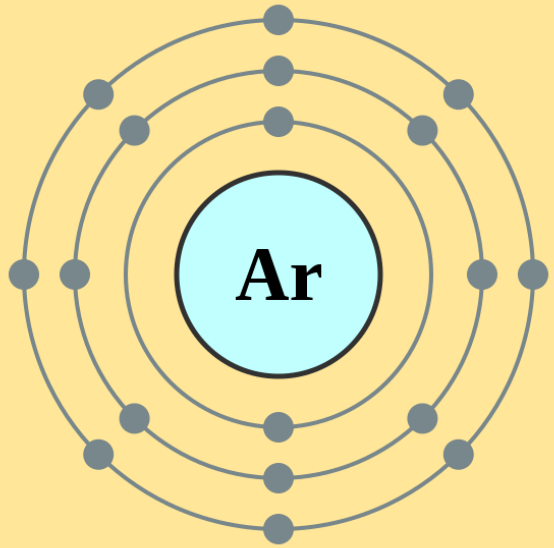


R. Casiday and R. Frey, Washington University

Argon

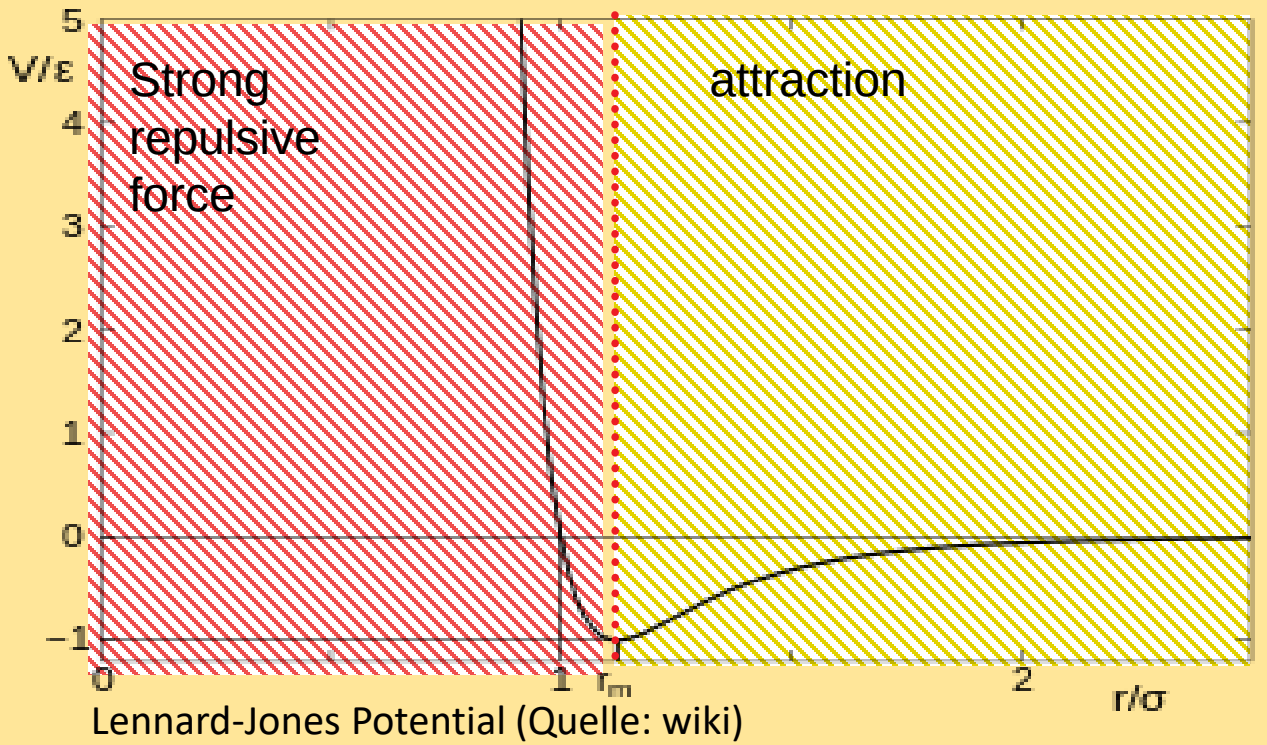
- Noble gas → inert
- Does not react
- Monoatomic in all phases
- Simple Force-Field
- apolar





https://id.wikipedia.org/wiki/Berkas:Electron_shell_018_Argon_-_no_label.svg

Force-Field

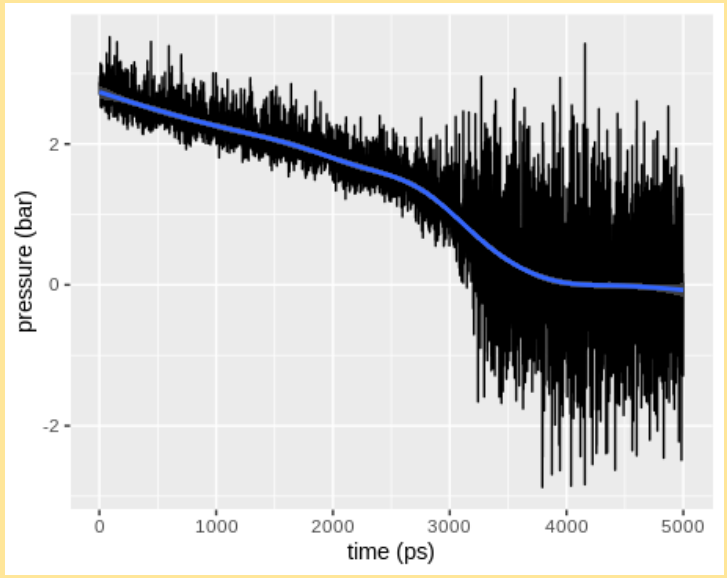


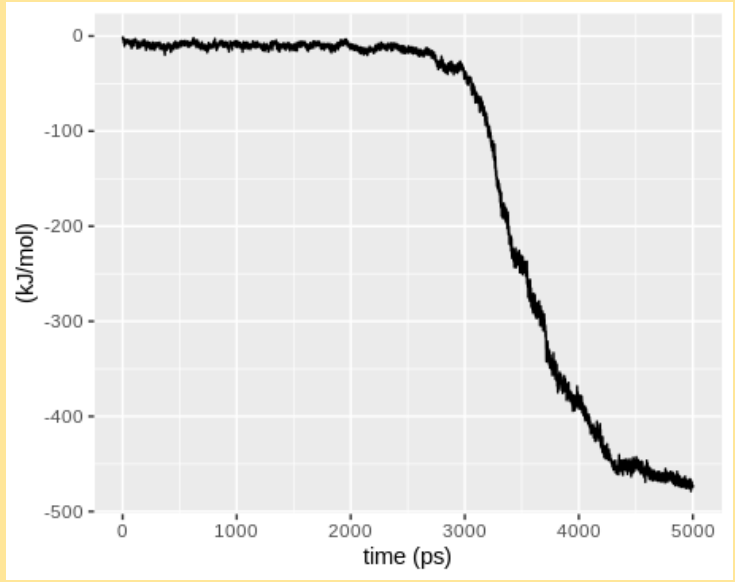
Lennard-Jones Potential (Quelle: wiki)

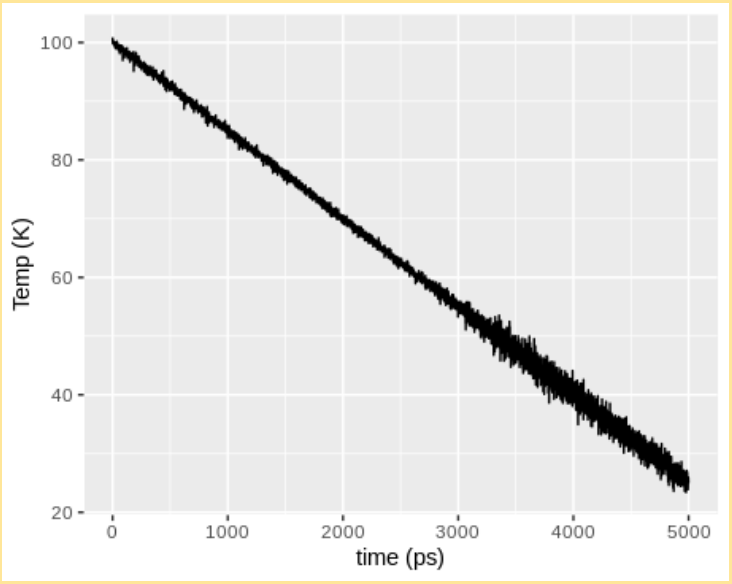
- Pauli-Repulsion
  - Prevents overlapping
- London-Dispersion
  - Induced dipol-dipol interaction

→ Lennard-Jones Potential

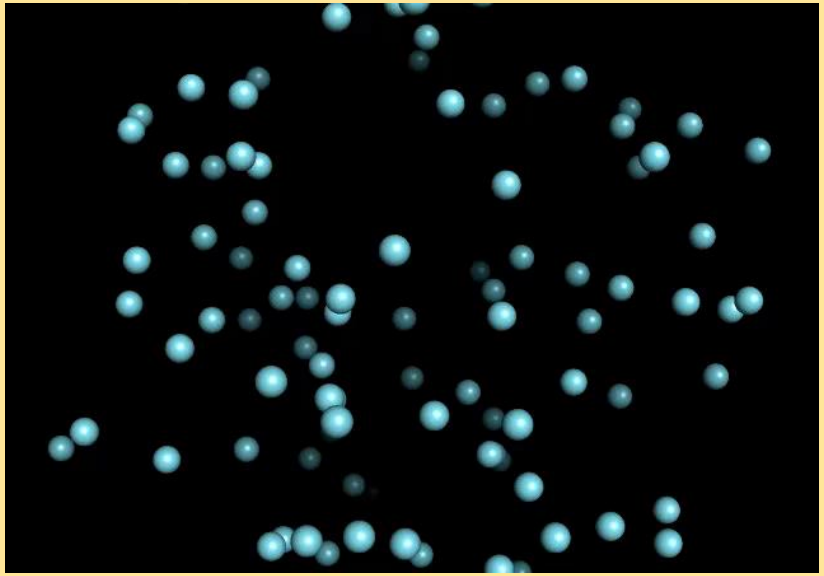
Cooling (gas → liquid)



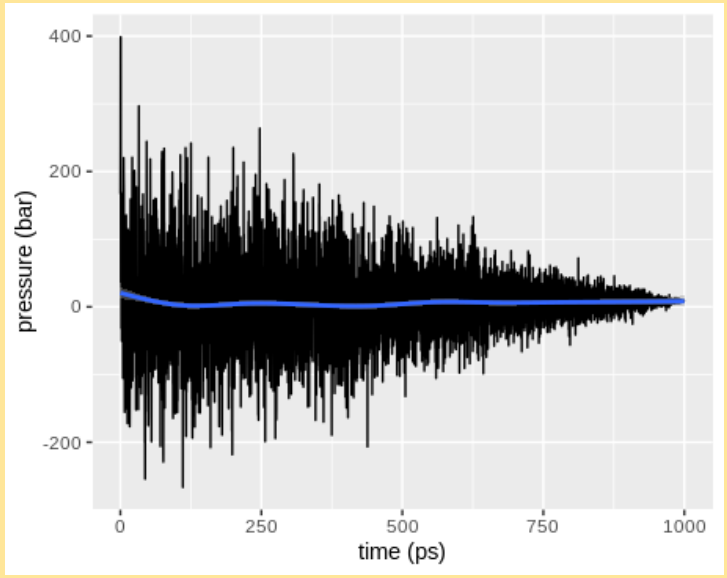


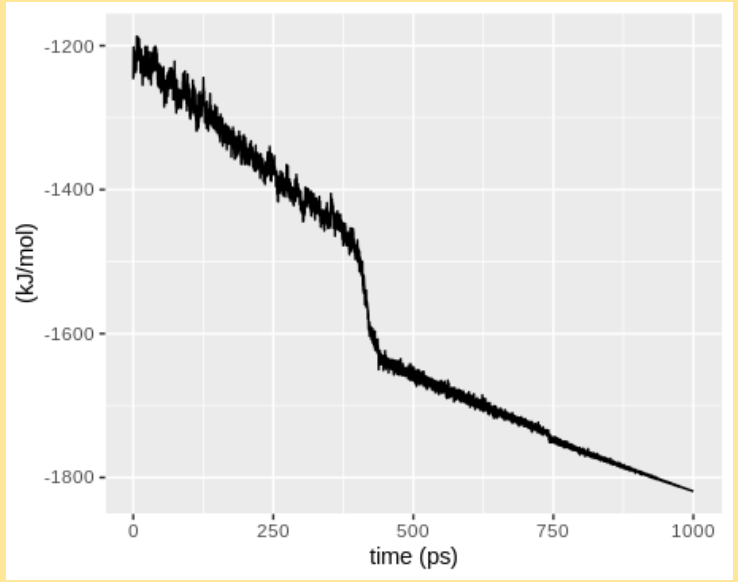


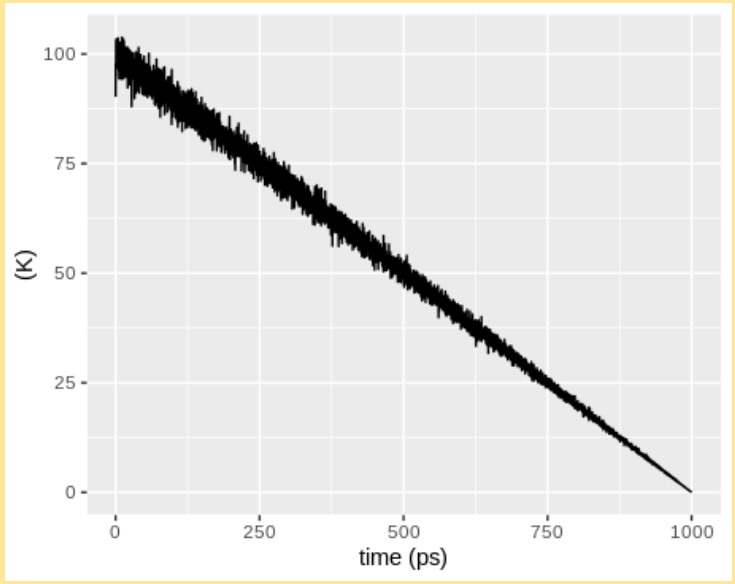
- Conditions:
  - controlled: atom count (fixed), volume (fixed) & temperature (decreasing: 100 → 25°K)
  - Variable: pressure
  - Time: 5000 picoseconds



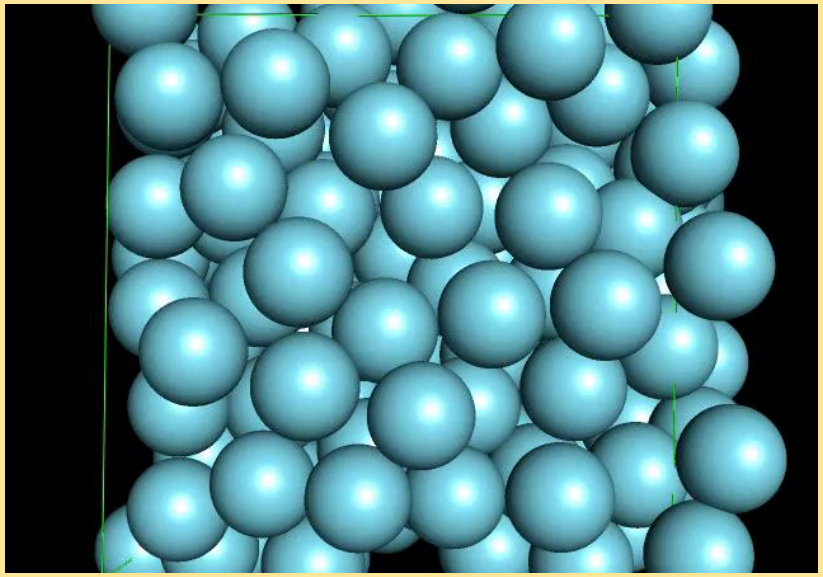
Cooling (fluid → solid)



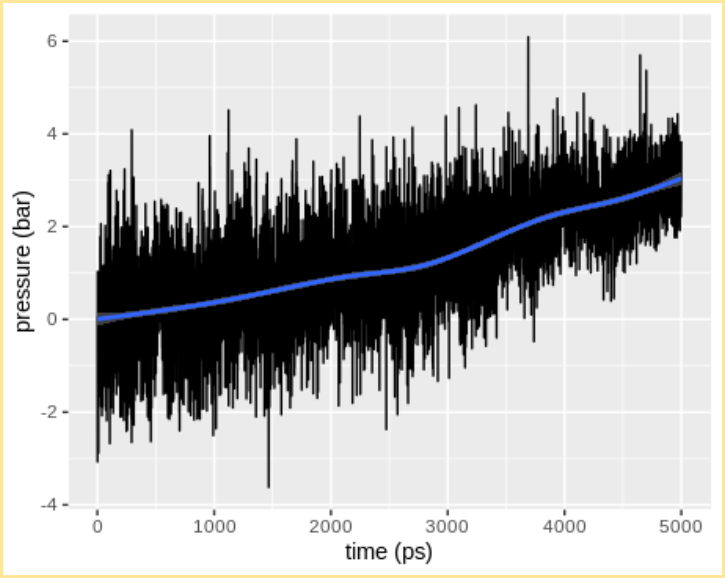


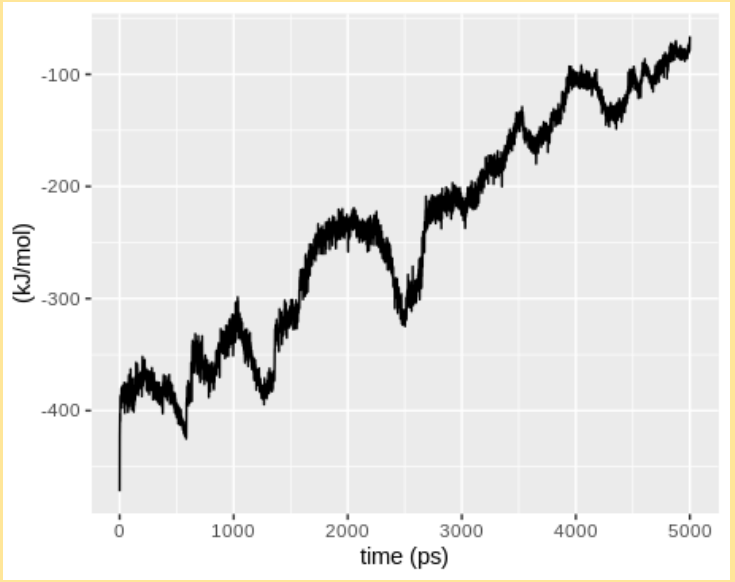


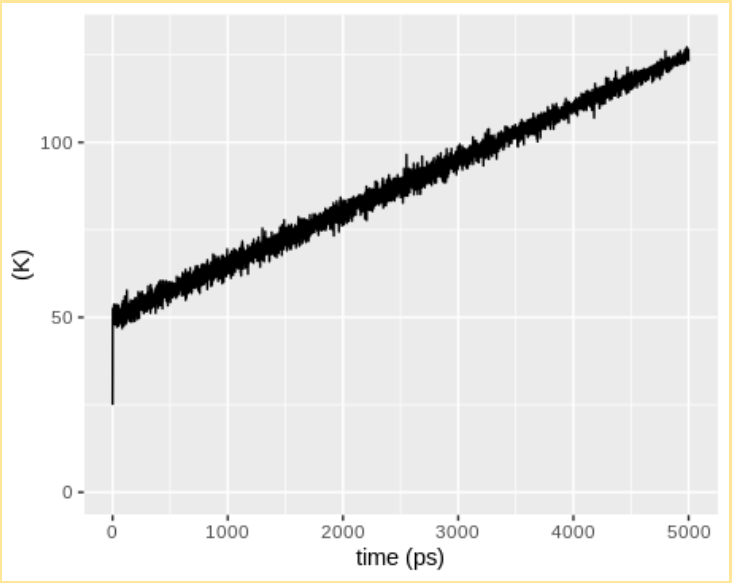
- Conditions:
  - controled: atom count (fixed), volume (fixed) & tempereture (decreasing: 100 → 0°K)
  - Variable: pressure
  - Time: 1000 picoseconds



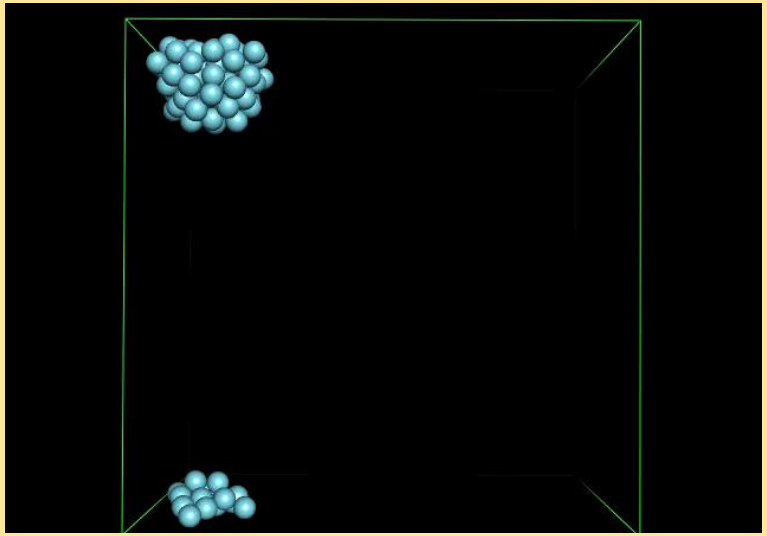
Heat up (fluid → gas)





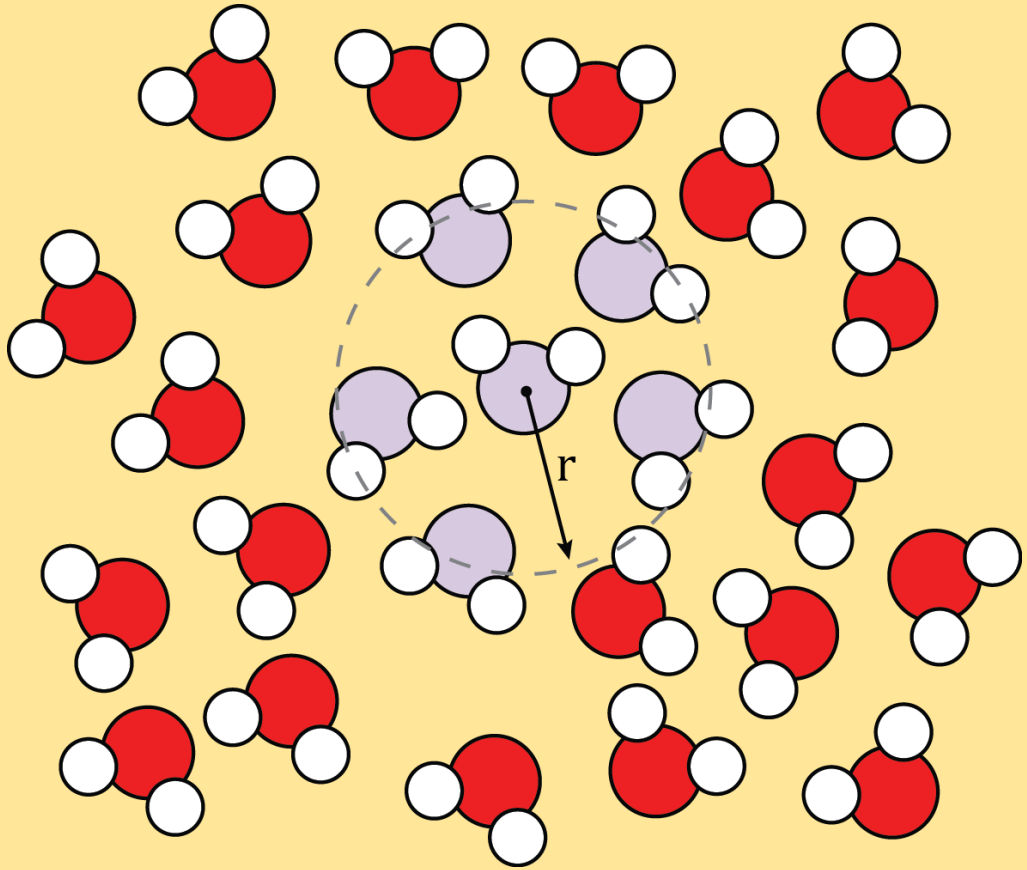


- Conditions:
  - controled: atom count (fixed), volume (fixed) & tempereture (increasing: 50 → 125°K)
  - Variable: pressure
  - Time: 5000 picoseconds



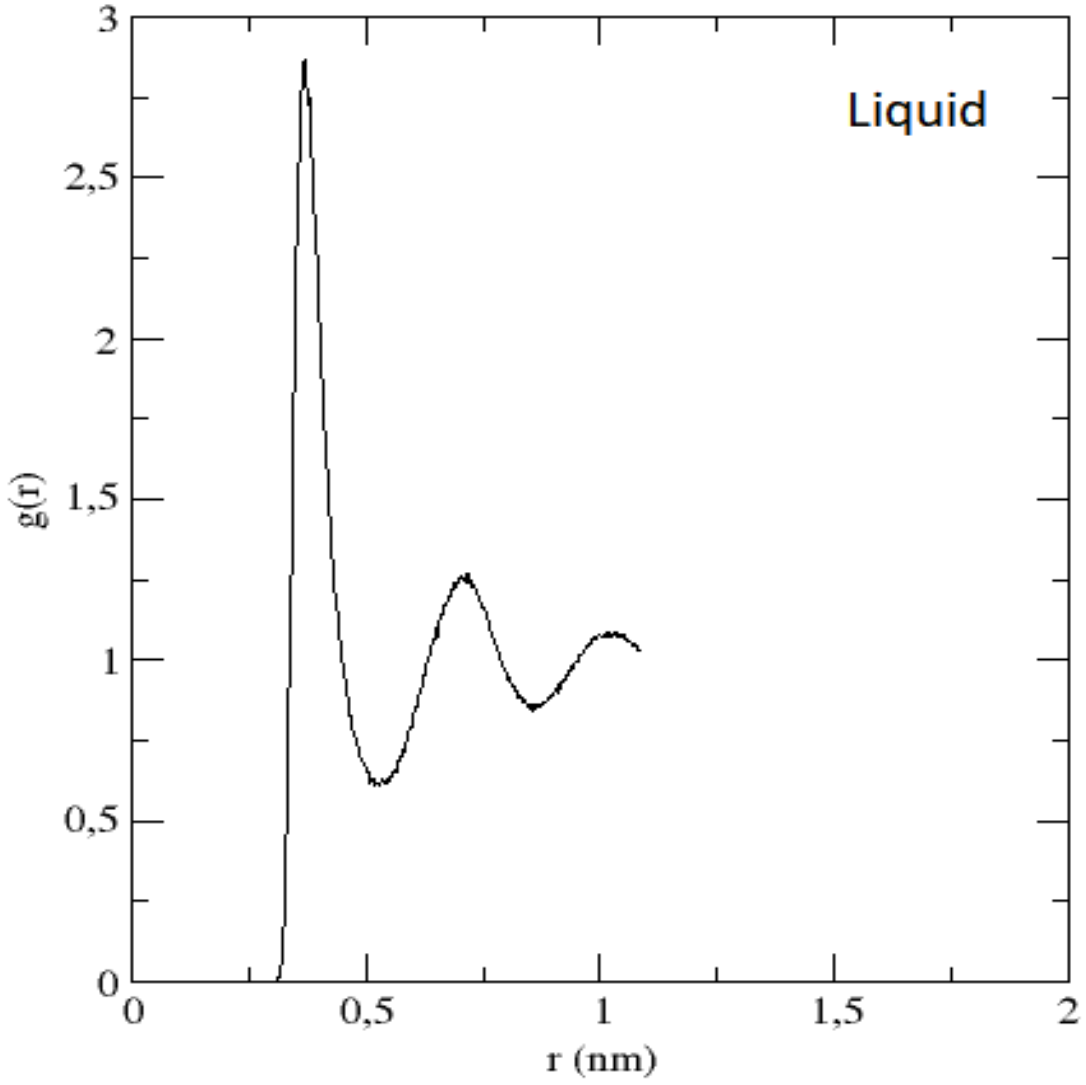
Radial Distribution Density-Function

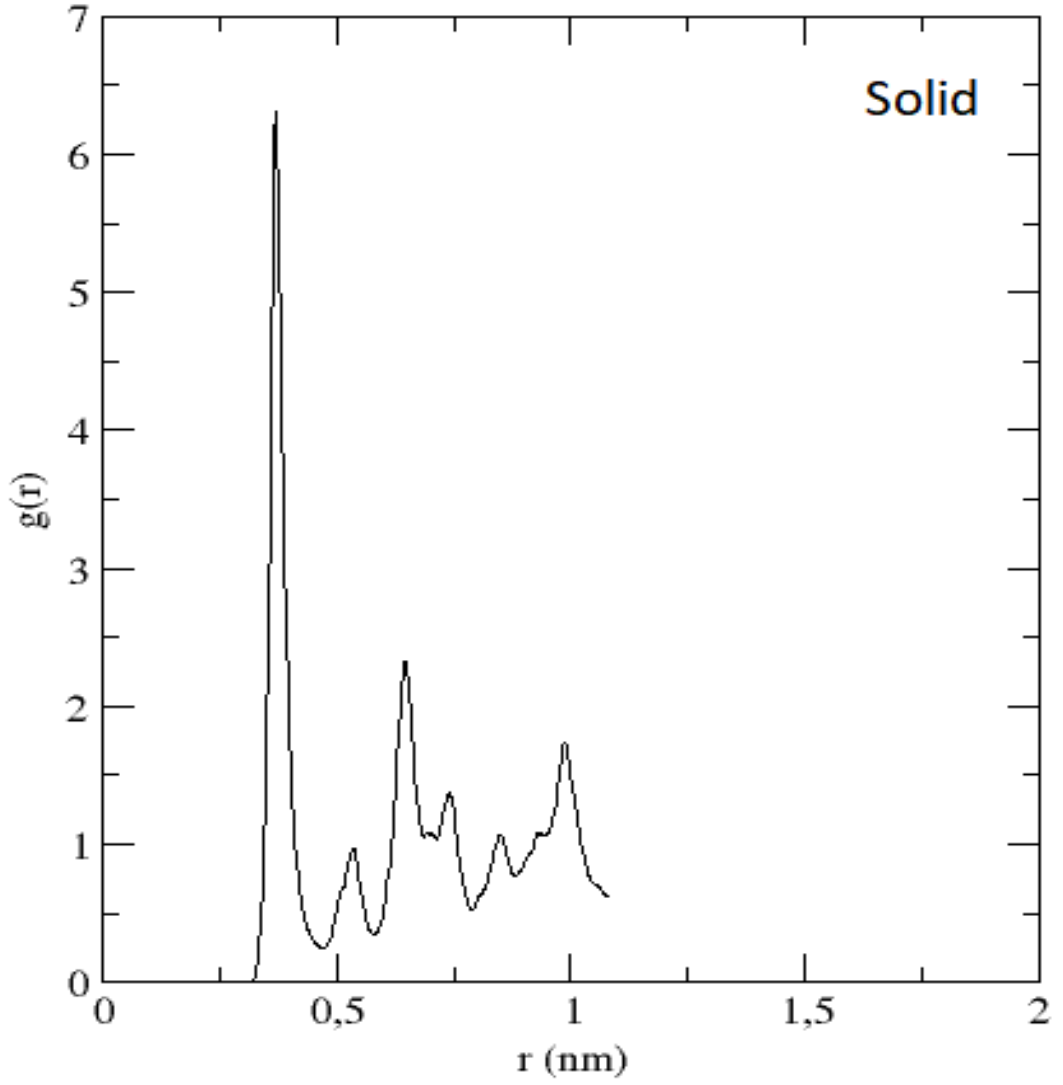
- Defines probabilty to find other Atoms at distance *r* from a particle at the center



https://en.wikibooks.org/wiki/Molecular_Simulation/Radial_Distribution_Functions#/media/File:Molecular_Schematic_for_Interpreting_a_Radial_Distribution_Function.png

Radial Distribution Density-Function





Outlook

- Enhance Argon project:
  - Observe longer time period
  - Simulate: gas → fluid → solid or solid → fluid → gas
  - Use different ensemble: NTP
- Simulate different Atoms

Bibliography

- Tutorial: http://cmb.bio.uni-goettingen.de/pract/p1/
- Introduction to molecular dynamics: https://www.neutron-sciences.org/articles/sfn/pdf/2011/01/sfn201112009.pdf
- used programs: GROMACS (http://www.gromacs.org/), VMD (https://www.ks.uiuc.edu/Research/vmd/), pymol (https://pymol.org/2/), R (https://www.r-project.org/), ggplot2 (https://ggplot2.tidyverse.org/)