

A brief introduction to LAMMPS

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The basics

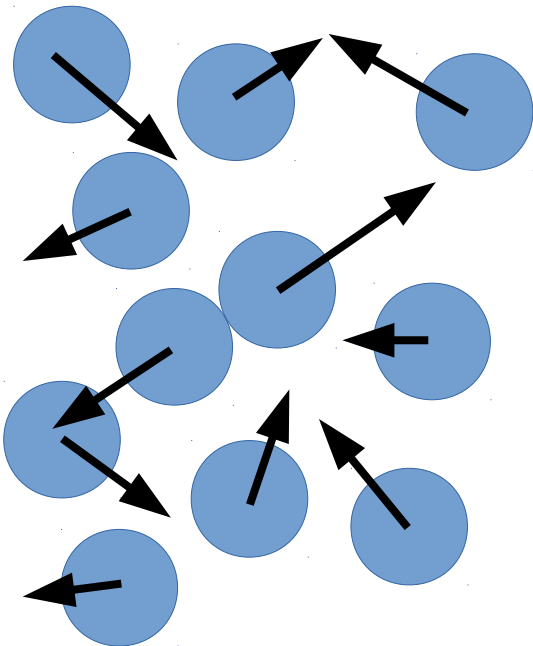
- LAMMPS – Large-scale Atomic/Molecular Massively Parallel Simulator
 - Developed by Sandia National Laboratories and by its wide user-base
 - Can be downloaded from:
<https://lammps.sandia.gov/download.html>
- Everything we are covering today (and a lot of other info) can be found in the LAMMPS User Manual:
<https://lammps.sandia.gov/doc/Manual.html>

Overview of this session

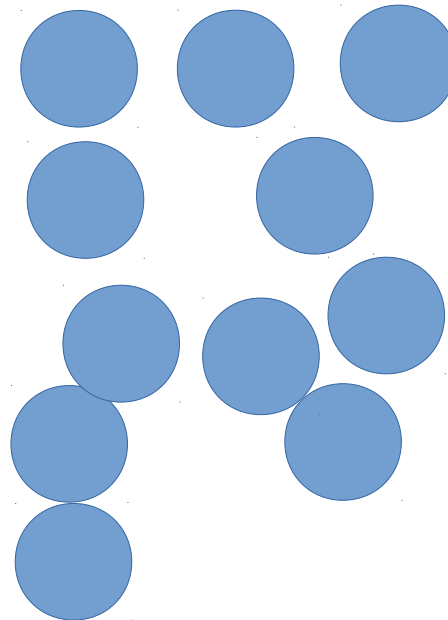
- Run first LAMMPS simulation on ARCHER
 - Briefly show how to run simulation locally
- Preparing a simulation:
 - How is simulation box prepared
 - How are particle interactions defined
 - Neighbour lists *etc*
- Coffee break
- Running a simulation
 - Fixes, computes, and variables
 - What can be output?
- Advanced options
- Questions & quick exercise

How molecular dynamics works

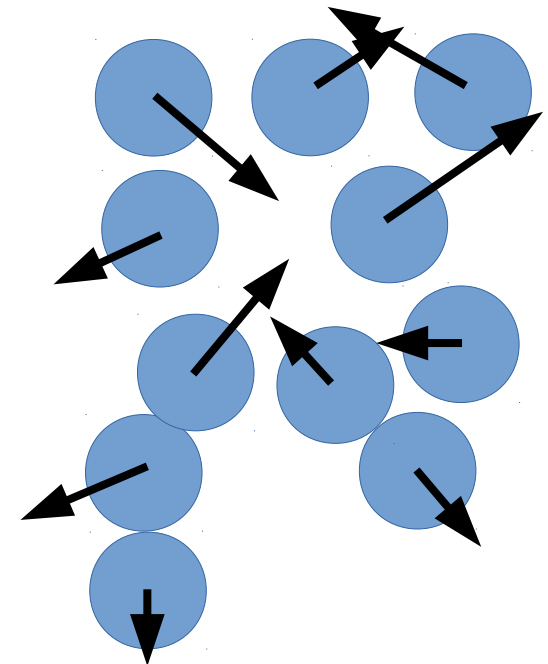
Start with all particle positions and velocities at time t



Update particle positions to time $t+\delta t$

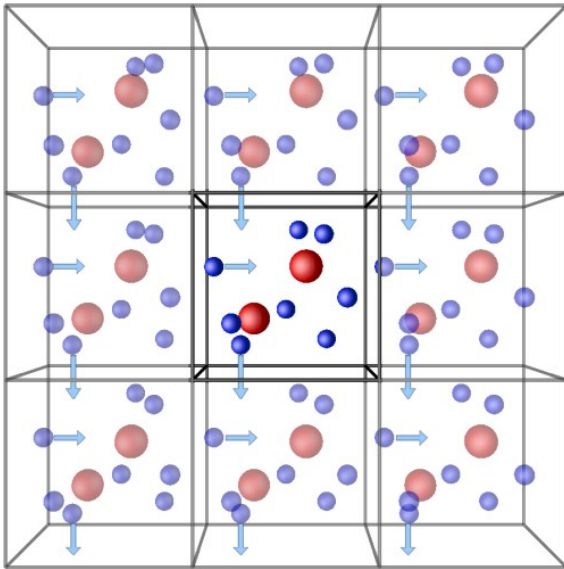


From new positions, find new potential energies, forces, and velocities at time $t+\delta t$

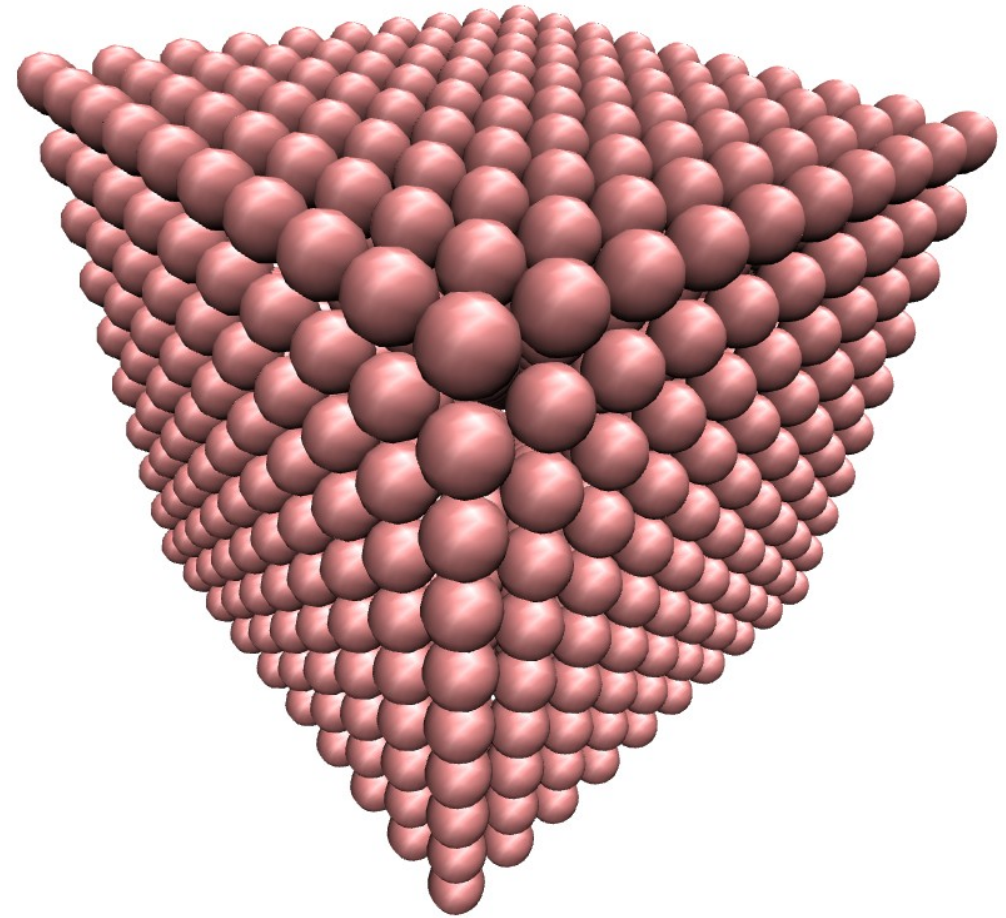


1) Simulation box setup

Periodic boundary conditions

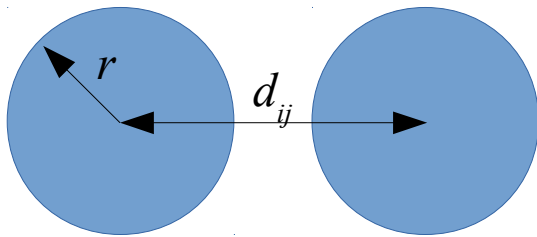
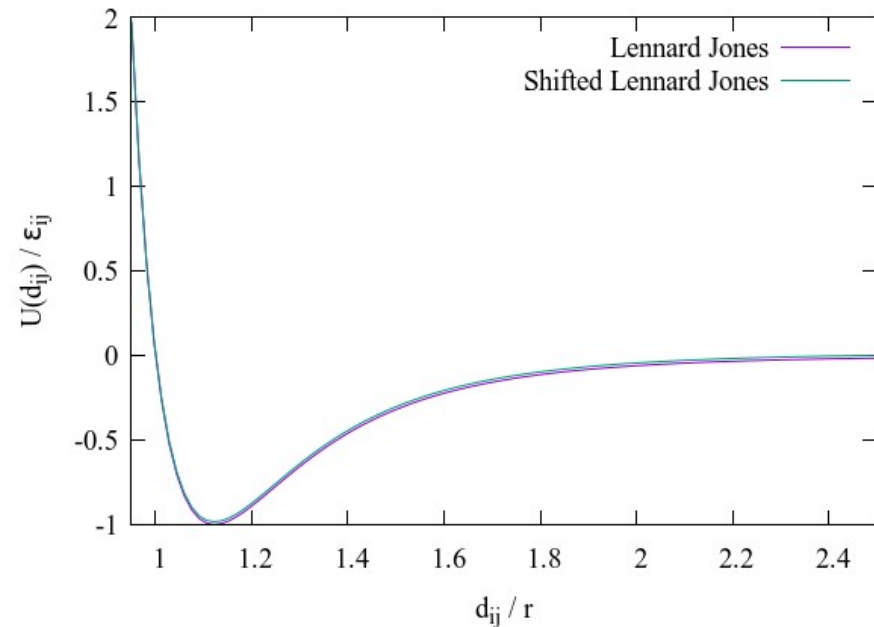


Starting simulation setup ($\rho \sim 0.4$)



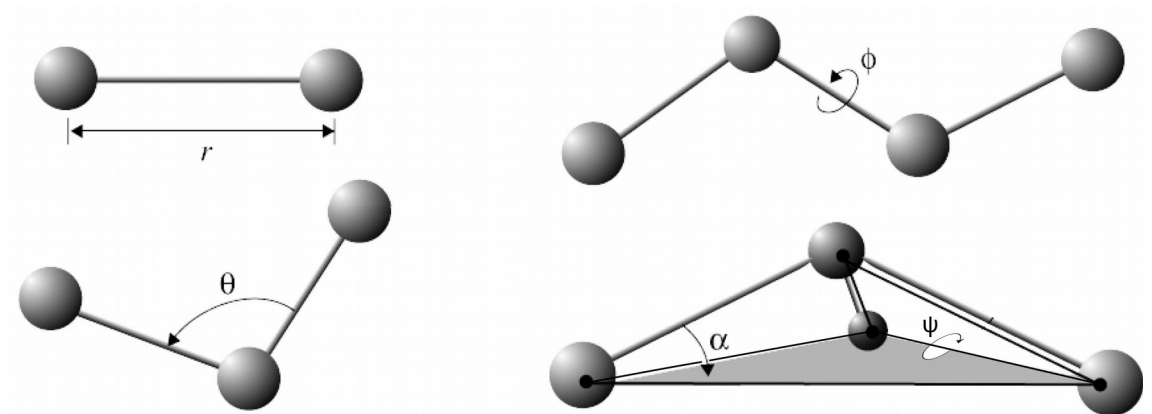
2) Interparticle interactions

- There are 221 different pair styles in LAMMPS

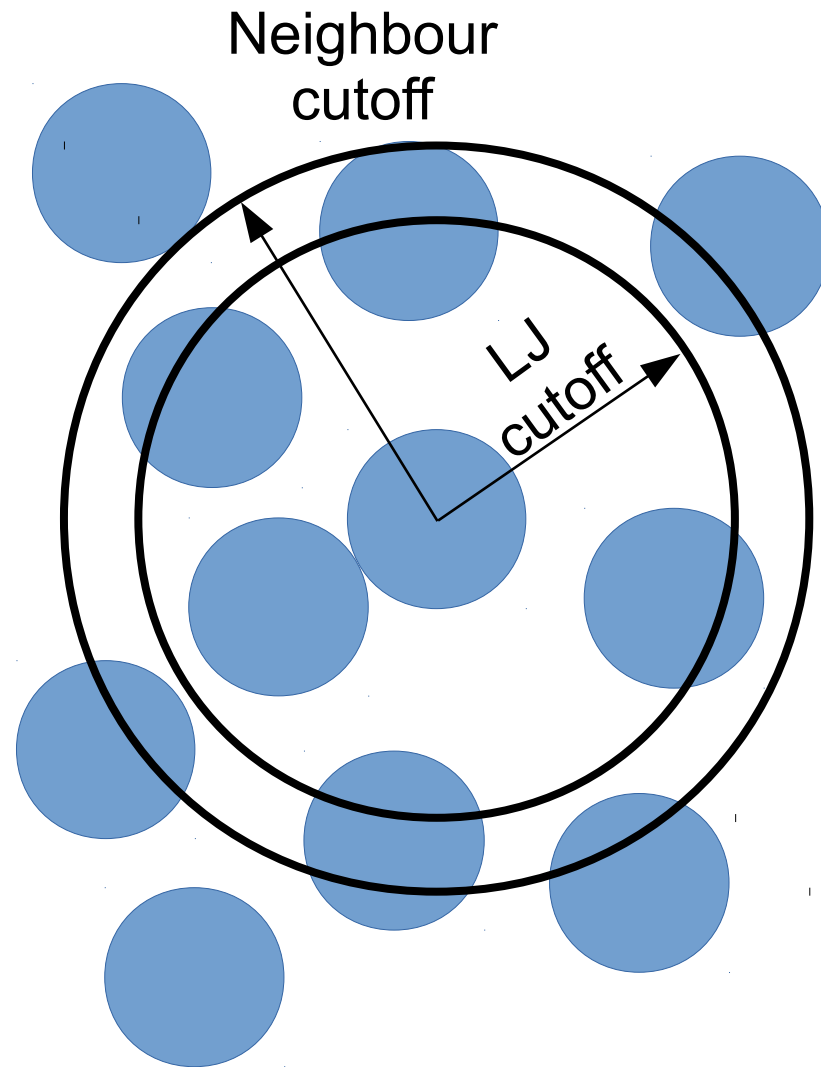


Not discussed here, but LAMMPS also has:

- 17 bond_style commands
- 22 angle_style commands
- 17 dihedral commands
- 13 improper_style commands
- Etc...



3) Neighbour lists



4) Fixes and computes

- 264 fixes
 - This sets general parameters
 - Temperature; pressure; gravity; viscosity; background flows; *etc.* defined by fixes
 - Our simple example has 2:
 - Fix NVT ensemble with temperature $T = 1.0$
 - Fix background flow to 0 (not needed)
- 138 computes
 - Where LAMMPS shines – these commands enable you to output ensemble or per-particle properties of interest

5) Simulation run and outputs

From known velocities and forces, update positions

$$\mathbf{r}(t + \delta t) = \mathbf{r}(t) + \dot{\mathbf{r}}(t) \delta t + \frac{1}{2M} \mathbf{F}(t) \delta t^2 + \mathcal{O}(\delta t^3)$$

From known forces, update velocities

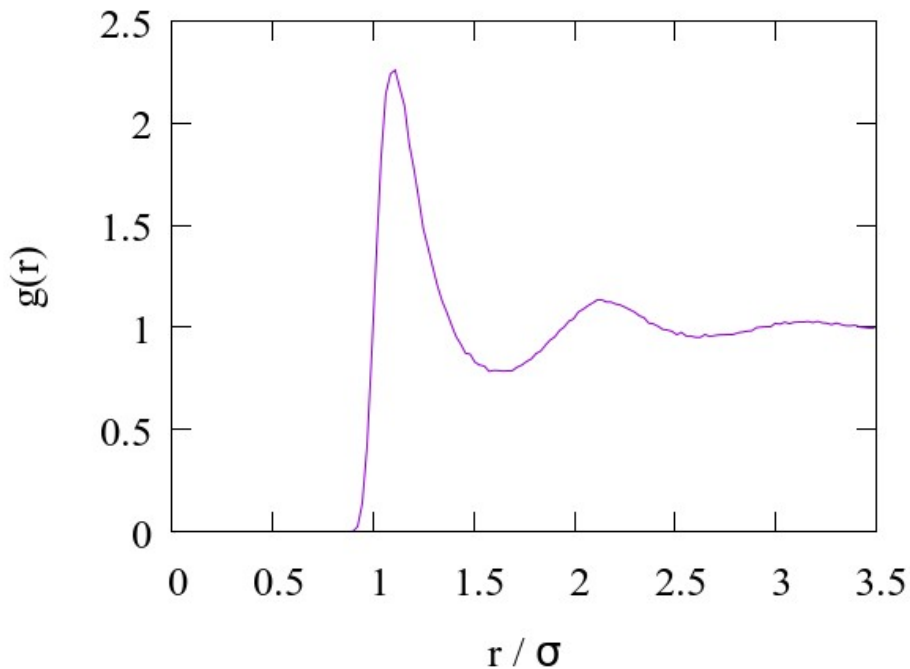
$$\dot{\mathbf{r}}(t + \delta t) = \dot{\mathbf{r}}(t) + \frac{\delta t}{2M} [\mathbf{F}(t) + \mathbf{F}(t + \delta t)] + \mathcal{O}(\delta t^3)$$

From known positions, update energies and forces

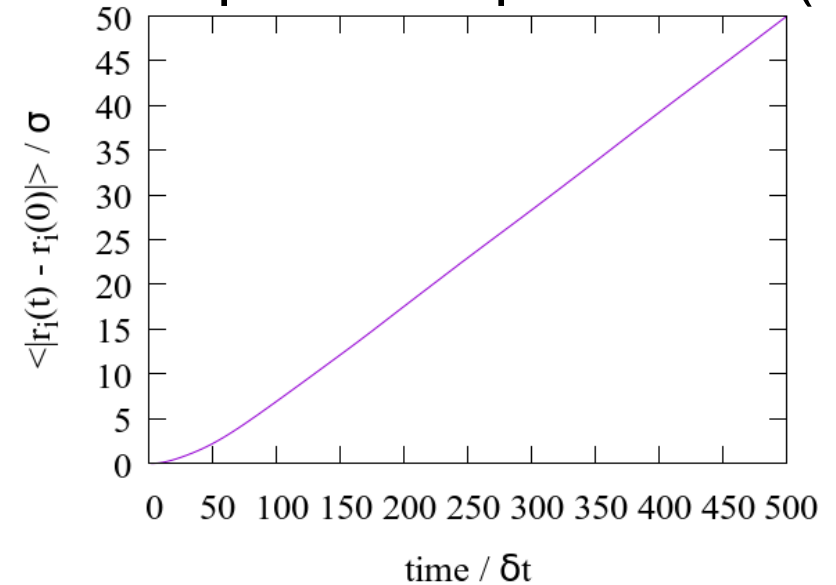
$$\mathbf{F}(t + \delta t) = -\frac{1}{|\mathbf{r}|} \nabla U[\mathbf{r}(t + \delta t)]$$

6) Advanced inputs

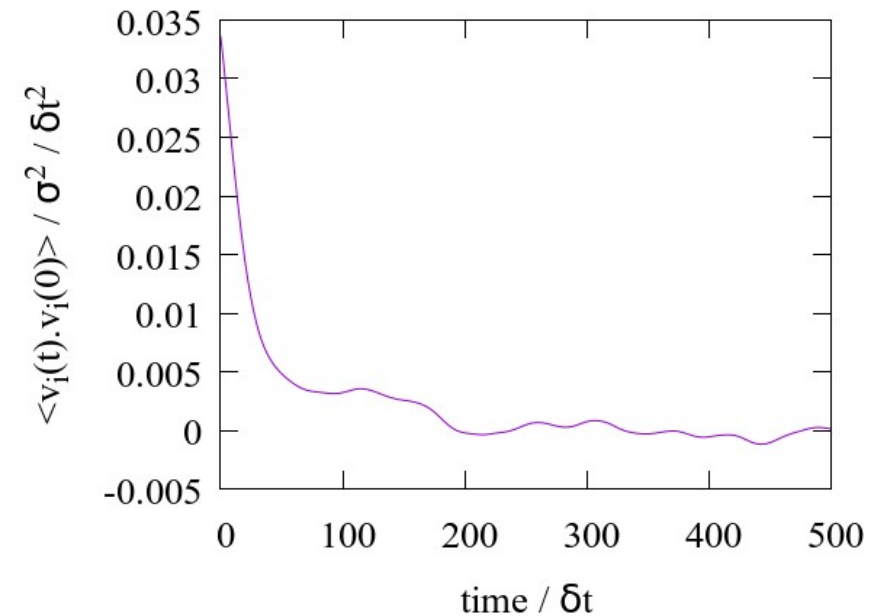
Radial distribution functions (RDFs)



Mean-squared displacement (MSD)

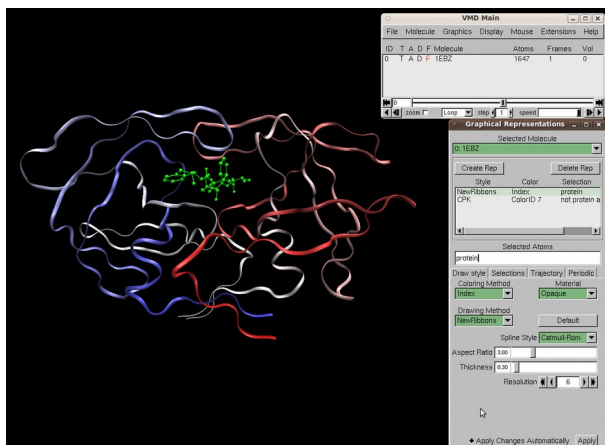


Velocity autocorrelation function (VACF)



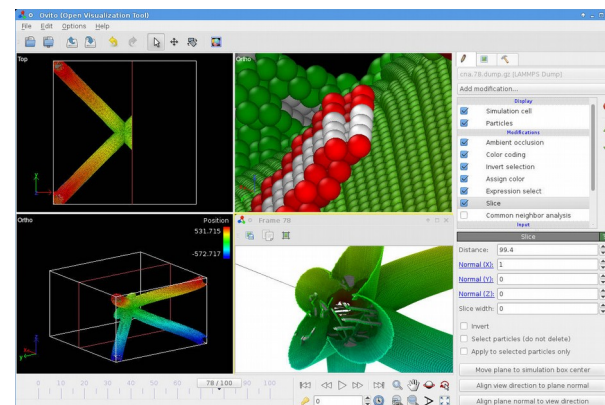
7) Useful third-party software

Visual molecular dynamics (VMD):
<https://www.ks.uiuc.edu/Research/vmd/>

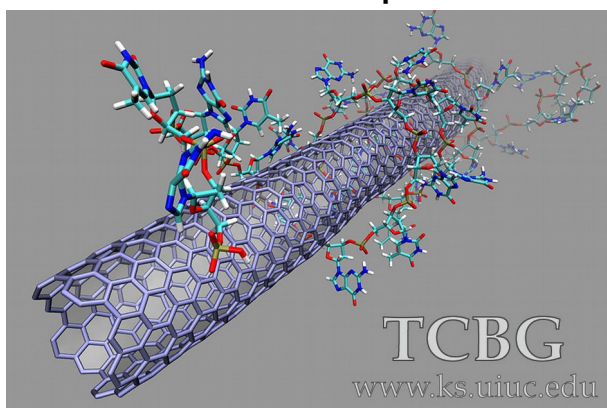


VMD GUI – Wikipedia

Open Visualization Tool (OVITO):
<https://www.ovito.org/>



OVITO GUI – Wikipedia



DNA binds to single-walled nanotube Xueqing Zou, 2013

Some Python pre- and post-processing packages:

- Pizza.py – <https://pizza.sandia.gov/>
- MDAnalysis – <https://www.mdanalysis.org/>
- PyLAT – <https://github.com/MaginnGroup/PyLAT>

8) Optional user exercise

- You have access to a LAMMPS input script called 'in.lj_exercise'
 - This is the same script as before with two changes:
 - The starting density is defined by the variable 'DENSITY'
 - A radial distribution function is output in the main simulation run
- For this exercise, you will look at how varying the system density affects the RDF
 - You should only vary the value of the variable 'Density'
 - In particular, I recommend looking at the RDFs output at densities $\rho = 0.05, 0.8, 1.4$

Overview for next session

- Questions from this session
- Compiling LAMMPS on Archer (similar to local compilation)
 - Packages, libraries, etc.
- Smarter domain decomposition commands
- Delving deeper into LAMMPS source code