PHYS 3061 Introduction to Computer Simulation of Physical Systems

LAB 3

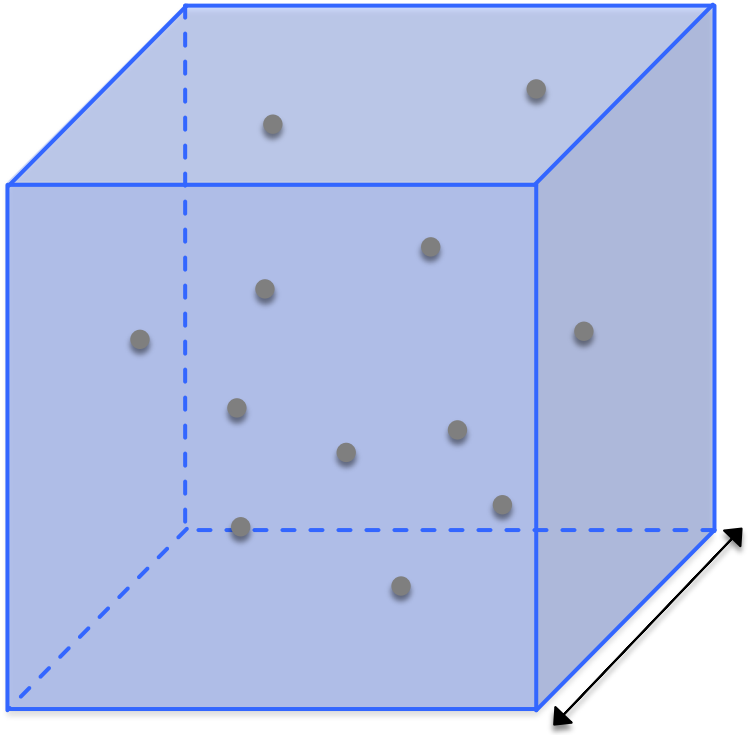
Goal of this session

- Initialize a system with center of mass velocity correction
- Apply Lennard-Jones potential
- Perform time evolution on the system

Centre of mass correction

- Motivation:
  - In the real case: imagine a box filled with gas molecules
    - The box is not moving

      ⇒ the center of mass velocity should be zero
- However, our velocity initialization may not include the zero center of mass velocity constraint
  - introduce an additional degree of freedom: the center of mass movement.
  - Such an additional degree of freedom may affect the statistics.



Centre of mass correction

- Apply center of mass correction before time evolution*:
  - Calculate the momentum of the center of mass (Identical particles are assumed)

$$\overrightarrow{p_{CM}} = \sum_i^n m\,\overrightarrow{v_i}^{\#}$$

  - Subtract every velocity by the center of mass velocity

$$\overrightarrow{v'_i} = \overrightarrow{v_i} - \overrightarrow{v_{CM}} = \overrightarrow{v_i} - \frac{\overrightarrow{p_{CM}}}{nm} = \overrightarrow{v_i} - \frac{\sum_i^n \overrightarrow{v_i}}{n}$$

  - The new velocity is the initialized velocity

One correction after the initialization will be good enough

i : each component; n: number of particles

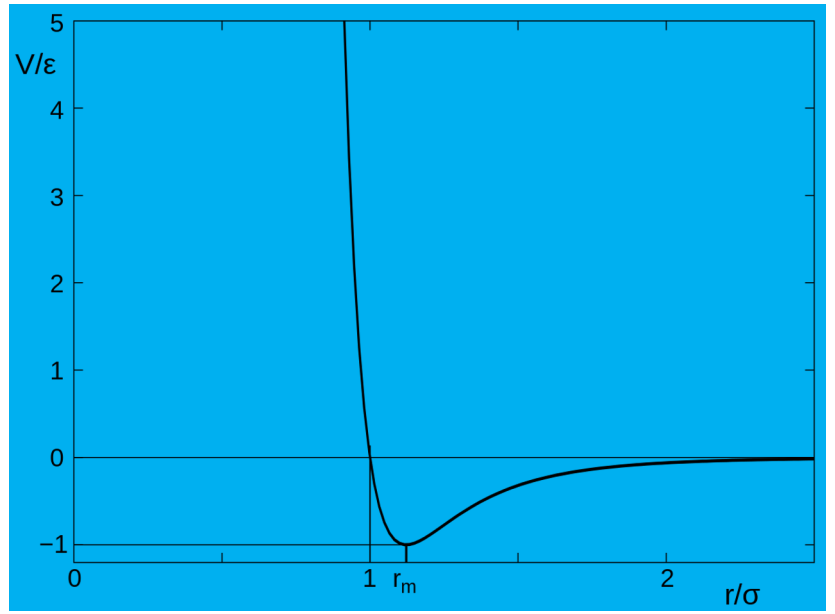
Lennard-Jones potential

- $V_{LJ} = 4\varepsilon\left[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}\right]$, where ε is the depth of the potential and σ is the zero-potential point

- Values of ε and σ vary depend on atom species.

For Argon: σ= 3.40 Å and ε= 1.65 × 10^{-21} J = 1.03 × 10^{-2} eV

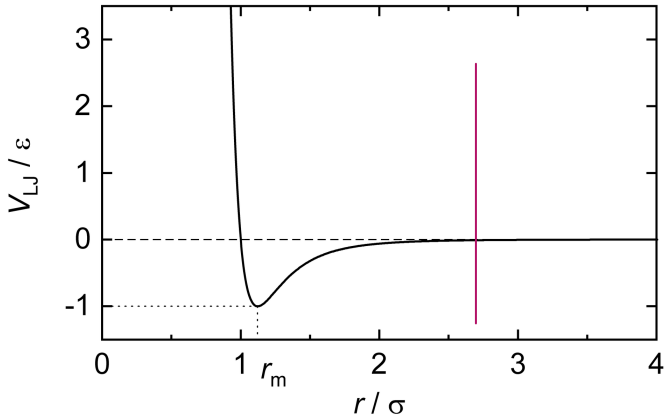
- You can switch the target atoms by replacing the correct values of σ and ε from literature. Please include the reference in your README file.



Lennard-Jones potential (cut-off and shifted form; optional)

- By default, you should calculate all the pairwise force based on LJ potential.
  - Optional: For very large systems with more than 1000 particles, you can apply the truncation to speed up the calculation
- However, if you do the truncation, it will introduce discontinuity of LJ potential, which may affect force calculations.
- One solution is to set an appropriate cut-off distance r_c and shift the whole L-J potential, the new shifted L-J potential is then:

$$V_{LJ-shift.} = \begin{cases} V_{LJ}(r) - V_{LJ}(r_c), r \leq r_c \\ V_{LJ}(r_c) - V_{LJ}(r_c) = 0, r > r_c \end{cases}$$



- Note the new V_{LJ} is shifted down by $V_{LJ}(r_c)$ to keep the continuity of V_{LJ}. However, it may affect the total energy calculations.

Force calculation

- The force can be calculated by differentiating the potential (Newton third law)

$$V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

- i.e.

The calculation of force or potential can be implemented through either the use of relative distance or simulation coordinate.

$$\vec{F}(\vec{r}_{ij}) = \frac{24\epsilon}{r_{ij}^2}\left[2\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]\vec{r}_{ij}$$

Force felt by j^{th} particle, due to i^{th} particle

$\vec{r}_j - \vec{r}_i$

Time evolution (Verlet method equation)

$$\vec{r_i}(t+\Delta t) = \vec{r_i}(t) + \vec{v_i}(t)\Delta t + \frac{\vec{f_i}(t)}{2m}\Delta t^2$$

$$\vec{v_i}(t+\Delta t) = \vec{v_i}(t) + \frac{\vec{f_i}(t+\Delta t) + \vec{f_i}(t)}{2m}\Delta t$$

where i stands for the i^{th} particle in both equations

What you need to do within a loop (or in one time unit Δt)

Where to check the boundary?

1. Update positions and partial velocities

$$\vec{r_i}(t+\Delta t) = \vec{r_i}(t) + \vec{v_i}(t)\Delta t + \frac{\vec{f_i}(t)}{2m}\Delta t^2$$

$$\vec{v_i}(t+\Delta t) = \vec{v_i}(t) + \frac{\vec{f_i}(t)}{2m}\Delta t$$

2. Update forces

$\vec{f_i}(t+\Delta t)$ *is only related by* $\vec{r_i}(t+\Delta t)$

3. Finalize velocities

$$\vec{v_i}(t+\Delta t) = \vec{v_i}(t) + \frac{\vec{f_i}(t)}{2m}\Delta t + \frac{\vec{f_i}(t+\Delta t)}{2m}\Delta t$$

Time evolution (Verlet method implementation)

Assume we have the positions, velocities and forces of particles at time t.

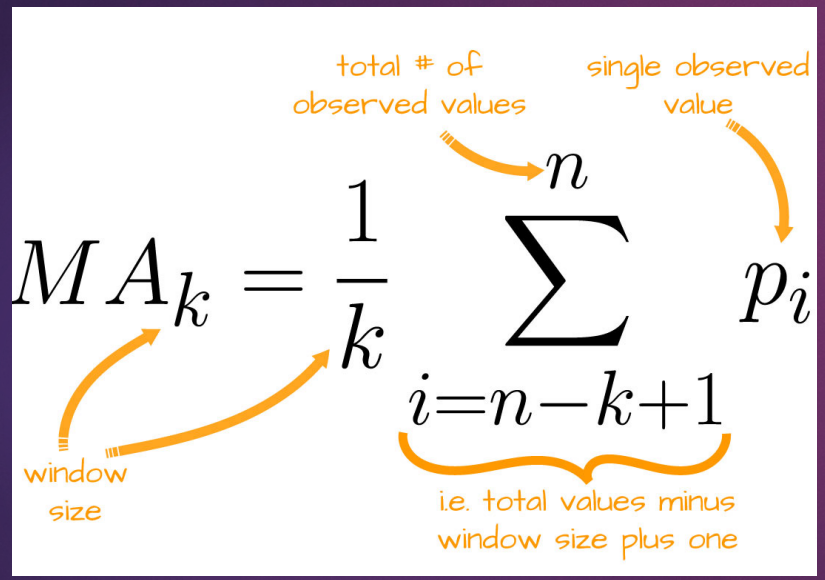
- At time $t + \Delta t$:
  - Compute the new positions and the partial velocities
  - Check the boundary
  - Calculate the forces
  - Finalize the velocities

Units

- Again, choose the meaningful units.
- Eg. Å, ps, ev, etc. You need to define the conversion constants and comment properly.
- Units can also be normalized to simplify calculation
- Example:
  - Recall $V_{LJ} = 4\varepsilon\left[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}\right]$ If we set $r' = \frac{r}{\sigma}$, then $V_{LJ} = 4\varepsilon\left[(\frac{1}{r'})^{12} - (\frac{1}{r'})^{6}\right]$
  - Same procedure can be done to V_{LJ}, which could be expressed in unit of ε

Notes: Explain your units and show your conversion condition in README

Check your result



- Calculate the kinetic energy (and the temperature), the potential energy and the total energy of the system and plot them against time
  - Recall $< \frac{1}{2}mv^2 >= \frac{3}{2}k_B T$ (or we can calculate the temperature based on the instant kinetic energy)
  - Compare with the T_0 used for initialization
  - Use instant KE to calculate "instant temperature" ? ill-defined!
  - Use moving average (MA) of KE to calculate the temperature
- The total energy should be conserved and both kinetic and potential energy should be stable (with small fluctuations) after equilibrium

Any comments on this equation?

Notes: Assume the temperature after the center mass correction is the initial temperature

Task for lab3

1. Initialize a system with
   - Same position and velocity requirement as in lab2
   - Center of mass correction applied
2. Apply Lennard-Jones potential

Deadline: 8th March 23:59

3. Use the Verlet method to evolve your system until it reaches equilibrium
   - Output every 100 simulation steps (suggested; time step dependent) as one frame in a .xyz file
   - Plot total energy, kinetic energy and potential energy against time
     - Two plots should be provided for each quantity: one for the full simulation process and another for the steps after reaching equilibrium (for temperature calculation)
   - Plot temperature against time and compare it with the initial temperature
     - Calculate the temperature using the moving average of velocity with proper window size

You need to submit **the code, the plots, readme and the .xyz file** before **8th March 23:59**.

No lab report is required in this lab.

The Simplified Flow chart

Suggestion:

Accumulate important physical quantities in the loop for statistic purpose.