Exercise 1

Zijian Sun

1. The Lennard-Jones potentials and the corresponding forces between particles for He, Ne, and Kr are shown in fig1-3. From the figures, the L-J potential becomes steeper as the atomic number increases from He to Kr. Correspondingly, the attraction and repulsion forces between particles become stronger in Kr than in He. The distance when L-J potential reaches its minimum also varies from He to Kr, He has the shortest distance and Kr has the longest distance.

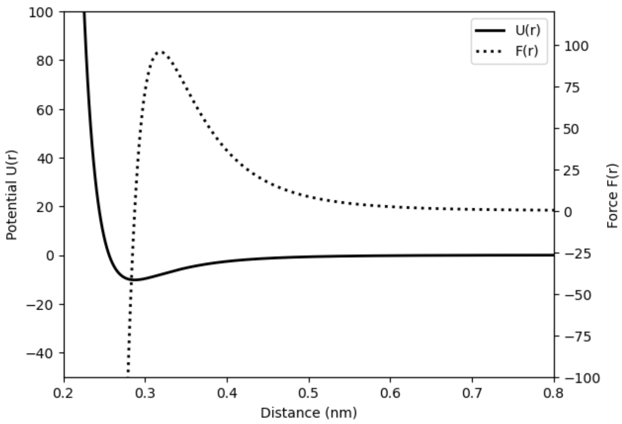

Figure 1: L-J potential and force for He

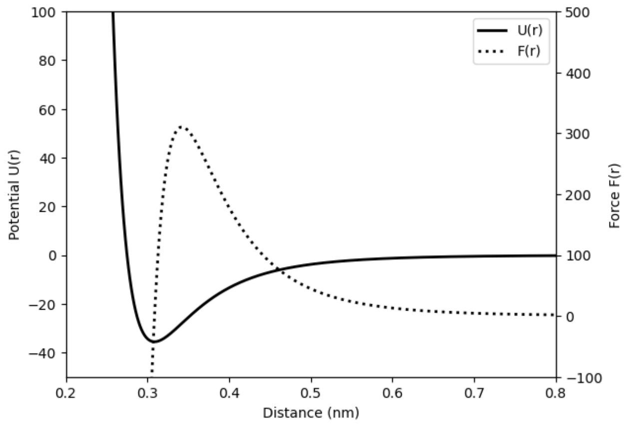

Figure 2: L-J potential and force for Ne

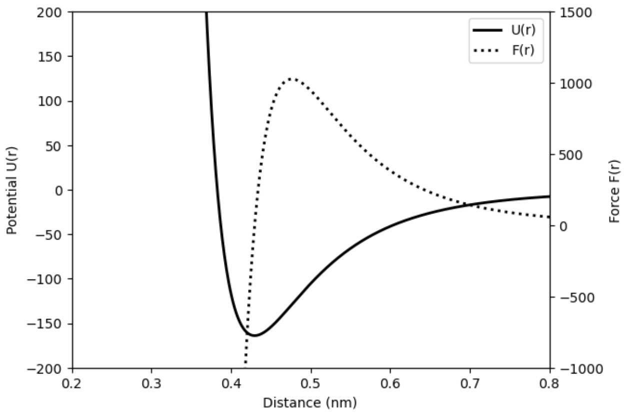

Figure 3: L-J potential and force for Kr

2. When we do not include the repulsion part of the L-J potential, the force between the particles will always be the attraction force, thus it will attract all the particles into one place, which is not physically right.

3. The calculated densities by LAMMPS as well as the density from the database are shown in table1. When the time is short, the discrepancy between the density by MD simulation and the standard database is significant. As the simulated time increasing, the simulated density gradually become close to the real value. This result supports the ergodic hypothesis.

Table 1: Densities from simulation and NIST Database

Time (ps)	Density (kg/m^3)
1	101.416
2	132.749
5	0.827
10	0.8
20	0.816
100	0.829
NIST	0.8058

4. $r_{12} = 1.1, r_{13} = 0.922, r_{23} = 1.2728$. Base on the distance, the molecule has two OH bonds, while the two H atoms do not form a HH bond. The energy can be calculated as

$$
\begin{aligned}
E = {} & 4\epsilon(H)\left[\left(\frac{\sigma(H)}{r_{23}}\right)^{12} - \left(\frac{\sigma(H)}{r_{23}}\right)^{6}\right] + k_{OH}(r_{12} - R_{OH})^2 \\
& + k_{OH}(r_{13} - R_{OH})^2 + k_{HOH}(\theta_{231} - \theta_{HOH})^2 \\
& = 4 \times 0.25 \times \left[\left(\frac{2}{1.2728}\right)^{12} - \left(\frac{2}{1.2728}\right)^{6}\right] + 1000 \times (1.1 - 1)^2 \\
& + 1000 \times (0.922 - 1)^2 + 0.25 \times (77.4712 - 105)^2 \\
& = 417.0784 kJ/mol
\end{aligned}
$$