Exercise II
Force in atomic level

1 Lennard-Jones potential

Given the Lennard-Jones potential:

$$U_{L-J}(r) = 4\epsilon \left[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6} \right] \tag{1}$$

it is possible to find the equilibrium position r_0 with the derivative of the previous expression:

$$\frac{\partial}{\partial r}(U_{L-J}(r)) \quad = \quad 4\epsilon \left[12\frac{\sigma^{12}}{r^{11}} - 6\frac{\sigma^{6}}{r^{5}} \right]$$

To find the equilibrium position we can find the minimum of the potential, solving the equation

$$\begin{aligned} \frac{\partial}{\partial r}(U_{L-J}(r)) &= 0 \\ 4\epsilon \left[12\frac{\sigma^{12}}{r^{11}} - 6\frac{\sigma^{6}}{r^{5}} \right] &= 0 \end{aligned}$$

$$r^6 = 2\sigma^6$$

The only real and positive value is

$$r_0 = \sqrt[6]{2}\sigma$$

and the minimum energy is

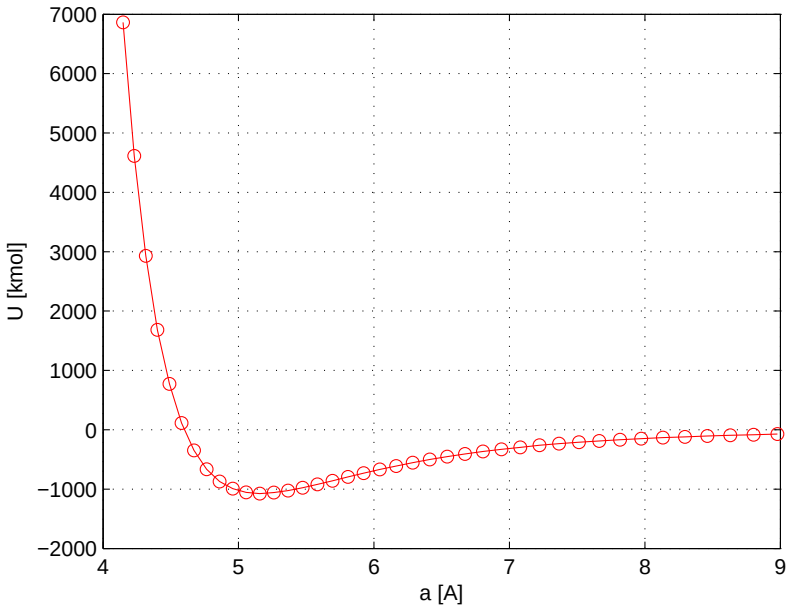
$$U_0 = U_{L-J}(r_0) = -\epsilon$$

2 Lattice constant of *fcc* Ar crystal

With LAMMPS it is possible to determine the lattice constant a and the per-atom cohesive energy U_c at T=0 K. Using the following script:

```
# L-J fcc cohesive energy calculation.
#
units real
atom_style atomic
boundary p p p

variable m equal 39.948
variable epsilon equal 0.25337
variable sigma equal 3.345
variable a0 equal 1.24*${sigma}
variable cutoff equal 4.0*${sigma}
print "epsilon = ${epsilon}"
print "sigma = ${sigma}"
print "cutoff = ${cutoff}"
print "a0 = ${a0}"
print "mass = ${m}"

lattice fcc ${a0}
region BOX block 0 5 0 5 0 5
create_box 1 BOX create_atoms 1 box

mass 1 $m
pair_style lj/cut ${cutoff}
pair_coeff 1 1 ${epsilon} ${sigma}

thermo_style custom lx pe

variable i loop 40
label loop
run 0
displace_box all x scale 1.02
displace_box all y scale 1.02
displace_box all z scale 1.02
next i
jump in.coh loop
```

In the first part there are the parameters typical for Ar-Ar interaction, in the appropriate measurement units. After the specifications for the crystal generation, the input script contains a loop (without time integration) in which the box increases with a rate of 2%. The outputs are the x length of the box and the potential energy. After collecting the numerical values from the output file, the graph of the results is the following:



In particular it can be noticed that the numerical simulation gives these values:

$$a = 5.1573\,\text{Å}$$

$$U_0 = -1074.4\,kcal$$