Project 1
Molecular Dynamics
FYS-4460

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March 4, 2015

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1 Part 1:

1.1 Task a: Creating a FCC lattice

This task is implemented in the function createFCCLattice()

The noble gas argon should have a stable lattice structure when a solid, by letting the system start in a stable situation we avoid a lot of energy to be infused into the systems temperature due to it minimizing potential energy. The implementation is done by going through several nodes, R_i, put on a grid in the box and then placing 4 atoms around each node. Let c_l be the length between nodes.

$$\mathbf{R}_{ij} = \mathbf{R}_i + \mathbf{r}_j \qquad j = \{1,2,3,4\} \qquad i = \{1,2,...,4\mathrm{N}_{\mathrm{atoms}}\}$$

$$\begin{aligned}
\mathbf{r}_1 &= 0\hat{\mathbf{i}} + 0\hat{\mathbf{j}} + 0\hat{\mathbf{k}} \\
\mathbf{r}_2 &= \frac{c_l}{2}\hat{\mathbf{i}} + \frac{c_l}{2}\hat{\mathbf{j}} + 0\hat{\mathbf{k}} \\
\mathbf{r}_3 &= 0\hat{\mathbf{i}} + \frac{c_l}{2}\hat{\mathbf{j}} + \frac{c_l}{2}\hat{\mathbf{k}} \\
\mathbf{r}_4 &= \frac{c_l}{2}\hat{\mathbf{i}} + 0\hat{\mathbf{j}} + \frac{c_l}{2}\hat{\mathbf{k}}
\end{aligned}$$

1.2 Task e: Computing forces

We will be using the Lennard-Jones potential to approximate the forces between the molecules, which work quite well, given it's simplicity, for neutral particles, especially noble gases, as we are dealing with in this study [1]. The formula is given below.

$$U(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$$

At short distances the term to the twelfth power dominates and represents a repulsive force, Paulie exclusion principle, while at longer distances the term to sixth power dominates and represents the attractive van der Waal force. The σ is the distance at which the potential is 0, while ϵ is the depth of the well. $\sigma = 3.405$Å and $\varepsilon/k_B = 119.8$K are chosen to fit the physical properties of the system for Argon.
The force felt between the molecules is given by the negative gradient of the potential.

$$\mathbf{F}(r_{ij}) = -\boldsymbol{\nabla} U(r_{ij})$$

The potential only has a nonzero derivative along $\mathbf{r}_{ij}$, the axis between then particles, so it is natural to evaluate the gradient in that coordinate system before projecting it onto the xyz coordinates used by the program.

$$\begin{aligned}
\mathbf{F}(r_{ij}) &= -4\epsilon \partial_{r_{ij}} \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right] \hat{\mathbf{r}}_{ij} \\
\mathbf{F}(r_{ij}) &= -4\epsilon \left[-\frac{12}{r_{ij}} \left(\frac{\sigma}{r_{ij}} \right)^{12} + \frac{6}{r_{ij}} \left(\frac{\sigma}{r_{ij}} \right)^{6} \right] \hat{\mathbf{r}}_{ij} \\
\mathbf{F}(r_{ij}) &= 24\epsilon \left[2 \left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right] \frac{\mathbf{r}_{ij}}{r_{ij}^2} \\
m_i \frac{\partial^2 r_i}{\partial t^2} &= \sum_j 24\epsilon \left[2 \left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right] \frac{\mathbf{r}_{ij}}{r_{ij}^2}
\end{aligned}$$

1.3 NonDimensionality

Now we introduce some new units to get a nondimensional equation of motion. $\begin{cases} r & \to \sigma r' \\ t & \to \tau t' \end{cases}$

$$\begin{aligned}
m_i \frac{\partial^2 \sigma r'_i}{\partial (\tau t')^2} &= \sum_j 24\epsilon \left[2 \left(\frac{\sigma}{\sigma r'_{ij}} \right)^{12} - \left(\frac{\sigma}{\sigma r'_{ij}} \right)^{6} \right] \frac{\sigma \mathbf{r}'_{ij}}{\sigma^2 r'^2_{ij}} \\
\frac{\partial^2 r'_i}{\partial (t')^2} &= \frac{24\epsilon\tau^2}{m_i \sigma^2} \sum_j \left[2 \left(\frac{\sigma}{\sigma r'_{ij}} \right)^{12} - \left(\frac{\sigma}{\sigma r'_{ij}} \right)^{6} \right] \frac{\mathbf{r}'_{ij}}{r'^2_{ij}}
\end{aligned}$$

Choosing $\tau = \sigma\sqrt{m/\varepsilon}$ then gives the dimensionless equation

$$\frac{\partial^2 r_i'}{\partial(t')^2} = 24\sum_j \left[2r_{ij}'^{-12} - r_{ij}'^{-6}\right] r_{ij}'^{-2}\mathbf{r}_{ij}'$$

1.3.1 Algorithm to implement force

The implementation of the force will be along the following steps:

- Find vector between the two particles $\mathbf{r}_{ij} = \mathbf{r}_i' - \mathbf{r}_j$
- Calculate $r_{ij}'^2$, $r_{ij}'^6$ and $r_{ij}'^{12}$ for a particle pair
- Calculate the modified force $24\sum_j \left[2r_{ij}'^{-12} - r_{ij}'^{-6}\right] r_{ij}'^{-2}\mathbf{r}_{ij}'$
- Add the force to both particles force account, halves the necessary computations. One positive one negative

A Unit scheme

We want to use a unit system so all the numbers are computed on a unity scale, this ensures that there will be no overflow and it is easy to check that the number are approximately correct.

The program uses a more natural set of units which let's Boltzmann's constant be 1.

$$\begin{aligned}
1 \text{ mass unit } &= 39.948 \text{ a.m.u } = 39.948 \times 1.661 \times 10^{-27} \text{ kg} && (1)\\
1 \text{ length unit } &= 3.405 \text{ Å} = 3.405 \times 10^{-10} \text{ m} && (2)\\
1 \text{ energy unit } &= 1.651 \times 10^{-21} \text{ J} && (3)\\
1 \text{ temperature unit } &= 119.735 \text{ K} && (4)
\end{aligned}$$

All the other units are then expressed in term of these units.

Boltzmann constant translates between temperature and energy, in SI-units it is $k_B = 1.381 \times 10^{-23}$ J K^{-1}, which in the previously defined units becomes

$$k_B = 1.381 \times 10^{-23} \left(\text{ J K}^{-1}\right) \left(\frac{\text{energy unit}}{1.651 \times 10^{-21} \text{ J}}\right) \left(\frac{119.735 \text{ K}}{\text{temperature unit}}\right) \tag{5}$$

$$k_B = 1 \, \frac{\text{energy unit}}{\text{temperature unit}} \tag{6}$$

References

[1] Wikipedia `http://en.wikipedia.org/wiki/Lennard-Jones_potential`.