Exercise 5 – Computational Materials Engineering

Prof. M. Moseler – WS 2020/2021

Goals:

- Understand the calculation of forces.
- Understand how the time step in molecular dynamics works.

In lecture 3, the forces on atom K for a system of N atoms interacting via the superposition of pairwise Morse potentials was found to be

$$\vec{F}_K = -\sum_{\substack{J=1 \\ J\neq K}}^{N} \frac{du_M(R_{KJ})}{dR_{KJ}} \quad \frac{\overrightarrow{R_{KJ}}}{R_{KJ}}, \tag{1}$$

where

$$u_M(R) = D_0\left[e^{-2\alpha(R-R_0)} - 2e^{-\alpha(R-R_0)}\right]. \tag{2}$$

It is recommended to create a new directory for this exercise and save all the scripts in that folder.

Tasks

Task 1: Consider two particles 1 and 2 with positions $\vec{r}_1 = (0,\ 0,\ z_1)$, $\vec{r}_2 = (0,\ 0,\ z_2)$ and calculate the force vectors acting on both atoms by evaluating equation (1) for $z_1 = 0$, $z_2 = 0.5$ and $D_0 = 1$ eV, $\alpha = 1\ \text{Å}^{-1}$ and $R_0 = 1$ Å .

Task 2: Download *dimer.py* and *MorseCalculator.py* from ILIAS. *MorseCalculator.py* contains the information how the energy and forces are calculated. You need to save the file in the same folder as *dimer.py*. Open and run *dimer.py*. Try to understand what it does. Compare the forces the script calculates with the forces that you obtained in Task 1.

Task 3: As we now know how forces are calculated, we have all ingredients to do a molecular dynamics simulation using the velocity-Verlet propagator as discussed in lecture 4. Before we perform the actual simulation, we calculate manually what to expect. Use the formulae

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \vec{v}_i(t)\Delta t + \frac{1}{2}\frac{\vec{F}_i(t)}{m_i}\Delta t^2 + O(\Delta t^3) \tag{3}$$

$$\vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \frac{1}{2}\frac{\vec{F}_i(t)+\vec{F}_i(t+\Delta t)}{m_i}\Delta t + O(\Delta t^3) \tag{4}$$

to determine the velocities and positions of a dimer after a single time step of *1 fs*. The dimer has the initial positions $\vec{r}_1 = (0,\ 0, 0)$, $\vec{r}_2 = (0,\ 0,\ 0.5)$**,** interacts via the Morse potential from Task 1 and has zero initial velocity. The mass of each atom is 1.008 *u* (unified atomic mass unit).

Note: Handling the units correctly is tricky. If you use the units as given during this exercise sheet, it might be useful to know that the conversion factor from $[\frac{\text{eV}}{\text{Å}\,u}\ \text{fs}^2]$ to [Å] and from $[\frac{\text{eV}}{\text{Å}\,u}\ \text{fs}]$ to $[\frac{\text{Å}}{\text{fs}}]$ is approximately 0.00964853322 (these are useful for the "$\frac{\vec{F}_i(t)}{m_i}\Delta t^2$ " and the " $\frac{\vec{F}_i(t)}{m_i}\Delta t$" terms).

Task 4: Download, open, understand and run the *dimer_dynamics.py* script. You need to download the *Verlet.py* script and save it in the same folder. Compare the values that the script prints to your screen with the values that you calculated in Task 3.

Task 5: Open *Verlet.py* and try to understand the implementation of the velocity-Verlet algorithm (i.e. everything that is written below "*def step(self, f=None)*").

Results:

Task1:

$$\vec{F}_K = -\sum_{\substack{J=1 \\ J\neq K}}^{N} \frac{du_M(R_{KJ})}{dR_{KJ}} \quad \frac{\overrightarrow{R_{KJ}}}{R_{KJ}}$$

$$u_M(R) = D_0\left[e^{-2\alpha(R-R_0)} - 2e^{-\alpha(R-R_0)}\right]$$

Calculation for k=2, j=1 (N=2, k ≠j) [Force acting on the second atom]

$$\vec{F}_2 = -\frac{du_M(R_{21})}{dR_{21}} \quad \frac{\overrightarrow{R_{21}}}{R_{21}}$$

Calculate Components of the formula:

$$\overrightarrow{R_{21}} = \begin{pmatrix} 0\text{Å} \\ 0\text{Å} \\ 0.5\text{Å} - 0\text{Å} \end{pmatrix} = \begin{pmatrix} 0\text{Å} \\ 0\text{Å} \\ 0.5\text{Å} \end{pmatrix}$$

$$R_{21} = \sqrt{\left(R_{21x}\right)^2 + \left(R_{21y}\right)^2 + (R_{21z})^2}$$

$$R_{21} = \sqrt{(R_{2x} - R\_1x)^2} = \sqrt{\left(0\text{Å} - 0.5\text{Å}\right)^2} = 0.5\text{Å}$$

$$\frac{du_M(R_{KJ})}{dR_{KJ}} = D_0 2\alpha\left[-e^{-2\alpha(R-R_0)} + e^{-\alpha(R-R_0)}\right]$$

Insert calculated components and values ($z_1 = 0, z_2 = 0.5$ and $D_0 = 1$ eV, $\alpha = 1$ Å^{-1} and $R_0 = 1$ Å):

$$\vec{F}_2 = -\frac{du_M(R_{21})}{dR_{21}} \quad \frac{\overrightarrow{R_{21}}}{R_{21}}$$

$$\vec{F}_2 = -1eV\ 2\ \text{Å}^{-1}\left[-e^{-2\text{Å}^{-1}(0.5\text{Å}-1.0\text{Å})} + e^{-\text{Å}^{-1}(0.5\text{Å}-1.0\text{Å})}\right]\begin{pmatrix} 0\text{Å}/0.5\text{Å} \\ 0\text{Å}/0.5\text{Å} \\ 0.5\text{Å}/0.5\text{Å} \end{pmatrix}$$

$$\vec{F}_2(t) = \begin{pmatrix} 0\ \text{eV/Å} \\ 0\ \text{eV/Å} \\ 2.139\ \text{eV/Å} \end{pmatrix}$$

The force is acting towards positive z-direction on the second atom. Carry out the same computation with k=1, j=2 (N=2, k ≠j) [Force acting on the first atom]:

$$\vec{F}_1(t) = \begin{pmatrix} 0\ \text{eV/Å} \\ 0\ \text{eV/Å} \\ -2.139\ \text{eV/Å} \end{pmatrix}$$

The only difference is the $\overrightarrow{R_{12}}$ vector: $\overrightarrow{R_{12}} = \begin{pmatrix} 0\text{Å} \\ 0\text{Å} \\ 0\text{Å} - 0.5\text{Å} \end{pmatrix} = \begin{pmatrix} 0\text{Å} \\ 0\text{Å} \\ -0.5\text{Å} \end{pmatrix}$

Task 3: Velocity verlet procedure:

1. Calculate new positions $\overrightarrow{r_1}(t+\Delta t), \overrightarrow{r_2}(t+\Delta t)$ [using formula 3]
2. Calculate new forces $\overrightarrow{f_1}(t+\Delta t), \overrightarrow{f_2}(t+\Delta t)$ [same procedure than Task1]
3. Calculate new velocities $\overrightarrow{v_1}(t+\Delta t), \overrightarrow{v_2}(t+\Delta t)$ [using formula 4]

1) $\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \vec{v}_i(t)\Delta t + \frac{1}{2}\frac{\vec{F}_i(t)}{m_i}\Delta t^2 + O(\Delta t^3)$

$$\vec{r}_1(t+1fs) = \begin{pmatrix} 0\text{Å} \\ 0\text{Å} \\ 0\text{Å} \end{pmatrix} + 0\frac{\text{Å}}{fs}\,\Delta t + \frac{1}{2}\frac{\begin{pmatrix} 0\ \text{eV/Å} \\ 0\ \text{eV/Å} \\ -2.139\ \text{eV/Å} \end{pmatrix}}{1.008u}(1\text{fs})^2\ 0.0096485\frac{\text{Å u}}{eV\ fs^2}\ \text{Å} + O(\Delta t^3)$$

$0.0096485\frac{\text{Å u}}{eV\ fs^2}$ Å is the conversion to Å.

$$\vec{r}_1(t+1fs) = \begin{pmatrix} 0\text{Å} \\ 0\text{Å} \\ -0.010237\text{Å} \end{pmatrix}$$

Same procedure for $\vec{r}_2(t+1fs)$

$$\vec{r}_2(t+1fs) = \begin{pmatrix} 0\text{Å} \\ 0\text{Å} \\ 0.510237\text{Å} \end{pmatrix}$$

2) $\vec{F}_K = -\sum_{\substack{J=1 \\ J\neq K}}^{N} \frac{du_M(R_{KJ})}{dR_{KJ}} \quad \frac{\overrightarrow{R_{KJ}}}{R_{KJ}}$

$$\vec{F}_1(t+\Delta t) = \begin{pmatrix} 0\ \text{eV/Å} \\ 0\ \text{eV/Å} \\ -1.98783\ \text{eV/Å} \end{pmatrix},\ \vec{F}_2(t+\Delta t) = \begin{pmatrix} 0\ \text{eV/Å} \\ 0\ \text{eV/Å} \\ 1.98783\ \text{eV/Å} \end{pmatrix}$$

3) $\vec{v}_i(t+\Delta t) = \vec{v}_i(t) + \frac{1}{2}\frac{\vec{F}_i(t)+\vec{F}_i(t+\Delta t)}{m_i}\Delta t + O(\Delta t^3)$

$$\vec{v}_1(t+1fs) = 0\frac{\text{Å}}{fs} + \frac{1}{2}\frac{\begin{pmatrix} 0\ \text{eV/Å} \\ 0\ \text{eV/Å} \\ -2.139\ \text{eV/Å} \end{pmatrix} + \begin{pmatrix} 0\ \text{eV/Å} \\ 0\ \text{eV/Å} \\ -1.98783\ \text{eV/Å} \end{pmatrix}}{1.008\,u}1\text{fs}\ 0.0096485\frac{\text{Å u}}{eV\ fs}\ \frac{\text{Å}}{fs} + O(\Delta t^3)$$

$$\vec{v}_1(t+1fs) = \begin{pmatrix} 0\frac{\text{Å}}{fs} \\ 0\frac{\text{Å}}{fs} \\ -0.01975\frac{\text{Å}}{fs} \end{pmatrix}, \text{ analogous } \vec{v}_2(t+1fs) = \begin{pmatrix} 0\frac{\text{Å}}{fs} \\ 0\frac{\text{Å}}{fs} \\ 0.01975\frac{\text{Å}}{fs} \end{pmatrix},$$