Exercise 5 – Computational Materials Engineering

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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)*").