Exercise 2 – Computational Materials Engineering

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Goals:

- Understanding the Morse potential.
- Getting acquainted with the software.

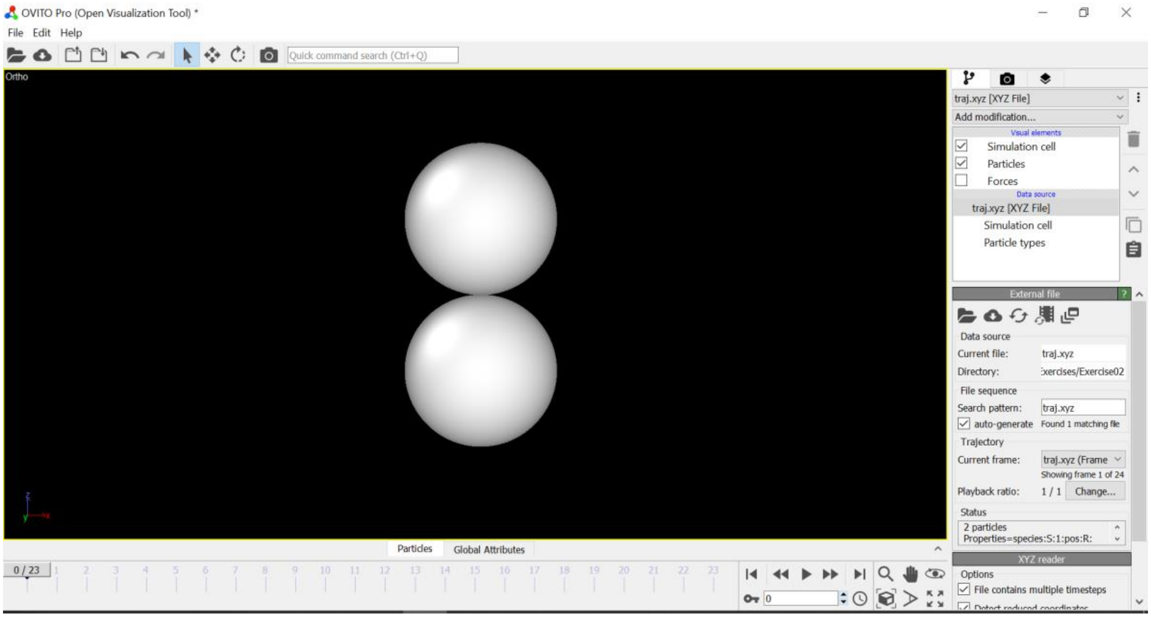
In many cases the Morse potential is a convenient model for the interaction of two particles. For two particles separated at a distance R it is given by

$$U_M(R) = D_0\left[e^{-2\alpha(R-R_0)} - 2e^{-\alpha(R-R_0)}\right]. \tag{1}$$

D_0, α and R_0 are parameters, whose meaning will hopefully be clarified during this sheet.

Tasks

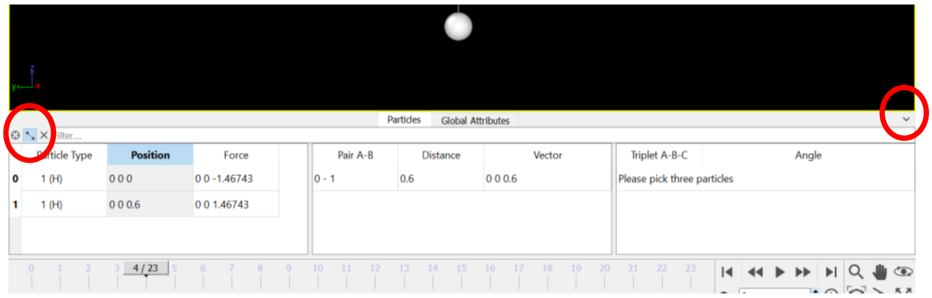
Task 1: OVITO is a scientific visualization tool for atomistic and particle simulation data. Download the *traj.xyz* file from ILIAS and open it with OVITO (File → Load file). Mark the checkbox “File contains time series”.



Task 2: Visualize the movement of the particles by using the “Play animation” button.

Task 3: Play around with OVITO. Change the color, the radius and the shape of the particles.

Task 4: Measure the distance between the particles. For this purpose, open the Data Inspector under the visualization window by clicking the tab bar. Click the *Show distances and angles* button on the left. Select particles with the button *Select in viewports* (ctrl + mouseclick)



(Version 2.9: Use the “Inspect particles” tool under “Utilities” (the hammer symbol) and select both particles.)

Task 5: The energy of the two particles depends on their distance. Use formula (1) with $D_0 = \alpha = R_0 = 1$ to explicitly calculate the energy of the system for $R = \{0.5, 1.0, 1.5\}$. Interpret the results.

Task 6: *traj.xyz* is a simple text file that contains all the information that OVITO displays. Open *traj.xyz* with Spyder and try to understand what is written in the file. Can you spot the energies that you calculated in Task 5?

Task 7: *traj.xyz* was created using the “Atomic Simulation Environment” (ASE). ASE is a set of tools and Python modules for setting up, manipulating, running, visualizing and analyzing atomistic simulations. Download *morse.py* from ILIAS and open it with Spyder. Try to understand what it does.

Task 8: Adjust the parameters of the distances array (line 22) and rerun the Python script (Play button in Spyder) such that the created *traj.xyz* only consists of three images at the distances $R = \{0.5, 1.0, 1.5\}$. Visualize the newly created file with OVITO.

Task 9: Compare the energies that the Python script calculates and prints with your manually calculated values from Task 5.

Task 10: Matplotlib is a Python plotting library which produces publication quality figures. Uncomment the plt.plot(…) command (i.e., remove the hash-sign at the beginning of the line) and rerun the script to create an energy-distance diagram. Vary again the parameters of the distances array.

Task 11: Try to understand the meaning of the parameters of the Morse potential by rerunning the script with varied parameters. You can fix the limits of the y-axis of the plot using the command *plt.ylim([-1.2, 0.5])*.

Task 12: Prove the meaning of D_0, α and R_0 you suspect from Task 11 by explicitly calculating the derivatives of the Morse potential with respect to R.

Task 13: Feel free to further play around with OVITO (https://www.ovito.org/manual/) and Python (https://www.python.org/) including ASE (https://wiki.fysik.dtu.dk/ase/), matplotlib (https://matplotlib.org/) and numpy (https://numpy.org/).