Exercise 02

Force Fields

Deadline: Please hand in your protocol in **pdf format** by **Thursday, 18th May, 10.15 a.m.** to **stevan.aleksic@fu-berlin.de**. The proctol should contain analytical solutions, short discussions, Python code, and plots.

2.1 Lenard-Jones Potential (30 Points)

Non-binding interactions are often modeled with a Lenard-Jones potential according to the following equation:

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

where r is the distance between two atoms, and constants σ, and ϵ depend on the given atom types.

1. Estimate the distance r_m at which the potential energy is minimal. (**7 Points**)
2. Sketch the potential. Explain the mathematical, and physical implications of a such plot. (**8 Points**)
3. Approximate Lenard-Jones potential with a Taylor series for $r = r_m$ for the first three terms. What is the value of the second derivative of the potential $U''(r = r_m)$? (**8 Points**)
4. How can one construct a harmonic oscillator potential in order to approximate L-J U(r)? What is the value of respective force constant? (**7 Points**)

2.2 Water Force Field (30 Points)

Consider a typical modeling of a water dimer in the terms of a classical force field representation. Atoms are annotated as follows : H_1 - O_2 - H_3 , and H_4 - O_5 - H_6.

1. Provide all the terms of a force field representing the binding interactions between two water molecules. (**6 Points**)
2. Provide all the terms of a force field representing the non-binding interactions between two water molecules. (**6 Points**)
3. In which energy range would you place the different force field terms (1 kJ/mol, 10 kJ/mol, 100 kJ/mol)? (**6 Points**)
4. How would you model the tetraedric coordination between water molecules? (**4 Points**)
5. How does the number of binding, and non-binding interactions increase with the increasing number N of the water molecules in a system? What are the difficulties in computation of interactions for a very big number N of water molecules? What is solution to this problem? (**8 Points**)

2.3 Critical Points of the Pontential Energy Surface (40 Points)

Consider the following function in 2D space:

$$U(r) = (r_x^2 - 1)^2 + \frac{5}{4}\left(r_y - \frac{1}{2}r_x\right)^2$$

1. Calculate the gradient, and the Hessian matrix of the function U(r) ? (**10 Points**)
2. Provide the location of the all critical points. (**4 Points**)
3. Characterize the critical points as minima, maxima, or saddle points. (**6 Points**)
4. Write a Python script which plots this function as a 3D potential energy surface. Provide 2D projection of the 3D potential energy suface as a contour plot , and mark all the critical points. (**20 Points**)