Molecular Dynamics Project

FYS-MEK1110 - Mechanics

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Part 1: 2-atom model

Bare legger en liten mal her på oppgavene jeg har programmert så langt. Veldig overfladisk oppgavetekst, kan og bør endres underveis.

a)

Plot the LJ-potential curve. What does the different terms in the potential do?

b)

Find the force corresponding to the potential from a), and plot the result. For what distance r is this force 0? Is this force conservative? *What's different with this force compared to say Newton's Law of gravitation?*

c)

Say we place one atom at $\vec{r_1} = [0, 0, 0]$ and the other at $\vec{r_2} = [1.5, 0, 0]$, with no initial velocities. Describe qualitaively what the motions of the atoms will look like. Support your arguments with the LJ potential curve.

If we place the second atom at $\vec{r_2} = [0.95, 0, 0]$ instead, what do you expect then? Explain by again using the potential curve from task a).

d)

Develop a code to simulate a system of two atoms with the LJ-forces being the only ones acting. Use the Euler-Cromer integration method (?). Simulate the system with the initial conditions (both cases) from task c), and plot the distance between the atoms r as a function of time. What do you see?

e) (optional)

Download a visualization tool (i.e. Ovito), and write a function that writes the positions of the atoms at every time step to a xyz.-file. Load this file into *Ovito* and describe what you see. Does this fit well with the assumptions you made in task c) ?

f)

Implement different integration methods so that you have the Euler, Euler-Cromer and Velocity-Verlet methods available for your simulations. Run simulations with the same initial conditions as in the

first case in task c) ($\vec{r_1} = [0, 0, 0]$, $\vec{r_2} = [1.5, 0, 0]$) for all three methods, and plot the mechanical energy for all three with $\Delta t = 0.01$. Compare the results for all three methods. How does these methods perform in terms of energy conservation?

a) g) (I tvil om denne skal med)

Run simulations for all three methods implemented in the previous task, and find the an approximation to the largest time step (Δt) required to keep the integration from exploding. Whats the difference between these methods, and why does some of them perform better than others?

Part 2: N-atom model

Part 3: Let's do some science!