FYS-4096 Computational Physics: Exercise 12

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Week 16

General:

- You should have access to `ex12_help` on teacher's repo.
- There you will find, e.g., files `md_simple.py` that will most likely be useful in this exercise.
- **Deadline before noon on Monday April 26!**

Problem 1: Lennard-Jones potential

- Lennard-Jones potential can be expressed as

$$u_{\mathrm{LJ}}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]. \tag{1}$$

a) Analytical derivations (pen and paper, LaTeX, etc.):

  - Find the distance $r = r_{\min}$ where the potential has its minimum value. What is the value of the potential at that specific point?
  - Derive the analytical expression for the force due to the Lennard-Jones potential.
  - Notice: You should get $r_{\min} = 2^{1/6}\sigma$ and $u_{\mathrm{LJ}}(r_{\min}) = -\epsilon$, but you need to derive the expression for $r_{\min}$ and use that to calculate $u_{\mathrm{LJ}}(r_{\min})$.

b) Numerical visualization:

  - Define Lennard-Jones parameters (i.e., σ and ϵ) for the H-H interaction based on the equilibrium distance $1.4a_0$ and dissosiation energy 0.1745 Hartree of H_2 molecule.
  - Plot the potential and force as a function of r.

- Include the derivations and relevant figure(s) to your repository.

Problem 2: Molecular dynamics code

- Study `md_simple.py` to understand the basic structure and modify the necessary parts in order to make it work for solving H_2 molecule with Morse potential.
- There should read `# ADD` where something needs to be added.
- Add comments for better understanding, especially for all the `# ADD` parts.
- With the default settings you should get roughly -0.17274 Hartree for the total energy once the code is working correctly (and roughly 0.000877 Hartree for the kinetic energy).
- What are the default settings: update/integration algorithm, boundary conditions, and dimensions of the system?
- Plot the total energy vs. time from the simulation observables. Make figure and add it to your repository.

Problem 3: Adding observables

- Include the calculation of temperature, interatomic distance and heat capacity into your md_simple.py code.
- What values do you get with the default settings?
- Plot the behavior of these observables as a function of time. Add relevant figures to your repository.
- What is the standard deviation of the temperature in your simulation?

Problem 4: Evaluation of performance and feedback

- Answer the following inquiries:
  - Mention two to four new / useful / interesting things you have enjoyed getting more familiar with during the course.
  - Do you think the subjects will benefit you in your future endeavors? Why?
  - How well have you performed in terms of understanding and performance?
  - What has been challenging to you in the course?
  - Have you been able to schedule a suitable amount of time for the course?
  - How would you improve the course and its contents?
- Write the answers into a text file problem4.txt and remember to add the file into your repo. Feel free to be verbal in your response. You may give your answers either in English or in Finnish.

Returning your exercise

1. Make a new folder "exercise12" to your existing Computational Physics repo.
2. Create a file solvedProblems.txt in the "exercise12" folder. Inside it, write a comma separated list of problems you have solved, e.g., 1,2x,4.
3. Make sure all your source files and relevant figures etc. are under version control and push them to GitLab.
4. Push your commits to GitLab before noon on Monday April 26:
   ```
   git push --all && git push --tags
   ```