FYS-4096 Computational Physics: Exercise 12

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General:

- You should have access to `exercise12_help_files` on teacher's repo.
- There you will find, e.g., files `md_simple.py` that will most likely be useful in this exercise.

Problem 1: 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.

Problem 2: Adding observables

- Include the calculation of temperature, interatomic distance and heat capacity.
- What values do you get with the default settings?
- Plot the behavior of these observable as a function of time.
- What is the standard deviation of the temperature in your simulation?

Problem 3: Lennard-Jones potential

- For Lennard-Jones potential

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

show analytically that the minimum is at $r_{\min} = 2^{1/6}\sigma$ and that $u_{\mathrm{LJ}}(r_{\min}) = -\epsilon$.

- Define Lennard-Jones parameters (i.e., σ and ϵ) for the H-H interaction based on the parameters you used in problem 1 with the Morse potential.
- Plot the two potentials and respective forces as a function of r.
- Modify the code to enable usage of Lennard-Jones potential and report the energetics for the default case.

Problem 4: Temperature behaviour

- Using either the Morse or the Lennard-Jones potential consider the temperature dependence of the energetics, interatomic distance and heat capacity.
- That is, calculate the above mentioned observables at about 10 different temperatures, e.g, $T \in [100, 4000]$ Kelvin.
- Plot the observables as a function of temperature and also consider the uncertainty of the temperature (at each temperature).

Returning your exercise

1. Create a new git repo or make new folder to your existing Computational Physics repo.
2. Create a file problems_solved.txt at the root of your "exercise12" git repo. Inside it, write a comma separated list of problems you have solved, e.g., 1,2,3.
3. Make sure all your source files are under version control and push them to GitLab.
4. Tag your final solution (git commit) with "final" tag: `git tag final`
5. Push your commits and the final tag to GitLab before Friday's exercise session:
   `git push --all && git push --tags`
6. Remember to share your GitLab project with the teacher before or right after the final git push. Be careful in providing proper permissions, so that the teacher can also access the data. (Teacher's GitLab account: kylanpaait, ilkka.kylanpaa@tuni.fi).
7. **If you are using the same repo for all exercises, send the teacher an email once you are done with the weeks exercise!**