SC9502B – Scientific Computing. Winter 2024
> *Instructor: Dr. M. Karttunen*

Assignment 1. Due: Mon. Feb. 5, 2024 by 23:59.
See the template(s) for presenting the results + all answers should be returned using GitHub.
Each problem is of equal value.
Use the lecture notes posted on Jan 22, 2024.

1. Lecture notes: Problem 1.1.

2. Read through the lecture notes (the chapters included in the Jan 22 posting). Excluding the typos that have been posted by some you on the Discord channel, find 5 errors (not grammar) in the notes (there are at least 5). They may be in the text, code bits or elsewhere.

3-13. Lecture notes: Problems 5.1-5.11. Each one is a separate problem (=11 problems)

14. Lecture note: Problem 8.1

For the following, return your answer as a Jupyter notebook (.ipynb) [you can and should integrate the answers to the above questions as a part of that same Jupyter notebook but it is also ok to post the above separately as a pdf file]. It should contain both the code, its comments and your explanations. Download the two data sets from the Discord channel posted on Jan 22. The data set are have the names `energy-check-argon-nve-rlist09.xvg` and `energy-check-argon-nve-rlist10.xvg`. Do not rename the files. The two files have data from molecular dynamics simulations of argon. The first column is time in picoseconds and the second column is energy in kJ/mol (the same in both cases).

15. Write a python script to read and plot the data from the two files in one single plot at the level of publication quality. You have examples of this in the lecture notes.

16. Find python package, or write your own code, to fits for the two data sets (linear regression is totally suitable). Justify your choice of method. Plot as above in a single plot

17. Use `pandas`, `numpy` or such to find the statistical descriptors of the data.

18. Plot the distribution (or histogram) of the fluctuations for the case of `energy-check-argon-nve-rlist10.xvg`. Can the data be fitted to a simple distribution (if so, give the usual data descriptors)?