Introduction to Computational Physics SS2023

Lecturers: Rainer Spurzem, Stefan Reißl, Ralf Klessen
Tutors (group number in brackets): Jeong Yun Choi (1), Patricio Alister (2), Vahid Amiri (3), Matheus Bernini Peron (4), Bastián Reinoso (5), León-Alexander Hühn (6), Florian Schulze (7), Marcelo Vergara (8)

Exercise 1 from April 19, 2023
Return before noon of April 28, 2023

1 General Comments

Tutorials take place Friday or Monday afternoon. We recommend that you *work in teams of up to two students*; working alone is allowed but not recommended. Groups 1,2,4,5 are in presence in the CIP pools, and groups 3,6,7,8 are online in zoom rooms with breakout rooms for each team. During the tutorial sessions tutors will answer questions to the current tutorial number n (issued previous Wednesday); they expect you to return on Friday tutorial $n-1$, and will discuss with you the solutions of tutorial $n-2$. Every student should *at least once present some exercise to the group* (either piece of homework or piece of preparation task).

The first tasks of any tutorial sheet should normally be done during the tutorial hours with help and advice from your tutors (preparation tasks). The second part is a homework task, for which you have 9 days to prepare it and solve it. Then please submit the solution of your homework assignment to the tutor in electronic form, *in one single file containing all necessary pieces of your solution, like programs, graphs or tabular values* (do not forget to add all names of your team members).

Preferred way to submit is a PDF file obtained from your python notebook. Your tutor may accept also python notebooks directly, but you should make sure it can run without the need for specialized packages. Do not force the tutor to install specific non-standard packages for it to work. One way to achieve that is to convert the python notebook into a PDF, and hand in the PDF to the tutor. You may use any other computer language, **but** we strongly encourage you to use python (e.g. with Jupyter notebooks).

The main course webpage is given in the footnote[1]. New tutorial sheets, messages and other up-to-date material you will find in the moodle system[2] of Heidelberg University. Tutorial sheets will also be provided in the "uebungen" web system[3] of the Faculty of Physics and Astronomy, via the menu item "Exercise Sheets" ("Übungsblätter"), where you may also submit your solution files, make sure to check this with your tutor.

[1] https://wwwstaff.ari.uni-heidelberg.de/spurzem/lehre/SS23/compphys/compphys.php.en
[2] https://moodle.uni-heidelberg.de/course/view.php?id=16108
[3] https://uebungen.physik.uni-heidelberg.de/v/1637

2 Basic Exercises (PREPARATION WORK)

- Get acquainted with the Unix/Linux operating system. For example the Unix commands ls, cd, ps, less, etc. Also try out a text editor which you can use for programming, e.g. emacs, vi, joe. Start your favourite plotting program and try to plot a few simple functions as in the lecture notes (simple gnuplot can be used for example). If you use a home computer without Linux - make sure you can handle these tasks on your operating system.
- Practice writing a basic computer program and run it (e.g. define some vectors or matrices, add or multiply them, plot some functions, preferrably in a jupyter notebook).
- Consider a simple quadratic equation $x^2 + x + c = 0$. One of the solutions clearly is $x_1 = (-1 \pm \sqrt{1-4c})/2$. Write a simple computer program that writes out this solution for input values $0 \le c \le 1/4$. Experimentally find out how small c has to become before the resulting solution becomes erroneous. Can you find a way to rewrite your program in such a way that these errors do not occur?
- If interested, also try to get acquainted with Mathematica (CIP pool computers should have license). The old lecture manuscript linked a bit down in our static webpage gives some inspirations for it in Sect. 3.2.6. The entire Sect. 3 gives introductory hints to classical programming tools, like compilers, preprocessors, Makefiles, etc. This is **NOT** required anymore for this course, however, you may encounter these issues later in your studies or work.

3 Numerical Integration (HOMEWORK)

In this exercise we will numerically evaluate the integral

$$y_n = y_n(a) = \int_0^1 \left(\frac{x^n}{x+a}\right) dx \; = \; \frac{1}{n} \; - \; a \, y_{n-1} \; .$$

(a) Plot the integrand for $a = 5$ and $n = 1, 5, 10, 20, 30, 50$ in the domain $0 \le x \le 1$. (7 points)

(b) Write a computer program that reads the value of a, the starting values n_0 and y_0, and the final value n_1, and performs the iteration from n_0 to n_1 (either backward or forward, depending on whether $n_1 < n_0$ or $n_1 > n_0$). (7 points)

(c) Experiment how this series behaves for iterations from $n_0 = 0$ to $n_1 = 30$ for $y_0 = \ln[(1+a)/a]$ with $a = 5$. Also try starting with $n_0 = 50$ and iterate back to $n_1 = 30$ for any starting value y_0. (6 points)

NOTE, for this and all following homework exercises, which require writing a computer program, it is necessary to submit all parts of the program written by you, together with the results. It must be comprehensible for your tutor how your program generates your results.