Introduction to Computational Physics SS2017

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Exercise 1 from April 19, 2017
Return by noon of April 28, 2017

1 Basic Exercises

Notice: The first part of any tutorial sheet should normally be done during the tutorial hours with help and advice from your tutors. You can also go independently to any CIP pool and work out the tutorial sheets by yourself (but we recommend to work in a group of 2-3 students). Or you may use your own computer. Please note that our tutors can only help with the main programming languages. You are free to use any language, but you may be on your own. Please check with your tutors.

- 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 the plotting program gnuplot and try to plot a few simple functions as in the lecture notes.

- Practice writing a simple computer program in a language of your choice (e.g. C, C++, Fortran, python). Compile the program, as in the lecture, from source code via object code to executable.

- The main lecture webpage is http://wwwstaff.ari.uni-heidelberg.de/mitarbeiter/spurzem/lehre/SS17/compphys/compphys.php.en. New tutorial sheets, messages and other up-to-date material you will find in the course pages in the "Moodle"-System of Heidelberg University: https://uebungen.physik.uni-heidelberg.de/uebungen/liste.php?vorl=748.

- Use the gnuplot tutorial (Section "More Info" on Lecture Webpage) to do some exercises on how to plot data - you can use the example datafile "myfile.txt").

- 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 $0 \leq c \leq 1/4$. 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?

- Start Mathematica and start experimenting with it. Make plots of simple functions, solve quadratic or cubic equations. How does Mathematica behave when solving $x^2 + x + c = 0$ for very small c?

- Also, try to get acquainted with python.

2 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 $0 \leq x \leq 1$. (7 points)

(b) Write a compute 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 iteration from $n_0 = 0$ to $n_1 = 30$ for $y_0 = \log[(1 + a)/a]$ 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)

3 Some General Comments

General comments, also valid for future exercises:

- Please hand in the computer programs, graphs or tabular values (if no graphs are required) by email to the Tutor(s).
- Do this by making a PDF document containing all these items using latex. You can use the template provided by the tutors.
- One document per group is sufficient.
- Please write the names of the group members in the document.
- Tutorials are grouped together on Friday and Monday the following week.