Tutorial Introduction to Computational Physics SS2012

Lecturers: Ralf Klessen & Rainer Spurzem

Tutors: Tobias Brandt & N.N.

Sheet 1 (April 18, 2012)

Return by noon of April 25, 2012)

1 Basic Exercises – use Script Chapters 1-3 for help and reference

- 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-90). Compile the program, as in the lecture, from source code via object code to executable.
- 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"). See Links on http://www.ari.uni-heidelberg.de/lehre/SS12/compphys/compphys.php.en
- 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?

2 Numerical Integration (homework)

In this exercise we will numerically evaluate the integral

$$y_n = y_n(a) = \int_0^1 dx \frac{x^n}{x+a} = \frac{1}{n} - a y_{n-1}$$

- 1. (7 pt) Plot the integrand for $a = 5$ and $n = 1$, 5, 10, 20, 30, 50 in the domain $0 \leq x \leq 1$.
- 2. (7 pt) 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 $n_1 > n_0$).
- 3. (6 pt) 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.

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 suchcient.
- Please write the names of the group members in the document.