Computational Physics I

Dr. S. Recksiegel — Winter Term 2024/25

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Lecture Moodle: https://www.moodle.tum.de/course/view.php?id=101063

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1. **Account**

   Make sure that you can login to the computers in the CIP pool room. As a physics student, your TUM login (ga12abc) and password will give you access. If you are not a physics student, please send an email to cipadmins@ph.tum.de to have your account enabled for the CIP pool.

2. **Mathematica**

   Find out how to start Mathematica and look at the Tutorial at
   `http://users.ph.tum.de/srecksie/teaching/mathematica.nb`

3. **C**

   Write and compile a simple C program that prints some message on the screen. Do not worry if you have no programming experience, the tutors will help you and explain exactly what to do. If you do not have a favourite editor or IDE yet, we recommend that you have a look at the program `geany`, which is easy to use for beginners but still has a lot of features. (If geany's output window does not open, make sure you have something like `/usr/bin/xterm -e "/bin/sh %c"` in Preferences → Tools → Terminal.)

   If you have no idea what to write, use the source code below.

```c
#include <stdio.h>
int main() {
        printf("Hello World!\n");
        return 0;  }
```

The following exercises will be discussed on October 22, 2024. You should try to solve them on your own before that date.

1. **Recursion relations**

   Reproduce the evaluation of the integral

$$p_n = \int_0^1 \mathrm{d}x\, x^n e^x$$

   via recursion in both directions as shown in the lecture. Compare your results with those obtained using Mathematica and `NIntegrate`.

2. **Machine precision**

   Determine the approximate machine precision in the following way: Declare `floats` `eps` and `x`, set `eps=1` and repeat the following steps: Divide `eps` by 2, set `x=1+eps`, print out `eps` and `x` and determine when, according to the computer, `x` is equal to 1. Try both `float` and `double`. *Output of floating point numbers to a custom precision using printf:* `printf("%.nf",var);` *where n is the number of digits to be shown –after– the decimal point.**

3. **Truncation of power expansions**

   Compute $\sin x$ for a reasonable value of x via the C-function `sin(x)` (hint: `#include<math.h>` and `-lm`) and via the power expansion of the sin function. Observe what happens when you use higher and higher powers. Try both `float` and `double`.
   $*$ *Advanced problem, if you do not feel challenged enough: Write your data into a file and plot it using* `gnuplot` $*$

4. **Stability of Algorithms**

   Compute one of the roots of

   $$y^2 + 2py - q = 0, \tag{1}$$

   first by the obvious formula

   $$y_1 = -p + \sqrt{p^2 + q},$$

   then by the analytically equivalent, alternative formula

   $$y_1 = \frac{q}{p + \sqrt{p^2 + q}}.$$

   Use the parameters $p = 1000$ and $q = 10^{-10}$. Check the accuracy of the result using the original equation (1). Which algorithm is better? Can you explain why?

5. **Plotting Functions in Mathematica**

   Plot the following functions:

   (a) $f(x) = x^2$

   (b) $f(x) = \ln x$

   (c) $x = 4\cos(\phi) + 2\cos(2\phi), \quad y = 4\sin(\phi) - 2\sin(2\phi), \quad 0 < \phi < 2\pi$
   (hint: `ParametricPlot`)

Practise your C skills:

1. Write a program to output the numbers 1-10, all odd numbers from 1-100, all even numbers from 0-99 and the characters of the alphabet using `for,while` and `do-while` loops. Use each loop structure at least once.

2. Write a program to output the numbers 2,3,5,9,15,23,45,82,94,95,97,99. You should use loops, and `if` or `switch`. **Advanced: Use an array to store the numbers you want to print and iterate over the array.**

3. Write a program to calculate the first few digits of PI using an iterative algorithm. Compare your result to the constant `M_PI` of the C math library (hint: `#include<math.h>` and `-lm`). **Try Wikipedia for algorithms.**

4. **Advanced:* Print out the characters of the sentence *"Without fame, he who spends his time on earth leaves only such a mark upon the world as smoke does on air or foam on water."* in alphabetical order **Hint: use qsort()** Try again with the sentence *"The quick brown fox jumps over the lazy dog."*.