Numerical Methods in Physics WS 2013/2014

2 VL (515.421) + 2 UE (515.422)

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Time and place of the lecture:

Lect. (VL)   Tuesday, 8:30 to 10 a.m.
        Begin: Tuesday, 1st October 2013
        Seminarraum TDK PHEG016

Exercises (UE)   Tuesday (depending on group)
        Begin: Tuesday, 1st October 2013
        Computerraum Physik EG

Motivation and scope of this lecture

Learn the most important methods of "computational physics" and their application to the solution of non-trivial physical problems.

Lecture

The <u>main lecture</u> (Vorlesung) offers an introduction to the most important subjects of *computational physics*: Linear set of equations, point interpolation, determination of zeroes, eigenvalue problems, initial and boundary condition problems...

The lecture illustrates the basic mathematical principles and the advantages and disadvantages of the different methods, their numerical stability and a critical discussion of the possible methodological and rounding errors.

Script of the lecture:

The script of the lecture "Numerical Methods in Physics", ed. 2013/2014, can be downloaded from the web site from the 1st of october 2013 (English and german edition).

Exams for the lecture:

All the chapters of the script explicitely discussed in the course are material for the exam.

Exercises

In the <u>Exercises</u> of "numerical methods in physics" the students have to solve <u>four</u> numerical exercises. It is a tradition of this lecture to put emphasis on physically interesting problems from different areas of physics.

- It is not possible to cover in the exercises all the themes and methods explained in the script of the lecture, and we will not attempt to do it.

- Each exercise will be introduced by a short script, that can be downloaded from the web page of the couse. This script covers the following points:
  description of the physical problem; suggestion on the numerical methods; possible programming problems; test data; suggestion on how to plot and interpret the results.

Organisation of the exercises

(see also the rules posted on the internet)

- **Tutors** for the exercises:

    Markus Stephan Krammer
    markus.krammer@student.tugraz.at

    Gernot Kraberger   **gkraberger@student.tugraz.at**

    Peter Wriesnik   **peter.wriesnik@student.tugraz.at**

- **General information** about the computer room on the ground floor of the Physics building are available on the internet at the address:

    **http://www.itp.tu-graz.ac.at → Computer Infrastr. →
    users**

    The "Handbuch für Benutzer der Unix und Linux Computer" contains useful information on how to obtain an account for the computer room.

- The **division in groups** will take place in the first hour of the exercise class on1st October 2013.
  Since all students registered for the exercise classes should have access to their own workstation in the computer room participants will be divided into groups of max. 14 students each.

- **Software:**
  The PC's in the computer room of the physics building are equipped with the LINUX operating system.

- **Programming language:**
  Students are free to choose between *C* and *MATLAB*.

- **IMPORTANT:** Experience in the last few years has shown that many students use the numerical exercises to learn a second programming language (typically C); obviously, we have nothing agains this, and the tutors will also try to help in a reasonable way.
  We have to stress however that the lecture "Numerical methods in physics" **is not a programming course**. However, in order to allow you to familiarize yourself with a new programming language, the first exercise will be easier than the rest.

- **A big simplification** for you is that the C version of all the <u>structure charts</u> contained in the script of the main lecture will be uploaded to the internet.

- Students of this lecture who want to realize the exercises in **MATLAB** can use all the special libraries of this programming tool. In this case, we assume that they have at least a basic knowledge of MATLAB.

- In all cases you should have a clear understanding of the structure charts contained in the main script.

- <u>**Requirements for a positive evaluation of the exercise class:**</u>

  You will receive extensive information on this subject in the first lecture and during the exercises.

  The **two basic rules** are the following:

  1. We require a **documented** attendace of at least 10 (out of 15) exercise classes (we will provide signature sheets).
  2. The students are required to succesfully present <u>all</u> 4 problems "at the computer" before the **10th of March 2014**.

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Internet

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- The internet address of the lecture "Numerical methods in physics" is

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http://www.itp.tu-graz.at/LV/boeri/NUM_METH/

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  On this web page you can find:

  - Information about the lecture and exercises.
  - The script of the lecture in pdf format (English and German versions).
  - "Mini-scripts" on different subjects (i.e. a small introduction to LINUX, selected software problems, tips on plotting data, etc) Most of these "mini-scripts" are ASCII-files with extension .txt
  - Material relevant to the single exercises (divided in C und MATLAB):
      Description of the exercises as PS files,
      Software with numerical programs,
      Test data for the problems,
      Demos for the exercises.

- If you have other question, you can ask them during the exercise classes, or require an appointment per email:

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- The structure charts and programs presented in the lecture "numerical methods in physics"are meant as an introduction to the most important methods of *Computational Physics*. For this reason they are formulated very didactically and optimised in terms of computational speed.

  However, in "real" scientific work it is often better to resort to professional software. At the end of each chapter of the script you will find information on how and where to access ready-to-use numerical software on the internet.