

Course Manual PRA1004: Scientific Computing

Period 5

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1 Introduction

Mathematical models form the core of many scientific studies across all academic disciplines. Especially in exact sciences, it is difficult to overstate the role of such models. However, the complexity of such models directly implies the need of computers in order to estimate their parameters and/or use them for prediction. Scientific computation deals with problems that frequently arise when implementing mathematical models on a computer, paying particular attention to issues that arise by making the transition from mathematics to the finite representations used by computers.

This skills provides a first introduction to scientific computing by introducing the students with high-level scientific programming languages like Matlab and Mathematica. It presents a broad overview of numerical methods for solving selected problems in scientific computing, including linear and nonlinear equations, interpolation, differential equations, integration, optimization, random numbers and simulation.

2 General Information

2.1 Course Coordinator

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2.2 Schedule and Location

The course will consist of 6 lab sessions on Fridays 9:00–15:00, at UB 0.204. A detailed schedule of topics is listed in Section 4.

2.3 Text Book & Course Materials

The course will make use of a number of sources, such as handouts with assignments and slides. In addition, it makes use of the following text book:

- *Introduction to MATLAB*. Delores M. Etter. 2nd ed.
<http://amzn.to/X774fX>

Further Recommendations

Many of the method of scientific computing build upon linear algebra. While this course will not go into any detail, I highly recommend everybody who is interested in exact sciences to own a text book on linear algebra. The linear algebra course offered by the Maastricht Science Program uses the following book:

- *Linear Algebra and Its Applications*. David C. Lay. 4th ed.

For students interested in further exploring numerical methods and numerical analysis, I highly recommend the following book for further reading:

- *Numerical Methods. An introduction to Scientific Computing Using MATLAB*. Peter Linz, Richard L.C. Wang.

3 Objectives

This course serves two goals:

1. To make students familiar with the concepts of programming and the get them accustomed with high-level languages like Matlab en Mathematica.
2. To provide an overview of some of the issues and problems that arise in scientific computation, such as (non-)linear systems, numerical and symbolic integration, differential equations and simulation.

After this course the student should be able to understand simple mathematical models and scientific problems (such as finite capacity growth models, fitting a line through data points, etc.) and implement a solution in an adequate scientific programming language (such as matlab, mathematica).

4 Schedule

The proposed schedule is as follows (and subject to changes):

Week	Topic
1	Introduction Mathematica. Difference equations.
2	Introduction Matlab
3	Matrices. Interpolation & Curve Fitting.
4	Integration & Differentiation.
5	Simulation: the simple programming approach to difference equations.
6	Differential Equations

5 Attendance

MSC imposes a 85% attendance requirements on skill courses. This means that you can miss only one session. Also take into account that if you are supposed to show your work for the assignment of previous week (see 'assessment' below), so not being present will lead to a '-' grade, unless the work was already complete and shown in the previous week.

6 Assessment

Students will have to work individually and will be assessed on individual basis. The final grade will be composed of two parts:

1. The grade will for 60% be determined by the assessment (good/neutral/bad) of the explanation of and answering questions about the assignments.
2. The other 40% will be determined by mini-reports about certain parts of the assignments.

Part 1: Explanation of Assignments. Students will be required to show and explain parts of the assignments of the previous lab at the beginning of the next lab. Each assignment will be graded good(+), bad(-) or neutral (0). Additionally, there will be occasional surprise questions which will also be marked (+/0/-). A weighted average of these will form part 1 of the grade. (The following numerical translation will be applied: good=10, neutral=6, bad=2).

Part 2: Hand in of Mini-reports. For a small number (2 or 3) of assignments, students will need to hand in written reports, these count for 40% of the grade. For these assignments, it is important to follow the guidelines and hand in the work in the way described. Not following guidelines will lead to subtraction of points. Also, for these reports, there will be a strict deadline. Failing to hand in work on time will lead to subtractions:

- 0-1 day late: -1
- 1-7 days late: -2
- More than 1 week late: fail, without resit opportunity.

Resit Opportunity At the end of the course there will be the possibility of a 'resit'. This will be in the form of an extra assignment which can increase your final grade with 2 points.

Other Remarks

- The work for this course has to be done individually. While students are encouraged to help each other, copying each others work will not be tolerated.