Numerical Methods for Chemical Engineers
Study guide for 6E5X0, 2016-2017

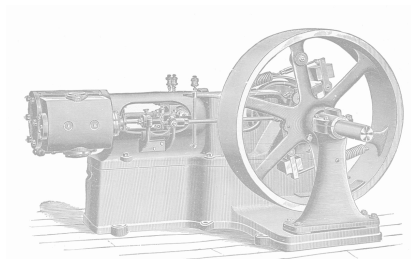Ivo Roghair, Martin van Sint Annaland

Chemical Process Intensification
Eindhoven University of Technology

14 November 2016

Numerical Methods

"Simulation and mathematical modeling will power the twenty-first century the way steam powered the nineteenth."
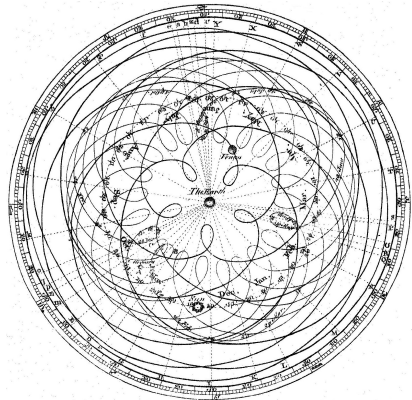
— W.H. Press[*]

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[*]Author of Numerical recipes, in "The Nature of Mathematical Modeling" by Neil Gershenfeld

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Ptolemy and the almagest

~150 AD. Development of numerical approximations to describe the motions of the heavenly bodies with accuracy matching reality sufficiently.

Numerical Methods

- Numerical analysis is concerned with obtaining approximate solutions to problems while maintaining reasonable bounds of error...

- ...because it is often impossible to obtain exact answers ...

- Numerical analysis makes use of algorithms to approximate solutions

Relevance

- Important to the world!
- E.g. in astronomy, construction, agriculture, architecture, ...
- And of course in Engineering!

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...Chemical Engineering...

- Description of reactors and separators (dynamic and steady state)
- Computational fluid dynamics
- Thermodynamic equations of state
- Optimizing process performance
- Design and synthesis of processes
- Regression of data, e.g. isotherms, kinetics, ...

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Course Schedule

Lecture	Date	Topic	Teacher
1	14/11/2016	Programming and algorithms (1)	IR
2	17/11/2016	Programming and algorithms (2)	IR
3	21/11/2016	Numerical errors	IR
4	24/11/2016	Linear eqns: direct methods	IR
5	28/11/2016	Linear eqns: iterative methods	IR
6	01/12/2016	Non-linear equations	MSA
7	05/12/2016	Interpolation + integration	IR
8	08/12/2016	ODEs (1)	MSA
9	12/12/2016	ODEs (2)	MSA
10	19/12/2016	PDEs (1)	MSA
11	22/12/2016	PDEs (2)	MSA
12	12/01/2017	Regression and optimization	IR

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Course Objectives

- Gain experience with programming basics and algorithm design
- Acquire knowledge of and experience with different techniques for the numerical solution of systems of linear and non-linear algebraic and differential equations, as well as data analysis and optimization.
- Being able to solve various numerical problems using Matlab or Excel.

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Prerequisites

The following subjects should give you enough hold-on to follow
this course comfortably:

- Calculus A and B
- Linear Algebra
- Some basic MATLAB experience
    - We will shortly cover some aspects on MATLAB programming
      in the first lectures. Detailed documents and courses are
      provided on Canvas, for your own reference.
- Laptop with Matlab and Excel installed

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Course Materials

- Lecture slides
- MATLAB scripts
- Additional articles
- There are some useful books:
  - Numerical recipes, W.H. Press et al.
  - Numerical methods for chemical engineering, K.J. Beers
  - Numerical methods for chemical engineers, A. Constantinides
  - Essential matlab-for engineers ,B.D. Hahn
  - Introduction to Numerical Methods and Matlab Programming for Engineers, T. Young and M.J. Mohlenkamp

> Look on Canvas for the slides, exercises, scripts, assignments and additional documentation on MATLAB.

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Assessment

5 assignments

- Each 20% of the final result
- Done in groups of 2 persons
  - Form groups via Canvas
  - Make sure that you have similar intentions!
- Short report (template provided, Canvas)
- Resit: 1 assignment + oral exam can be re-done

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About the 5th assignment

- Short assignment + oral exam (in groups)
- Oral exam covers *all assignments and topics*
- Individual knowledge is assessed
- Grade needs to be at least a 5.0

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Assignment grading

We will use rubrics to grade your reports. The following categories will be looked at.

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- Use of numerical methods: e.g. built-in solvers vs. show
  implementation numerical methods

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- Analysis of results: just the number is provided vs. high detail analysis and interpretation
- Programming skills: unstructured code, difficult to change vs. readable code with comments and UI

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- Visualisation: unreadable graphs with no axes labels or legend vs. publication quality graphs, consistency between datasets

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The first assignment will be graded via peer-review.

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Assignment handout and deadlines

Hand-in your assignments via Canvas

- Deadlines are given on Canvas as well
- Deliver the report in PDF format
- Send along the scripts + necessities in a .zip

> When delivering your final assignment, suggest a timeslot for the oral exam (e.g. via Canvas/assignment comment section or as Canvas message).

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Contact information

Ivo Roghair

- Contact via Canvas is preferred!
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- Office: STW 0.37

Martin van Sint Annaland

- E-mail: m.v.sintannaland@tue.nl
- Office: STW 0.39

Ramon Voncken and Alessandro Battistella

For help with the exercises, Ramon and Alessandro (STO 1.28) will help out during the lectures.

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Some last remarks

- Tell us if something is not clear.
- We try to make the lectures interactive, working on examples and creating scripts as we go. Please work along with us to get the most out of this course!
- The exercises are meant to provide a jump start towards the assignments.
- We will always answer questions on the exercises. We may didactically answer questions on the assignments.
- We will distribute the assignments via Canvas. During the lectures/tutorials we first and foremost work on the exercises. If they are done, you can work on the assignment if you want.

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Some Acknowledgements

Some Real Acknowledgements

- To Roel Verstappen of Groningen University
- To Johan Hult of Cambridge University
- To Edwin Zondervan, now at Universitt Bremen