Numerical Methods for Chemical Engineers

Study guide for 6E5X0, 2018-2019

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Chemical Process Intensification
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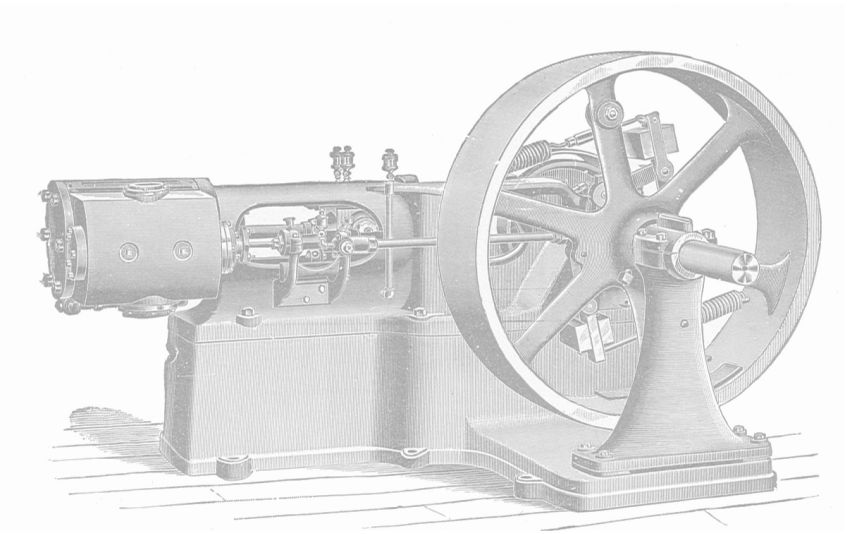
Numerical Methods

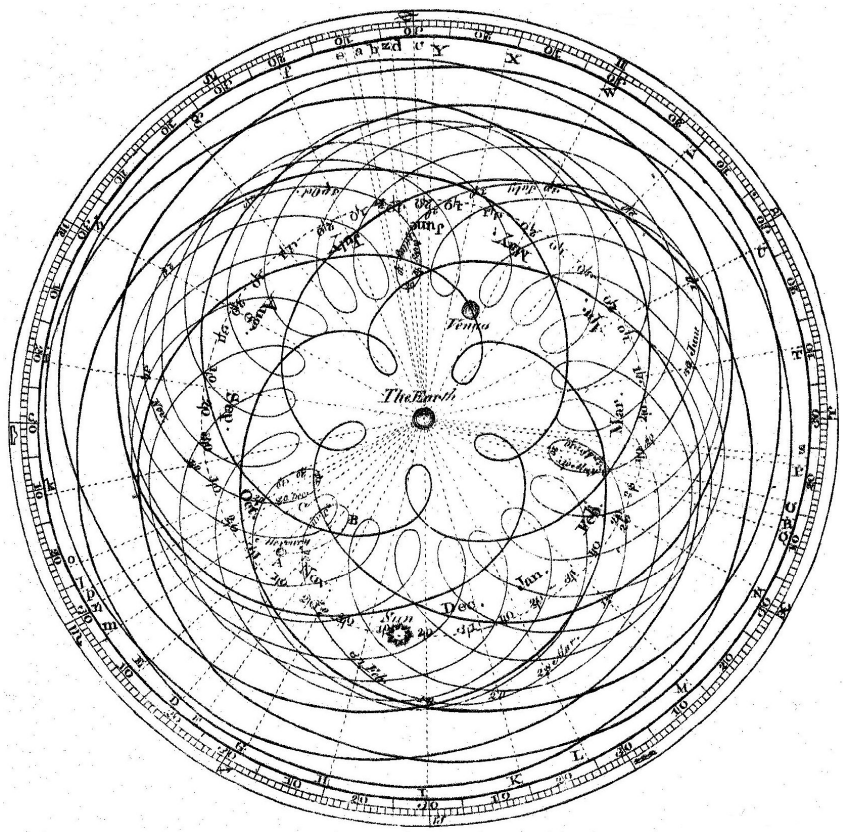
"Simulation and mathematical modeling will power the twenty-first century the way steam powered the nineteenth."

— W.H. Press*



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

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!

...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, ...

Course Schedule

Lecture	Date	Topic	Teacher
1	12/11/2017	Programming and algorithms (1+2)	IR
2	15/11/2017	Numerical errors	MSA
3	19/11/2017	Linear eqns: direct methods	IR
4	22/11/2017	Linear eqns: iterative methods	IR
5	26/11/2017	Non-linear equations (1)	MSA
6	29/11/2017	Non-linear equations (2)	MSA
7	03/12/2017	No lecture	
8	06/12/2017	No lecture	
9	10/12/2017	Interpolation + integration	IR
10	13/12/2017	ODEs (1)	MSA
11	17/12/2017	ODEs (2)	MSA
12	20/12/2017	PDEs	MSA
13	07/01/2018	Q&A session	IR
14	10/01/2018	Regression and optimization	IR

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.

Prerequisites

The following courses should give you enough background knowledge to follow this course comfortably:

- Calculus
- 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.

You will definitely need a laptop with Matlab and Excel installed!

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.

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)

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

Assignment grading

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

- Use of numerical methods: e.g. built-in solvers vs. show implementation numerical methods
- 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
- Visualisation: unreadable graphs with no axes labels or legend vs. publication quality graphs, consistency between datasets

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).

Contact information

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Dario Balice, Francesco Sabatino, Jasper van Kampen

For help with the exercises, Dario, Francesco and Jasper will help out during the lectures.

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. It is advised that you 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.
- 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.

Some Acknowledgements

Some Real Acknowledgements

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