Numerical Methods For Chemical Engineers

Study guide for 6E5X0, 2015-2016

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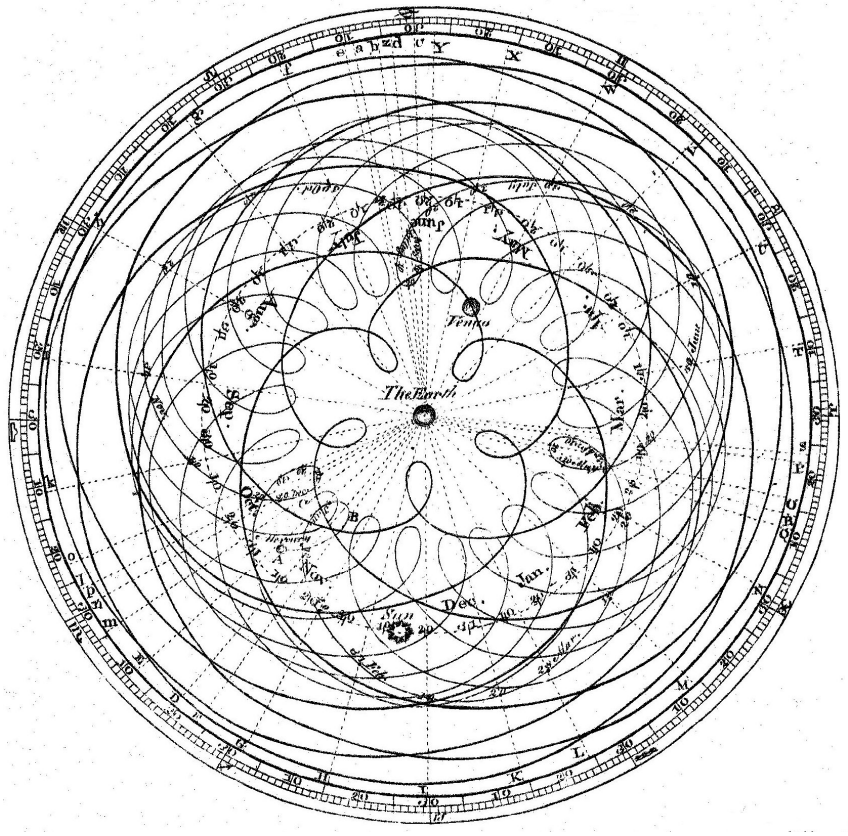
Chemical Process Intensification
Eindhoven University of Technology

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	9/11/2015	Programming and algorithms	IR
2	12/11/2015	Numerical errors	MSA
3	16/11/2015	Linear eqns: direct methods	IR
4	19/11/2015	Linear eqns: iterative methods	IR
5	23/11/2015	Non-linear equations	MSA
6	26/11/2015	Interpolation + integration	IR
7	30/11/2015	ODEs (1)	MSA
8	3/12/2015	ODEs (2)	MSA
9	7/12/2015	PDEs (1)	MSA
10	10/12/2015	PDEs (2)	MSA
	14/12/2015	Guest lecture	Mathworks
11	04/01/2016	Curve fitting and regression	IR
12	07/01/2016	Optimization	IR

Course Objectives

- 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 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 this first lecture. Detailed documents and courses are on OASE, for your own reference.
- Laptop with Matlab and Excel installed

Course Materials

- Lecture slides
- MATLAB scripts
- Additional articles
- Lecture book: A numerical primer for the chemical engineer by Edwin Zondervan (recommended)

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- There are other useful books:
  - Numerical recipes, W.H. Press et al., Cambridge
  - Numerical methods for chemical engineering, K.J. Beers, Cambridge
  - Numerical methods for chemical engineers, A. Constantinides, Prentice hall
  - Essential matlab-for engineers B.D. Hahn

Look on OASE 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 coupled yourselves)
- Results will be addressed in a short report (template provided, OASE)
- Typically 2 weeks for each assignment

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About the 5th assignment

- Consists of an assignment and an oral examination (groups)
- Oral examination covers *all assignments and topics*
- We will assess individual knowledge on the topics
- Mark needs to be at least a 5.0.
- Details on OWinfo

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

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The actual rubrics are provided on OASE (look in Assignments folder). If certain aspects are unclear, feel free to contact us.

Assignment handout and deadlines

Deliver your assignments via e-mail to i.roghair@tue.nl.

- Deliver the report in PDF format
- Name the files NM_X_lastname1_lastname2.pdf (with X the assignment number)
- Send along the scripts+necessities in a .zip

When delivering your final assignment,
suggest a timeslot for the oral exam.

Assignment handout and deadlines

Assignment	Provided	Deadline	Topic
1	9/11/2015	23/11/2015	Programming and algorithms, numerical errors
2	19/11/2015	07/12/2015	Linear and non-linear equations
3	03/11/2015	17/12/2015	ODEs, integration and interpolation
4	10/12/2015	04/01/2016	PDEs
5	04/01/2015	17/01/2016	All topics

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Contact information

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- Office: STW 0.37

Martin van Sint Annaland

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- Office: STW 0.39

Ramon Voncken and Alessandro Battistella

For help with the exercises, Ramon and Alessandro (STW 0.36) will help out during the lectures.
Ramon: r.j.w.voncken@tue.nl
Alessandro: a.battistella@tue.nl

Some last remarks

- This course was transferred to our group only very recently. Please mind there are some sharp edges occasionally.
- 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 jumping start towards the assignments. We will answer questions on the exercises, but not on the assignments.
- We will distribute the assignments via OASE. 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