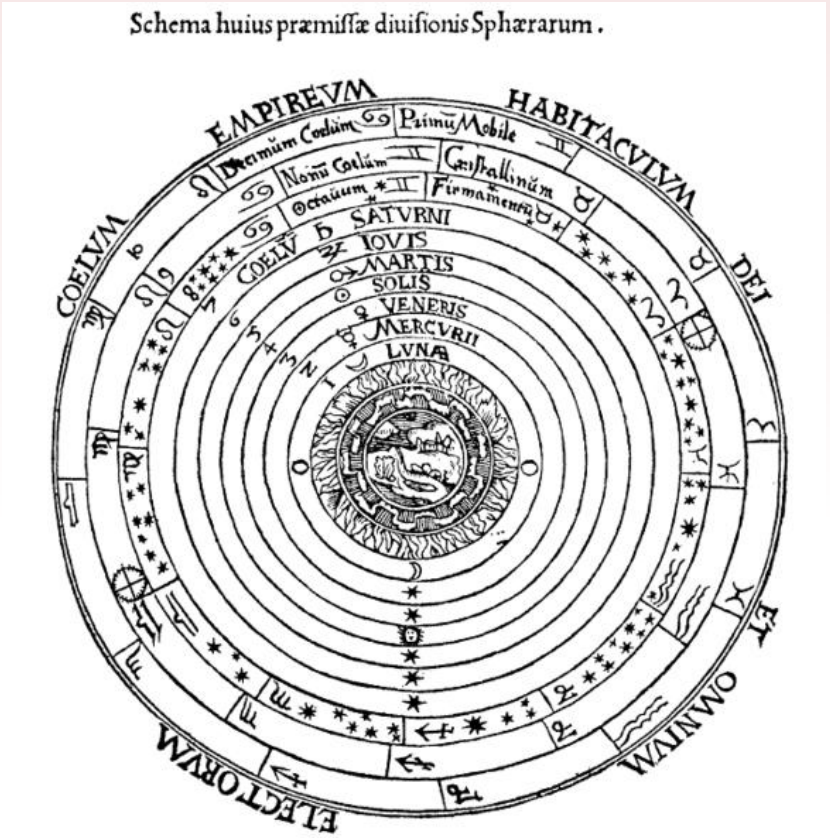
NUMERICAL METHODS FOR CHEMICAL ENGINEERS

Course outline
Autumn 2014

Edwin Zondervan, Ivo Roghair,
Martin van Sint Annaland

PTOLEMY AND THE ALMAGEST



~150 BC – 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

Datum	uur	Wat	Locatie	Onderwerp	Wie
10-nov	1+2	HC	PAV I.10	Intro + programming	IR/EZ
10-nov	3+4	WC	PAV I.10	Intro + programming	IR/EZ
13-nov	5+6	HC	PAV I.10	Errors in computer Simulations	IR
13-nov	7+8	WC	PAV I.10	Errors in computer Simulations	IR
17-nov	1+2	HC	PAV I.10	Linear + Elimination methods	EZ
17-nov	3+4	WC	PAV I.10	Linear + Elimination methods	EZ
20-nov	5+6	HC	PAV I.10	Elimination methods + Iterative methods	EZ
20-nov	7+8	WC	PAV I.10	Elimination methods + Iterative methods	EZ
24-nov	1+2	HC	PAV I.10	Nonlinear equations	IR/EZ
24-nov	3+4	WC	PAV I.10	Nonlinear equations	IR/EZ
27-nov	5+6	HC	PAV I.10	Integrals	IR
27-nov	7+8	WC	PAV I.10	Integrals	IR
1-dec	1+2	HC	PAV I.10	ODE's	MS
1-dec	3+4	WC	PAV I.10	ODE's	MS
4-dec	5+6	HC	PAV I.10	ODE's /PDE's	MS
4-dec	7+8	WC	PAV I.10	ODE's /PDE's	MS
8-dec	**1+2**			**No lecture**	
8-dec	**3+4**			**No lecture**	
11-dec	**1+2**			**No lecture**	
11-dec	**3+4**			**No lecture**	
15-dec	1+2	HC	PAV I.10	Data regression + Optimization	EZ
15-dec	3+4	WC	PAV I.10	Data regression + Optimization	EZ
18-dec	5+6	WC	PAV I.10	Guest lecture	Mathworks
18-dec				**Distribution of last assignment**	-

For the instructions: laptop with MATLAB is needed

COURSE OBJECTIVES

- After the course I hope you'll be able to
  - understand, solve and analyze datasets and different systems of equations (linear equations, nonlinear equations, ordinary differential equations, partial differential equations) using an appropriate programming platform (MATLAB).

PREREQUISITES

- The following subjects should give you enough hold-on to follow this course comfortably:
  - Calculus A and B
  - Linear Algebra

COURSE MATERIALS

- Lecture slides
- MATLAB scripts
- Additional articles
- **Lecture book (A numerical primer for the chemical engineer)**
- There are other useful books
  - Numerical recipes, W.H. Press, 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**

CHAPTERS IN OTHER BOOKS

Lecture:	K.J Beers	W.H. Press
1. Errors in computer simulations-	1.	-.
2. Linear equations	1.	2.
3. Elimination methods	1.	2.
4. Iterative methods	2.	3.
5. Non linear equations	2.	9.
6. Ordinary differential equations	4.	17.
7. Partial differential equations 1	6.	20.
8. Partial differential equations 2	6.	20.
9. Data fitting and regressions``	8.	15.
10. Optimization	5.	10.

ASSESSMENT

- You are required to execute **4 small assignments**
- You may work in couples
- Use the suggested report layout (from the web)
- Hand in the assignments in time!

- We will also give you time to solve **one larger assignment**
- You may work in a team of 4
- Write a report
- Present and discuss the results

ADDITIONAL INFORMATION

- Contact information
  - My e-mail: e.zondervan@tue.nl
  - My office: STW 1.22
  - My phone: 5433

  - Ivo Roghair (i.roghair@tue.nl)
  - Martin van Sint Annaland (M.v.SintAnnaland@tue.nl)

SOME ACKNOWLEDGEMENTS…

REAL ACKNOWLEDGEMENTS

- To Roel Verstappen of Groningen University
- To Johan Hult of Cambridge University