Numerical Methods in Chemical Engineering and Problem Solving

ChE 348 (Unique # 14600, 14605)

Spring 2016

Course Description: The purpose of this course is to learn basic computational methods for solving a variety of mathematical problems that cannot be solved analytically, and to develop your confidence in using computational tools for problem solving in engineering. The methods will be applied to several problems in chemical engineering. The methods and skills taught in this course will be valuable for future CHE courses (e.g., CHE 372 and CHE 360) and for many numerical solutions you might need to determine in industry and graduate school.

Prerequisites: CHE 210 (Introduction to Computing), CHE 317 (Introduction to Chemical Engineering Analysis) and M 427K (Advanced Calculations for Applications).

Lectures: TTh 11:00am - 12:15pm, CPE 2.220

Recitations: M 1:00pm - 2:00pm, CPE 1.418 (Unique # 14600)
W 1:00pm - 2:00pm, CPE 1.418 (Unique # 14605)

Instructor: Dr. Lea Hildebrandt Ruiz lhr@che.utexas.edu
Office Hours: Tuesday 12:15 - 1:00 pm and by appointment
CPE 3.470 Office Phone: 471-1050

Teaching Assistants: Dongyu (Simon) Wang dywang05@utexas.edu
Office Hours: Wednesday 3:00 - 4:30 pm, CPE 2.222

Course website: on Canvas http://canvas.utexas.edu


Assessment: Homework 12 %
Project 5 %
In-class participation 3 %
Matlab Exam 10 %
Midterm 1 17.5 %
Midterm 2 17.5 %
Final Exam 35 %

Anticipated course grade cut-offs are A: 90 % –100 %, B: 80 % –89.9 %, C: 70 % –79.9 % Depending on class performance the minimum grade to receive a letter grade may be lowered slightly, it will not be raised. No +/- grading will be used.

Exam Dates: Matlab Exam: Thur., Jan. 28, 11:00 am – 12:15 pm, CPE 2.220
Midterm Exam 1: Thurs., March 3, 11:00 am – 12:15 pm, CPE 2.220
Midterm Exam 2: Tues., April 12, 11:00 am – 12:15 pm, CPE 2.220
Final Exam: Tuesday, May 17, 9:00 am – 12:00 pm, location TBA
Notify instructor by January 27, 2016 if you have a time conflict during the exam periods. Make-up exams will only be given in extenuating circumstances documented by an official letter (e.g. from the student health center). Notify instructor as soon as possible.

Homework is due on Thursdays at 11 am and includes paper submission (in class) and electronic submission of computer code (upload to Canvas). Late homework will be accepted only until the time when solutions are posted. The penalty will be -20% per 24 hour period. This penalty is assessed after normal grading and is cumulative with any points lost (e.g. a homework that would normally receive 80% of total points would receive only 40% if handed in within 48 hours). Late homework must be submitted via e-mail to the instructor and the undergraduate grader (Anais Dotis-Georgiou, dganais@gmail.com).

Students are expected to bring a laptop computer to lecture with access to MATLAB. The instructor will write example code during class, and it will be instructive for students to follow along. Also, there will be some time during lectures for students to work on problems in small groups.

COURSE EXPECTATIONS

Knowledge, abilities and skills students should have entering this course:

1. This course has the following strict prerequisites: CHE 210, CHE 317 and M 427K with a grade of C at least in each of them. The only exceptions to this policy are students who have already acquired permission from me to waive the prerequisites.
2. Ability to program in MATLAB (at the level of CHE 210). This includes being able to write scripts and function files, plot graphs, understand and be able to use control structures like for loops, if loops and while loops, understand and be able to use relational and Boolean operators.
3. Complete understanding of algebra, trigonometric and logarithmic functions (Math 305G)
4. Familiarity with matrices and their properties (CHE 210).
5. Ability to work with and manipulate partial derivatives, integration, Taylor series expansions (Math 408C, 408D, 427).
6. Ability to analytically solve linear ordinary differential equations of first and second order (Math 408C, 408D, 427).
7. Understanding of scientific units, absolute temperature (CHE 317)
8. Complete understanding of the behavior of ideal gases and some familiarity with the properties of real gases (CHE 317, CH 302).
9. Fundamental understanding of mass and energy balances (CHE 317)
10. Stoichiometry and equilibrium constants (Ch 301, 302, 353)

Knowledge, abilities and skills students should gain from this course:

This course has several objectives. The foremost is to introduce several computational techniques which are important in the solution of a variety of mathematical problems that cannot be solved analytically. By the end of this course, students should be able to:
1. Successfully solve mathematical problems with a computer.
2. Be able to formulate and write structured code in MATLAB.
3. Understand the foundation behind the basic numerical methods for matrix manipulations.
4. Solve sets of linear and nonlinear equations using numerical methods as well as built-in MATLAB functions.
5. Apply numerical methods and MATLAB functions to differentiate and integrate a function or a set of discrete points.
6. Apply explicit and implicit numerical methods and MATLAB functions to integrate single and multiple sets of initial value problems.
7. Apply shooting and finite difference methods to solve boundary value problems.
8. Apply finite difference and implicit methods to solve parabolic and elliptic partial differential equations.
9. Apply numerical methods and MATLAB functions to perform rudimentary optimization in the context of parameter estimation.

The programming environment incorporated into MATLAB will be used to introduce structured programming techniques. The major concepts taught in this course are broadly transferable to other software or computer languages.

**TENTATIVE COURSE SCHEDULE**

**This syllabus represents my current plans and objectives. As we go through the semester, those plans may need to change to enhance learning opportunities. Such changes are not unusual and will be communicated clearly.**

Suggested reading from *Numerical Methods for Engineers* is indicated for each lecture or set of lectures.

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<td>Successive Substitution, Newton and Secant Methods</td>
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<td>Explicit and implicit Euler Method and numerical stability</td>
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<td>Higher order and predictor – corrector methods</td>
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<td>Stiffness, Runge-Kutta methods</td>
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<td>Applications: Multiple reactions in a batch reactor and in a plug flow reactor</td>
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<td><strong>Ordinary Differential Equations (ODEs): Boundary Value Problem</strong></td>
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<td>17</td>
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<td>Introduction to BVPs, Finite difference method Application: reaction/diffusion in a catalytic disk</td>
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<td>18</td>
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<td>Additional example / practice with BVPs</td>
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<td>Shooting method Application: reaction/diffusion in a catalytic pellet. Incorporating derivative boundary conditions</td>
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<td><strong>Partial Differential Equations (PDEs)</strong></td>
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<td>Explicit Central Finite Difference Method Application: unsteady reaction/diffusion in a catalytic disk (Parabolic PDEs)</td>
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<td>24</td>
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<td>Application: Heat conduction in a rectangular plate (Elliptic PDEs)</td>
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**Reading**

- Skim Ch. 5
- §6.6, Skim Ch. 12
- PT6.1-6.3, Ch. 21
- PT7.1-7.3, §25.1-25.2
- p.768-772, Skim Ch. 28, 26.1, §25.3-25.4
- PT7.4-7.6
- §30.3-30.5, PT8.3-8.4
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<td><strong>Case Study:</strong> Parameter Estimation of Kinetic Data</td>
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<td>Final Review</td>
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<tr>
<td>30</td>
<td>05/05</td>
<td>Final Review</td>
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**FEEDBACK**

It is my goal to make this an excellent course and a positive experience for all of us. If you feel that the course is not meeting your expectations or you want to provide feedback on how the course is progressing for you, please contact me. I will also be circulating an early course evaluation in class in February. I will use your constructive comments as a way to improve the course where possible.

**POLICIES**

**Homework:** To develop your skills in solving a problem on the computer you need to practice, practice, practice. You must complete each problem by yourself in order to truly comprehend the material. It is acceptable to ask for advice from your classmates, the TA and me, but you need to understand everything you turn in as part of your homework assignment. This means, for example, that you should be able to explain every line of code you submit. You will be asked to submit your Matlab files electronically – please see Appendix A for instructions.

**Recitations:** The teaching assistants will conduct recitations in the computer teaching lab in CPE 1.418, where Matlab syntax and coding will be reviewed and/or a problem similar to problems on the homework will be given to be solved. This is an excellent opportunity to get advice while you are working on a computer. Please go to recitation and take advantage of it.

**Electronics:** If you choose to bring your cell phone, laptop or other personal electronic devices (PEDs) to class, please silence your PEDs before the start of lecture, and please do not use your phone during lecture. Also, laptops should only be used to follow along with Matlab code development or to take notes. Using you cell phone, laptop or other PEDs for other purposes will distract you and the students around you.
Academic Integrity

University of Texas Honor Code: The core values of The University of Texas at Austin are learning, discovery, freedom, leadership, individual opportunity, and responsibility. Each member of the university is expected to uphold these values through integrity, honesty, trust, fairness, and respect toward peers and community.

You will be required to turn in electronic copies of MATLAB script files used to solve homework and exam problems. Periodically these files will be examined with a software tool to check for plagiarism. Script files or homeworks that are discovered to be copied will receive no credit and the students involved will be reported to Student Judicial Services.

Cheating encompasses such behaviors as copying another student’s work, bringing materials into an exam that are not allowed, and a variety of other academically dishonest behaviors (a list of examples is included in Appendix B). As with plagiarism, students who are discovered to have cheated will receive no credit for an assignment or exam and will be reported to the Student Judicial Services.

Other University Notices and Policies

Use of E-mail for Official Correspondence to Students
All students should become familiar with the University's official e-mail student notification policy. It is the student's responsibility to keep the University informed as to changes in his or her e-mail address. Students are expected to check e-mail on a frequent and regular basis in order to stay current with University-related communications, recognizing that certain communications may be time-critical. It is recommended that e-mail be checked daily. The complete text of this policy and instructions for updating your e-mail address are available at http://www.utexas.edu/cio/policies/university-electronic-mail-student-notification-policy

Documented Disability Statement
Any student with a documented disability who requires academic accommodations should contact Services for Students with Disabilities (SSD) at (512) 471-6259 (voice) or 1-866-329-3986 (video phone). I will provide accommodations with an official accommodation letter from SSD. Please notify me as early in the semester as possible if you need disability-related accommodations.

Behavior Concerns Advice Line (BCAL)
If you are worried about someone who is acting differently, you may use the Behavior Concerns Advice Line to discuss by phone your concerns about another individual’s behavior. This service is provided through a partnership among the Office of the Dean of Students, the Counseling and Mental Health Center (CMHC), the Employee Assistance Program (EAP), and The University of Texas Police Department (UTPD). Call 512-232-5050 or visit http://www.utexas.edu/safety/bcal.
Appendix A: Instructions to submit the required files for ChE 348 on Canvas

File and Name Format

Include all required files in a zipped folder. The folder must be named as follows.

<EID of student>_PS<Problem set number>

Example: If your EID is abc123 and you want to submit the script files for Problem Set 1 the name of the zipped folder should be

abc123_PS1

Do *not* change the name of the files inside of the folder.

Submission through Canvas

The folder containing the required script files has to be submitted through Canvas

1. Login to Canvas
2. Select the course - ChE 348 - Numerical Methods in ChE and Problem Solving
3. Click on Assignments tab
4. Click on the Homework for which you are submitting files
5. Click on Submit Assignment on the right
6. Under File Upload browse and choose the file (zipped folder) to attach.
7. After choosing the file it will appear as a selected file.
8. Then click Submit Assignment to upload the file.
APPENDIX B: Examples of Cheating Behavior (a non-exhaustive list)

Exams
- Learning what is on an exam from someone who has already taken it
- Using a false excuse to delay taking an exam
- Copying from another student on an exam with or without their knowledge
- Helping someone else cheat on an exam
- Using unauthorized information: textbook, lecture notes, homework solutions, etc.
- Using unauthorized electronic devices to obtain information during an exam
- Using more time than allowed for an exam (take-home exam)
- Unauthorized communication during an exam
- Requesting a re-grade after modifying an exam

Homework
- Copying someone else’s computer code when asked for individual work
- Working with others on an assignment when not authorized
- Receiving unpermitted help from someone on an assignment
- Paraphrasing/copying material from a written/printed source without referencing it
- Paraphrasing/copying material from an internet source without referencing it
- Fabricating/falsifying a bibliography
- Turning in work copied from another
- Turning in work done by another
- Obtaining solutions from a database of previous years’ assignments/exams

Other work
- Fabricating or falsifying lab data
- Fabricating or falsifying research data