Syllabus

Computer Methods in Chemical Engineering

Fall 2019

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Instructor:

Nam Sun Wang
Class Hour: TuTh 12:30pm-1:45pm; location: CHE2110
Discussion Section Hour: M 11am-11:50am; location: CHE2108
Office Hours: MW 12noon-1pm, Computer lab: Rm2143 Chemical Engineering Bldg
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Graduate Teaching Assistant:

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Undergraduate Teaching Fellows:

Ziqi (Crystal) Lin
Office Hours: Tu 4:30pm-5:30pm, F 12noon-1pm, Room 2136 Chemical Engineering Bldg.
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Required Textbook:

- "Applied Numerical Methods W/Matlab, 4th Edition," Steven C. Chapra, McGraw-Hill, ISBN: 9780073397962

Recommended Reference Books

- "Essential Mathcad for Engineering, Science, and Math /w CD," Brent Maxfield, Elsevier, 2009. ISBN: 9780123747839 ($49.95 List, $39.95 from Barn& Nobel www.barnesandnoble.com). -- This comes with a full student version of Mathcad v14, which is what we have on Virtual Computer Lab.
- "Essential PTC Mathcad Prime 3.0: A Guide for New and Current Users," 1st Edition, Brent Maxfield, Academic Press (Elsevier), 2017. ISBN: 9780124104105, ISBN10:012410410X ($69.95 List, $34 from Amazon) -- This comes with a full student version of PTC Mathcad Prime 3.0, which is *not* what we have on Virtual Computer Lab.

Software Covered/Needed:

- Mathematical Application Programs
  - Mathcad
    (Version R14/R15 from PTC, R15 from Virtual Computer Lab.)
  - MATLAB
    (Version R2019a from Mathworks)

Prerequisites:

CHBE101 and ENES100. Some knowledge of computers (beyond gaming), operating systems, and preferably Matlab -- not strictly required -- we will take you through a crash course. Some experience with algebraic equations, differential equations, and preferably linear algebra (vectors & matrices).

Contents:

Coverage may include operating systems, text editing or word processing, graphics, structured programming (Matlab), numerical methods, mathematical packages (Mathcad), and numerical and symbolic computation. The overall goal of the course is to provide a general introduction to the use of computers and to familiarize a student with various computer tools that can aid in the numerical solution of chemical engineering problems. Examples will be drawn from chemical engineering.

- Numerical Methods
  - Linear Algebraic Equations
  - Matrix Inverse
  - Nonlinear Algebraic Equations
  - Linear and Nonlinear Regression (Data Fitting)
  - Definite Integral
  - Ordinary Differential Equations
- Programming
  - Matlab
- Mathematical Packages
  - Mathcad
- Chemical Engineering Simulation Packages
  - Aspen
  - Symbolic Computation (in Mathcad and MATLAB)

Objectives:

The primary objective of the course, as implied by the course content above, is to introduce computer methods to sophomore students in a hands-on approach. A significant fraction of the lectures are devoted to the specifics of the major computational tools introduced in this class:

- Mathcad
- Matlab

The other half of the lectures cover the numerical methods. Examples drawn from the chemical engineering field are solved with each of the two computational tools by applying appropriate numerical methods or by calling build-in functions. The course assumes only minimal computer background and does not assume any prior programming experience, although it certainly is advantageous to have prior exposure.

- Programming & coding of numerical algorithms
  Distributed throughout
- Call existing/build-in routines
- Solve problems taken from
  Material/energy balances
  Thermodynamics
  Transport
  Kinetics
  Data fitting & analysis of experimental data
  Steady-state & dynamic modeling

This is a required course for all chemical engineering students. Other engineering students who wish to be computer literate in the practical application of numerical methods will also benefit from the course. Upon successful completion of this course, the student should be able to recognize and solve, manually or with the help of a computer tool, most of the engineering problems involving:

- Linear & nonlinear algebraic equations
- Linear & nonlinear regression
- Integration & differentiation
- Ordinary differential equations

Grading:

Student assessment will be based on the following categories, and semester grade will be assigned based on the following scheme.

Homework	45%
Midterm Exam (10/01/19, 11/07/19)	30%
Final Exam (12/16/19, 1:30pm-3:30pm)	25%

Students are guaranteed the following letter grades. That means the instructor will not raise the cut-off points. However, the instructor shall reserve the right to lower the cut-off points at the end of the semester. Students study according to the grades they wish to receive.

Fraction of Points Earned	**Letter Grade**
0.80-	A (A+, A-)
0.67-0.80	B (B+, B-)
0.55-0.67	C (C+, C-)
0.40-0.55	D
0.00-0.40	F

For example, if you earn a total of 250 regular points out of a possible 300 points on the homework assignments, a total of 150 points out of a possible 200 points on the midterm examination, and a total of 120 points out of a possible 200 points on the final examination, your fractional grade at the end of the semester is:

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250/300*0.45 + 150/200*0.30 + 120/200*0.25 = 0.750
  Homework       Midterm       Final Exam
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The above lookup table shows that 0.750 translates to a semester letter grade of "B". For borderline cases, "+" and "-" will be appended to the letter grade. Thus, you can track your own letter grade during the semester.

We follow the University of Maryland policy on excused absence, typically for . unexpected medical reasons, death in the family, and religious observances.

Homework is due at the beginning of the class on the specified date; *no late homework will be accepted* unless individually arranged with the instructor *before* the due date with a valid excuse. In solving homework assignments, students may modify examples already posted on the class web page or worked out in class, and discussion among classmates is allowed. Likewise, seeking help from the TA, undergraduate teaching fellows, graders, and the instructor is certainly allowed (and highly encouraged). However, it is emphasized that **each student must ultimately do one's own work (i.e., absolutely no copying of homework from each other**). It is advised that students first go over the reading portion of the homework assignments and review the lecture notes, and subsequently make an honest concerted attempt at the submission portion of the homework assignments. Do not develop a habit of automatically and immediately default to external help; this will not help build your confidence and competency. A major discrepancy in the homework scores and exam scores is usually an indication of over-reliance on the help (or cheating/copying). After the semester is over, the instructor may process students' homework with one or more software plagiarism detection programs (such as Moss). Two midterm exams each lasting ~50 minutes will be given; absolutely no collaboration is allowed in exams.

Plagiarism and academic dishonesty absolutely will NOT be tolerated, and suspected incidence will be referred to the Student Honor Council of the Judiciary Programs. I subscribe to the zero-tolerance principle. It is your responsibility to consult the instructor whenever there is any doubt on the definitions of these terms or on the allowable materials on each specific homework assignments or quizzes/exams. See Policy on Academic Integrity.

If you have a documented disability and wish to discuss academic accommodations with the instructor, please do so as soon as possible.

Course Related Policies from Office of Undergraduate Studies has further information on, besides academic integrity, code of student conduct, sexual misconduct, non-discrimination procedures, attendance, etc.

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