

ChE352: Process Simulation and Mathematical Techniques for Chemical Engineers

Prof. Davis

Spring 2017 Syllabus

Class meeting times:

Mondays 4:00 – 5:50 PM in room 427

Thursdays 2:00 – 2:50 PM in room 427

Prerequisites and other requirements:

This course has one prerequisite, ESC340: Fluid Mechanics and Flow Systems. I generally assume that every student in the class is a junior in the chemical engineering major and has taken CS102: Introduction to Computer Science. I do not assume any previous knowledge of Matlab; I expect you to learn as we go. The course has a required textbook: Numerical Methods by J. Faires and R. Burden (4th ed.) ISBN# 0495114766. Go to BIGWORDS.com to compare prices: http://www.bigwords.com/details/book/Numerical_Methods/9780495114765/0495114766. I will generally be following the textbook through the course; you should purchase it and bring your copy with you to class. If you would like to prepare for class ahead of time, you can read the text by following the section numbers in the class schedule, but that is not essential. You will need materials to take notes and do problems during class (textbook, paper, pencil, A CALCULATOR, and different colors of pen) and access to a computer with Matlab to do most homework problems.

Course description:

In this course, numerical methods will be applied to chemical engineering problems in mass and energy balances, thermodynamics, fluid flow, heat transfer, separations, and chemical reactor analysis. Topics include: computer calculations and round-off error, algorithms and convergence, finding roots by bisection or Newton's method, exact curve fitting, interpolation, extrapolation, numerical integration and differentiation, numerical solution of initial value problems, stiffness, matrices and determinants, matrix properties, special matrices, methods of solution for systems of linear equations using matrices, eigenvalues, eigenvectors, solving systems of non-linear equations, and applications to unit operations. We will use numerical methods to simulate and solve various chemical engineering models, including the following specific methods: Euler's method, Runge-Kutta methods, the Finite difference method, and Newton-Raphson for vector systems of equations.

Sequence of topics:

The first half of the course (before the Midterm Exam) will cover:

- Mathematical Preliminaries and Error Analysis (Chapter 1)
- Solutions of Equations in One Variable (Chapter 2)
- Interpolation, Extrapolation, and Polynomial Approximation (Chapter 3)

- Numerical Differentiation and Integration (Chapter 4)
- Initial Value Problems (IVPs) for Ordinary Differential Equations (ODEs) (Chapter 5)

The second half of the course (from after the Midterm Exam to the Final Project) will cover:

- Direct Methods for Solving Linear Systems (Chapter 6)
- Iterative Techniques, Eigenvalues and Eigenvectors, and Optimization (Chapter 7)
- Numerical Solutions of Systems of Nonlinear Equations (SNLE) (Chapter 10)
- Boundary-Value Problems for ODEs (Chapter 11)
- Numerical Solutions to Partial Differential Equations (PDEs) (Chapter 12)

The textbook covers all the topics we will discuss in much more detail than we will get in to in a one semester course; for that reason, it is important that you come to class to learn the most important parts of each chapter.

Course goals and objectives:

The goal of this course is to prepare you to solve the chemical engineering problems you will encounter in ChE351, ChE361, and ChE381/382 numerically. I will not be evaluating you very much on:

- From a physical situation, derive or choose an appropriate model for an engineering system
- Derive or give all equations, variables, and parameters needed to solve for the model properties of interest in order to perform analysis, synthesis, optimization, or control

By the end of this course, you should be able to:

- Identify the general type of numerical method needed to solve a given problem type (e.g. IVP, SNLE, PDE, etc.)
- Choose the proper technique to solve a problem based on the characteristics of the equations which define the system/model
- Explain why we need to use numerical methods to solve problems
- Give bounds on the error in the numerical solution to a problem
- Solve for the root of a non-linear equation using bisection or Newton's method
- Write an algorithm to solve for a polynomial fit to a set of thermodynamic data
- Explain how one might solve for the derivative or integral of a function numerically
- Define what an initial value problem is and how it could be solved numerically
- Explain what Euler's method is and how it relates to solving ODEs
- Write an algorithm to solve a chemical reactor design IVP using a Runge-Kutta method
- Explain where a linear system of equations might come from and when they are solvable
- Solve a linear system of equations numerically
- Calculate the determinant, eigenvalues, and eigenvectors of a matrix
- Explain the properties of positive/negative definite/semi-definite matrices
- Explain what a convex function and convex set are and how they relate to optimization
- Write an algorithm to solve a set of non-linear equations from a chemical separation process using a numerical method

- Explain what a BVP is and why it's harder to solve than an IVP
- Explain what a PDE is and where they appear in chemical processes
- Use at least one numerical method to solve a PDE which has its origins in a chemical engineering heat, mass, and/or momentum transfer problem
- Effectively implement algorithms in Matlab to solve various problems from chemical engineering numerically

Homework assignments, projects, and exams:

You will be given six (6) homework assignments (HWs), a midterm examination (exam), and a final project. The HWs will be due before class on the date listed on the assignment and will be assigned at least one week prior to their due date. Homework assignments will consist of problems and essay questions which reinforce concepts from class and the text. Some assignments will take longer to complete than others, though I will do as much as I can to minimize this. I expect that you will spend about 6 hours per week outside of class on work for this class. I will have you submit how many hours per week you spend working on material for this course on your homework assignments. This has no bearing on your grade; it's for my records and may eventually be published anonymously. All homework submissions before the midterm exam must be hand-written (not typed); this does not include code printed from Matlab.

The Midterm Exam will be THREE HOURS LONG and cover the material in chapters 1 through 5 of the textbook which I go over in class and on the homework assignments. The portion of the exam corresponding to each topic will be approximately equal to the amount of time spent in class on each topic. The Final Project will cover the material in chapters 6 through 12 which I present in class and on the homework assignments, with more emphasis on PDEs and chapter 12.

Homework Groups:

You will be assigned a group at three (3) points in this class. You will work together on all HWs and be graded together on those assignments. Groups will be assigned by me on the first day of class. After HW2 has been submitted by each group, groups will be reassigned by me for HW3 and HW4. After HW4 has been submitted, you may choose your own group to work with (subject to my approval of your group) for HW5 and HW6. I reserve the right to reassign groups at any time without consent of any members of that group based on the following criteria: performance on homework assignments or the Midterm Exam (either too low or too high), well-founded complaints by one or many members of the group, or the need to split up another group (and thus break up two groups to form two new groups).

The HWs will be done in groups of two or three but each group member must submit THEIR OWN work. The same homework grade will be given to all group members. It is the responsibility of each group member to ensure that all assignments are of similar quality. The final project will be an individual assignment.

You are REQUIRED to put the names of ALL members of your group on your submissions. If any names do not appear on any submission, I reserve the right to give a zero grade to a person whose name does not appear at my discretion. You are also REQUIRED to submit a group member evaluation form for each group member you have during the semester. The evaluation form will be available to print out on Moodle.

Attendance and grading policy:

Attendance in class is mandatory. Please E-mail me before class if you cannot attend for whatever reason. If you miss class, please come to my office hours to find out what you missed. There will be no make-up or extra credit work associated with this class. Please ensure that you hand in your assignments on time and that you can attend the exam. All assignments and exams must be completed for a passing grade in the class. Students will be graded as follows:

	Homework	Midterm Exam	Final Project
% of grade	24	34	42

Letter grades will be determined at the end of the semester using each student's raw score from above, the average raw score for the class, and my discretion (in that order). My discretion will be based on class attendance / participation, effort on homework assignments, and improvement over the course of the semester. Generally, I have given anyone who gets 85% or better an A in my classes, though that is not a guarantee.

I will grade homework assignments, exams, and the final project based on what you have written or typed on your paper. All answers must be written in coherent, proper English. I can and will give you less credit for an answer which is illegible, poorly formed, unclear, or lacks basic information which is essential to the question at hand. Failure to follow directions is the most common mistake that students make on my assignments. If you disagree with a grade I have given on a question or an assignment, please do come see me; I am often wrong. However, I typically only give credit back to students on an assignment if I have clearly made a mistake in my evaluation (added up points incorrectly, forgot to grade your answer, etc.)

Office hours:

Office hours are hours I set aside in my schedule for you. If you have a question about the homework, about the class material, are confused about what a homework question means, etc., please come to my office hours. That is why I have them; they are for you.

T 3:00 – 4:00 PM, W 4:00 – 5:00 PM, and R 3:00 – 4:00 PM

Please do your best to bring questions to me during those times only. My E-mail address is bdavis@cooper.edu if you have a question which is brief or if you need to let me know you're going to be absent, late, etc. If you send me an E-mail, please put "ChE352" as the start of the subject, e.g. "ChE352 HW1 Question".

Resources which may (or may not) be helpful:

<https://www.mathworks.com/academia/courseware/introduction-to-matlab.html> - Introduction to Matlab resources / course materials

<http://rlburden.people.ysu.edu/index2.html> – Website for a similar textbook by the same authors, including all the algorithms in various programming languages

Numerical Analysis by R. Burden and J. Faires (10th ed.), ISBN# 0534392008

Mathematical Methods in Chemical Engineering by A. Varma and M. Morbidelli, ISBN# 0195098218

Getting Started with MATLAB: A Quick Introduction for Scientists and Engineers by R. Pratap, ISBN# 0199731241 (on reserve in the Cooper library)

Numerical Methods for Chemical Engineers with Matlab Applications by A. Constantinides and N. Mostoufi, ISBN# 0130138517 (on reserve in the Cooper library)

An Introduction to Numerical Methods for Chemical Engineers by J. Riggs, ISBN# 0896723348 (on reserve in the Cooper library)

<http://www.comsol.com/> – Comsol Multiphysics software website

<http://numericalmethods.eng.usf.edu/index.html> or <http://mathforcollege.com/nm/> – Website with a TON of resources on numerical methods, example problems, video lectures, etc.

ABET Outcomes for this Course:

ABET is a nonprofit, non-governmental organization that accredits college and university programs in the disciplines of applied science, computing, engineering, and engineering technology. As part of the accreditation process, engineering colleges are required to select, for each required course, student outcomes which are acquired by students who have taken that course. Student outcomes are succinct statements that describe what students are expected to know and be able to do by the time of graduation. These outcomes relate to skills, knowledge and behaviors that students acquire as they progress through the program. The outcomes I've associated with this course (taken from the ABET website) are:

- (a) an ability to apply knowledge of mathematics, science, and engineering**
- (c) an ability to design a system, component, or process to meet desired needs within realistic constraints such as economic, environmental, social, political, ethical, health and safety, manufacturability, and sustainability**
- (e) an ability to identify, formulate, and solve engineering problems**
- (g) an ability to communicate effectively**
- (i) a recognition of the need for, and an ability to engage in life-long learning**
- (k) an ability to use the techniques, skills, and modern engineering tools necessary for engineering practice**

Special accommodations for exams:

Students with disabilities or who need special accommodations for this class are required to meet with me and the Dean of Students immediately so that arrangements can be made. The Cooper Union has limited resources and extra lead time is required for such arrangements to be feasible.

In order to receive accommodations for an exam, you must notify me in writing at least two weeks before the accommodations are needed and you must also be registered with the Dean of Students. Students will not be afforded any special accommodations retroactively, i.e., for academic work completed prior to disclosure of the disability to myself and the Dean. This policy is modified from Monmouth University via Professor Topper.

Sequence of topics and class schedule:

Hour	Day	Date	Topic(s)	Due
X	Tues	1/17	Introduction / overview / syllabus	
1	Thu	1/19	Chapter 1.2: Motivation for process simulation, numerical methods, calculus review	
2,3	Mon	1/23	Chapter 1.3, 1.4: Taylor's theorem, error analysis, round-off	
4	Thu	1/26	Chapter 1.4, 1.5: Algorithms, rate of convergence, general v. special purpose	
5,6	Mon	1/30	Chapter 2.2: Bisection for root finding	HW1
7	Thu	2/2	Chapter 2.4: Newton-Raphson in Matlab	
8,9	Mon	2/6	Chapter 3.1, 3.2: Interpolation and polynomial approximation	
10	Thu	2/9	Chapter 3.2, 3.5: Lagrange polynomials, cubic splines	HW2
11,12	Mon	2/13	Chapter 4.2, 4.9: Numerical integration and differentiation	
13	Thu	2/16	Chapter 4: Basic quadrature, Advanced quadrature methods	
X	Mon	2/20	NO CLASS (Founder's Day / Presidents' Day)	HW3
14	Thu	2/23	Chapter 5.1, 5.2, 5.3: ODEs (IVPs), Euler's method, Taylor methods, Runge-Kutta methods	
15,16	Mon	2/27	Chapter 5.3, 5.4: RK4, related methods for solving IVPs	HW4
17	Thu	3/2	Chapter 5.6, 5.7: RKF45, IVP systems, RK4 for systems	
X	Mon	3/6	Midterm Exam (THREE HOURS , in class)	MT
18	Thu	3/9	Chapter 5.7, 5.8: Multivariable IVPs, higher orders, stiff IVPs	
X	Mon	3/13	NO CLASS (Spring break)	
X	Thu	3/16	NO CLASS (Spring break)	
19,20	Mon	3/20	Chapter 6.2, 6.4, 6.5: Linear systems, linear algebra, Gaussian elimination, inversion, factoring matrices	
21	Thu	3/23	Chapter 6.6: special matrices, Cholesky factors	HW5
22,23	Mon	3/27	Chapter 7.1, 7.2, 7.3: Large linear system methods, vector norms, matrix norms, eigenvalues, eigenvectors	
24	Thu	3/30	Chapter 7: Optimization, induced matrix norms	
25,26	Mon	4/3	Chapter 10.4: Iterative search, steepest descent, gradients, step size, search direction	
27	Thu	4/6	Chapter 7.6, 10: Iterative methods, condition numbers	
28,29	Mon	4/10	Chapter 10.2, 10.3: Newton's method for SNLE, quasi-Newton methods	
30	Thu	4/13	Chapter 11.2: Solving Linear BVPs	
31,32	Mon	4/17	Chapter 11.3, 11.5: Shooting, solving non-linear BVPs, finite difference methods	HW6
33	Thu	4/20	Chapter 11.4, 11.5: Solving non-linear BVPs	
34,35	Mon	4/24	Chapter 12.1, 12.2: Solving PDEs numerically, forward and backward finite differences	
36	Thu	4/27	Chapter 12.3: PDEs from transport / Crank-Nicolson	
37,38	Mon	5/1	Chapter 12.5: FEM / Comsol Multiphysics	
X	Thu	5/4	NO CLASS	
X	Thu	5/11	NO CLASS – Project due electronically by 11:59 PM	Project

Group work and academic integrity policy:

I believe group work is important to learning; I am requiring you to work in groups on your homework assignments. However, each student MUST submit their own work product for each HW. I will choose randomly each week which group member's homework submission I will grade. This means that you must work closely with your group members to ensure that you are all doing the work and that you are doing it correctly.

Plagiarism is the presentation of another person's "work product" (ideas, words, equations, computer code, etc.) as one's own. Whether done intentionally or unintentionally, plagiarism will not be tolerated in this class. You are plagiarizing if:

1. You present as your own work product (ESPECIALLY MATLAB CODE) a submission that includes the work product of your other group members
2. You present as your own work product a submission that contains the efforts or work product of other individuals aside from your other group members
3. You present as your own work product material from previous iterations of this course (old midterm exams, slides, old projects, homework solutions); representing my work as your own work is not only plagiarism, it keeps you from practicing forming and writing your own answers to my questions.
4. The help and contributions of other individuals are not acknowledged in writing on your submission (by writing their names or citing their published work)
5. You copy the work of other students on an in-class examination or communicate with other individuals in any fashion during an exam
6. You submit as part of a homework assignment or project material that has been copied from any source (including, but not limited to, a textbook, a periodical, an encyclopedia, the internet) without properly citing the source, and/or without using quotation marks. It is also prohibited to submit such materials in a minimally altered form without proper attribution. Improperly copied material might include text, graphics (computer or otherwise), computer source code, MATLAB SCRIPTS, etc.

If I have a strong suspicion that you have plagiarized your submission for an assignment (homework or project,) you will receive a zero on that assignment. If you commit another act of plagiarism during the course after this first act, I will refer the matter to the Dean's office. Other prohibited acts of academic dishonesty include (but are not limited to):

7. Attempting to obtain a copy of an examination before it is administered
8. Dishonesty in dealing with me or another professor, such as misrepresenting the statements of another professor
9. Bringing a text or study materials of any kind into an exam when forbidden to do so
10. Using an electronic device in class at any time when not expressly permitted by me
11. Bringing a device into an examination that allows communication with other individuals or computers or computer databases (i.e. no cell phones or laptops during exams)

If I have a strong suspicion that you have cheated on an examination, you will receive a zero on that examination and likely receive a D or F in the course. The above was modified from the course catalog from the 2009-10 academic year.