

COURSE INFORMATION	
Course Number and Title	CH E 310: Computational Methods in Chemical Engineering
Semester	Fall 2016
Class Meetings	Tue/Thu 12:40 - 2:00 in 1150 Sweeney
Instructor Philosophy Statement	<p>Welcome to ChE 310! This course will focus on the numerical (computer) tools that will help you solve the bulk of your engineering problems. It is my goal to give you a full toolbox to use for your remaining time at IA State and, more importantly, as you enter the workforce. In industry there is no clean answer key and no single solution method to a problem; instead there are pressing deadlines and a lot of messy data that needs to be transformed into accurate data-based decisions. As such, in this course you will find a lot of the exam questions are open-ended as to the method you use to derive an answer. My goal is to strengthen your ability and speed to chart a course to a satisfactory answer.</p> <p>As you progress in your career at Iowa State and beyond, I would be very interested to hear about any difficult engineering problems that were not addressed by the tools you acquired in this course. It will be my task to take this feedback and update the tool set we give future students, so they will be better prepared.</p> <p>I am looking forward to a great semester with you. – Dr. Reuel</p>
Catalog Course Description	Numerical methods for solving systems of linear and nonlinear equations, ordinary differential equations, numerical differentiation and integration, and nonlinear regression using chemical engineering examples.
Learning Outcomes	<p>By the end of this course you should be able to:</p> <ul style="list-style-type: none"> • Use Matlab to solve chemical engineering problems • Approximate function values using a Taylor Series • Convert differential equations to finite differences approximations • Apply root-finding methods to solve chemical engineering problems • Solve matrix equations • Solve systems of linear equations numerically • Solve systems of nonlinear equations numerically • Fit curves to data • Interpolate and extrapolate data • Apply numerical integration to solve chemical engineering problems • Apply numerical differentiation to solve chemical engineering problems
Prerequisites	<p>The prerequisites for this course are CH E 160, CH E 205*, CH E 210, MATH 265.</p> <p>*Note that Ch E 205 is new for the 2016-2017 catalog and does not affect those taking Ch E 310 at this time. You are not required to have taken it, nor will you need a prerequisite waiver.</p>

	<p>Course prerequisites will be enforced according to University policy: http://catalog.iastate.edu/informationaboutcourses/. This means that students who are enrolled in this course but have not met the prerequisite requirements must drop the course. The instructor will not grade any coursework submitted by a student who has not met the course prerequisites and if the student does not drop this course, the student will earn an “F” grade for this course.</p> <p>Students who do not meet prerequisites but do have equivalent preparation may submit a request for a prerequisite waiver to the instructor. Waivers are available on the CBE website.</p>
INSTRUCTOR INFORMATION	
Primary Instructor	<p>Dr. Nigel Reuel 3051 Sweeney reuel@iastate.edu 515-294-4592 Office hours: 9-11 am on Tuesday and 11-12 on Friday in Sweeney 1150</p>
Instructional Assistant	<p>Md Mir Hossen (Mir) mir@iastate.edu Office Hours: 9-12 on Friday in 1150 Sweeney</p>
TEXTBOOKS AND SUPPLIES	
Required Textbooks	<p><i>Applied Numerical Methods with Matlab for Engineers and Scientists</i>, Steven C. Chapra, McGraw Hill 3rd Edition, 2012.</p>
Supplement Text	<p><i>Street Fighting Mathematics</i> by Sanjoy Mahajan may be referenced. Electronic copy can be found free here</p>
Required Software	<p>We will make extensive use of MATLAB and some Microsoft EXCEL in this course. These software packages are installed in all College of Engineering computer labs and are also available via remote access (http://it.engineering.iastate.edu/remote-access/). MATLAB is available from the College of Engineering as a free download for use on your personal computer (http://it.engineering.iastate.edu/downloads). EXCEL is available as part of Microsoft Office for a nominal fee.</p>
Web Access	<p>Blackboard - http://bb.its.iastate.edu . All problem sets and answer keys will be distributed on Blackboard including your current grading status. It is important that you keep up-to-date with the course using this tool. Please let me know if you are unable to access this course online.</p>
ASSIGNMENTS AND EVALUATION	
In-Class Problems	<p>A simple problem set (1-3 multiple choice questions) will be given at the start of each course period to reinforce the assigned reading for that day and connect to the previous lecture. A new hyperlink to submit answers will be written on the board. No late submissions will be accepted (<i>i.e.</i> must come to class on time, have computer up and running and submit answers by 12:45). If you have read through the materials, the answers will be obvious and five minutes will be sufficient.</p> <p>Additionally during the class we will create VERY USEFUL code (m-files and scripts) that can be used in your problem sets and exams. This code is not turned</p>

	<p>in at the end of class, but it would behoove you to attend all of class and understand how the algorithms work. In this manner the pieces of code become tools in your toolbox to tackle future problems.</p>
Homework	<p>One problem set is assigned (2-5 problems) per week. It will be posted on Blackboard at 3:00 PM each Thursday and will be due the following Wed by 5 pm. These problems will reinforce the materials from the previous lectures, so you can get started on them immediately after they are posted on Blackboard (no need to wait for Tuesday lecture).</p> <p>Submission is done electronically via Blackboard. Submit a single M-file or Excel file for each problem. There will be no hard copy submissions for this course. Materials will be graded and commented on electronically as well.</p> <p>If your M-file program is unable to derive the answer (e.g. MATLAB m-file is not running correctly), first seek help from others (see collaboration note below and office hours above). If you still cannot get the program to run, write up WHY you think it is not working by using comment lines within your code. Detail the mental process you are trying to accomplish computationally to get to the answer. This is the only way partial credit will be assigned.</p> <p>If an Excel solution is submitted, the VBA scripts, macros should be contained in the file submitted and the answer clearly shown. If steps were taken (e.g. using a solver) to derive an answer in a cell, specify with text what was done.</p>
Teamwork/ Collaboration	<p>I encourage students to work together on problem sets but not to copy letter for letter the same program code. Use each other as sounding boards, lifelines, and guides when you undoubtedly get stuck or your code doesn't run properly. In your career, you will rarely work independently. (Sorry, Simon and Garfunkel enthusiasts—no, "I am a rock, I am an island" in real life.) You should get used to seeking and giving help.</p> <p>A lot of the tools (<i>i.e.</i> code) will be written together in class and copied throughout your problem set M-files. However, our in-class tools are only pieces of the larger solution. An individual's final problem set M-file should bear unique features (syntax, variable naming, code conciseness, etc.). Thus, I will be able to detect very quickly if a problem set file has been copied in its entirety from one person to the next. If this is detected, we will meet to discuss the similarities. Those found cheating on homework will receive a zero. So, write your own solution, run it on your own computer, and turn it in as your own work. This will only help you on exams where you will be tested on your own proficiency to weave together pieces of code. Plus, the points matter a whole lot more when you're flying solo (see break down below).</p>
Professionalism	<p>My expectation is preparation for future career. Be on time, be attentive, be courteous, and be engaged.</p>
Exams	<p>There are two in-class exams (not cumulative—see schedule for dates) and one comprehensive final (Monday, Dec. 12 from noon to 2:00 pm). All exams are administered on computers and are open note, open book, and open toolbox (<i>i.e.</i> all the code you have written to date can be accessed) but NOT open neighbor and</p>

	<p>NOT open internet. You will need to move fast in the exams; there will not be time to learn from the book on the spot. Having code already developed (from in-class work and problem sets) will give you a strong edge.</p> <p>NOTE: Problem set keys will be posted as scanned images, so you will not be able to lift this content during an exam. You will need to prepare ahead and have your own tools written and ready.</p>																				
Grading	<p>Point break down as follows</p> <p>Midterm Exam 1 = 20% Midterm Exam 2 = 20% Final Exam = 30%</p> <p>Daily start of class questions = 10% Weekly Problem Sets = 20%</p> <p>The minimum grade assignments will be:</p> <table border="1"> <thead> <tr> <th>If your course score is at least</th> <th>You are guaranteed at least this letter grade</th> </tr> </thead> <tbody> <tr> <td>93</td> <td>A</td> </tr> <tr> <td>90</td> <td>A-</td> </tr> <tr> <td>87</td> <td>B+</td> </tr> <tr> <td>83</td> <td>B</td> </tr> <tr> <td>80</td> <td>B-</td> </tr> <tr> <td>77</td> <td>C+</td> </tr> <tr> <td>73</td> <td>C</td> </tr> <tr> <td>67</td> <td>C-</td> </tr> <tr> <td>Less than 67</td> <td>F</td> </tr> </tbody> </table> <p>However, I reserve the right to adjust this scale in your favor, depending on the overall performance of the class.</p>	If your course score is at least	You are guaranteed at least this letter grade	93	A	90	A-	87	B+	83	B	80	B-	77	C+	73	C	67	C-	Less than 67	F
If your course score is at least	You are guaranteed at least this letter grade																				
93	A																				
90	A-																				
87	B+																				
83	B																				
80	B-																				
77	C+																				
73	C																				
67	C-																				
Less than 67	F																				
COURSE POLICIES																					
Attendance	Formal attendance is not taken, but start-of-class quizlets would necessitate being on time. If you cannot make a course for an approved reason (see University Policies below), please contact me at least 48 hr in advance to accommodate getting you class notes and allowing you to make up the daily quiz.																				
Late Assignments	Not accepted. You have a full week to submit. The deadline for each problem set is Wed at 5 pm for each week. If there are extenuating circumstances, please contact me ahead of time and I will do my best to accommodate.																				
Requests for Regrading	If you feel a problem set or exam has a grading error, please allow 48 hr. to pass before approaching the instructor or TA. This will allow you adequate time to look at the posted answer key.																				
Computer Use	Computers are to be used only for coursework. Do not peruse the internet; use email, Facebook or any other social network; play games; or indulge in other diversions. Again, during class we develop the tools (code) together that can be																				

	used in problem sets and exams. It is to your advantage to follow along and write your own tool set.
General Expectations	<p>You are expected to spend an average of nine hours per week preparing for class and completing homework assignments.</p> <ul style="list-style-type: none"> - Complete the reading assignment prior to class. - Bring your book, calculator, pencil, and paper to each class. - Ask questions if you do not understand the material. - Be on time to class. If you must be late to class, please enter quietly - Mute cellphones and any other electronic devices.
UNIVERSITY POLICIES	
Academic Dishonesty	<p>You are expected to practice academic honesty in every aspect of this course and all other courses. Information on academic misconduct and the consequences can be found on the Dean of Students webpage (http://www.dso.iastate.edu/ja/academic/misconduct.html). Students who engage in academic misconduct are subject to university disciplinary procedures, as well as consequences with regard to this course.</p> <p>Consulting a solution manual, student solutions from a previous semester, or using any unauthorized assistance from other people or resources (including the internet) is strictly prohibited. You are encouraged to seek help from the primary instructor, the teaching assistant, and your classmates to complete homework assignments and in-class problems. If you do seek help from your classmates, then you must acknowledge this help at the end of the assignment with the following statement: "Problem x.x was completed with assistance from [classmate's name]."</p>
Disability Accommodations	<p>Iowa State University complies with the Americans with Disabilities Act and Sect 504 of the Rehabilitation Act. If you have a disability and anticipate needing accommodations in this course, please contact the primary instructor to set up a meeting within the first two weeks of the semester or as soon as you become aware of your need. Before meeting with the instructor you will need to obtain a SAAR form with recommendations for accommodations from the Disability Resources Office, located in Room 1076 on the main floor of the Student Services Building (http://www.dso.iastate.edu/dr/). Retroactive requests for accommodations will not be honored.</p>
Harassment and Discrimination	<p>Iowa State University strives to maintain our campus as a place of work and study for faculty, staff, and students that is free of all forms of prohibited discrimination and harassment based upon race, ethnicity, sex (including sexual assault), pregnancy, color, religion, national origin, physical or mental disability, age, marital status, sexual orientation, gender identity, genetic information, or status as a U.S. veteran. Any student who has concerns about such behavior should contact his/her instructor, Student Assistance at 515-294-1020 or email dso-sas@iastate.edu, or the Office of Equal Opportunity and Compliance at 515-294-7612.</p>
Religious Accommodations	<p>If an academic requirement conflicts with your religious practices and/or observances, you may request reasonable accommodations. Your request must be in writing, and your instructor will review the request. You or your instructor may also seek assistance from the Dean of Students Office at 515-294-1020 or email</p>

	dso-sas@iastate.edu, or the Office of Equal Opportunity and Compliance at 515-294-7612 or email eooffice@iastate.edu.
Dead Week	<p>This class follows the Iowa State University Dead Week policy as noted in section 10.6.4 of the Faculty Handbook http://www.provost.iastate.edu/resources/faculty-handbook</p> <p>For each Fall and Spring semester, the last full week of classes before final examinations is designated as Dead Week. The intent of this policy is to establish a one-week period of substantial and predictable study time for undergraduate students. During the Dead Week period, regular lectures are expected to continue, including the introduction of new content, as deemed appropriate by the instructor. The restrictions established by this Dead Week policy are:</p> <ul style="list-style-type: none"> • Due dates for mandatory graded submissions of any kind that fall within Dead Week must be listed on the syllabus provided at the start of the course. <p>For ChE 310, there will be mandatory submissions of start of class questions and the last problem set (due Wed)</p> <ul style="list-style-type: none"> • Mandatory final examinations may not be given during the Dead Week period except for laboratory courses or courses that meet weekly and for which there is no contact during the normal final examination week. <p>In ChE 310, the Final Exam will be in class on Monday Dec. 12 from 12 to 2:00</p> <ul style="list-style-type: none"> • Registered ISU Student Organizations may not hold any meetings, functions, or sponsored events during the DeadWeek period. Any exception to these restrictions must be authorized in advance by Office of the Dean of Students.
COURSE SCHEDULE	
See attached schedule below	

Meeting	Date	Day	Topic	Reading Due	PSet Release (due following Wed @ midnight)
1	8/23/2016	T	Course Overview + Matlab Programming Basics	--	
2	8/25/2016	R	Matlab	Chp 1 and 3	Problem Set 1
3	8/30/2016	T	Matlab	Chp 2	
4	9/1/2016	R	Matlab	Chp 1-3	Problem Set 2
5	9/6/2016	T	Error, Taylor Series, and Finite Difference Approx	Chp 4	
6	9/8/2016	R	Plotting in Excel and Matlab	(will post to BB)	Problem Set 3
7	9/13/2016	T	Curve Fitting - Stats review and Excel	Chp 14 and 15	
8	9/15/2016	R	Curve Fitting - Matlab	Chp 14 and 15	Problem Set 4
9	9/20/2016	T	Polynomial Interpolation and Extrapolation	Chp 17	
10	9/22/2016	R	Splines and Piecewise Interpolation	Chp 18	Problem Set 5
11	9/27/2016	T	Intro to Unit 2 - Matrix math and Matlab	--	
12	9/29/2016	R	Midterm 1 - In Class	--	
13	10/4/2016	T	Root Finding - Bracketing Methods	Chp 5	
14	10/6/2016	R	Root Finding - Open Methods	Chp 6	Problem Set 6
15	10/11/2016	T	Optimization	Chp 7	
16	10/13/2016	R	Linear Algebraic Equations	Chp 8	Problem Set 7
17	10/18/2016	T	Gauss Elimination	Chp 9	
18	10/20/2016	R	LU Factorization	Chp 10	Problem Set 8
19	10/25/2016	T	Matrix Inverse and Condition	Chp 11	
20	10/27/2016	R	Iterative Methods	Chp 12	Problem Set 9
21	11/1/2016	T	Intro to Eigenvalues	Chp 13	
22	11/3/2016	R	Midterm 2 - In Class	--	
23	11/8/2016	T	Numerical Integration	Chp 19	
24	11/10/2016	R	Numerical Integration	Chp 20	Problem Set 10
25	11/15/2016	T	Numerical Differentiation	Chp 21	
26	11/17/2016	R	Ordinary Differential Equation Intro	Chp 22	Problem Set 11
	11/22/2016	T	THANKSGIVING BREAK - NO CLASS		
	11/24/2016	R			
27	11/29/2016	T	Ordinary Differential Equation	Chp 23	
28	12/1/2016	R	Ordinary Differential Equation	Chp 24	Problem Set 12
29	12/6/2016	T	Intro to Fourier Analysis	Chp 16	
30	12/8/2016	R	Intro to Designed Experiments	(will post to BB)	

- 12/12/2016 Final Exam - Noon to 2:00
- = Unit 1 - Matlab and Data
 - = Unit 2 - Roots, Matrices, and Systems of Eqns
 - = Unit 3 - Integrals and Differentials
 - = Introduction sections (basic level assessment)