

# CHeg 3145: Chemical Engineering Numerical Analysis, Fall 2017

## Course Syllabus and Schedule

**Instructor:** Prof. Matthew D. Stuber, PhD

Office Hours: Thu 2:00-3:00PM

Office: UTEB 276

Email: stuber@uconn.edu

Phone: (860) 486-3689

**Course Catalog Description:** Mathematical and numerical methods for solving engineering problems; description and computer modeling of physical and chemical processes with ordinary and partial differential equations; treatment and interpretation of engineering data. (3 credits, lecture)

**Lecture:** Tue/Thu, 11:00AM-12:15PM, GENT 131

### Teaching Assistants:

- Mr. Matthew Wilhelm (PhD Student), matthew.wilhelm@uconn.edu  
Office Hours: TBD
- Mr. Robert Ernst (UG Student), robert.ernst@uconn.edu  
Office Hours: TBD

### Textbook and Materials:

1. Dorfman, Kevin D., and Daoutidis, Prodromos. *Numerical Methods with Chemical Engineering Applications*. Cambridge University Press, 2017. ISBN: 9781107135116 (required)
2. *MathWorks*® *MATLAB*<sup>TM</sup> Software Package (required)
3. *Wolfram*® *Mathematica*<sup>TM</sup> Software Package (optional)

**Goals and Outcomes:** This course is designed to provide students with a sound foundation in numerical methods for solving engineering problems. Students will be introduced to computational mathematics, program methods on a computer, and formalize and solve engineering problems. Student progress towards the following ABET Engineering Objectives will be assessed:

- (a) An ability to apply knowledge of math, science, and engineering.
- (e) An ability to identify, formulate, and solve engineering problems.
- (k) An ability to use the techniques, skills, and modern engineering tools necessary for engineering practice.

Upon the completion of this course, students will be able to:

1. Interpret and solve chemical engineering problems by using techniques from applied mathematics. (ABET a, e)
2. Discriminate between various methods and software to select for characteristics appropriate for specific problem types and structures (ABET a, e, k).
3. Demonstrate proficiency in numerical analysis by solving chemical engineering problems using MATLAB. (ABET a, e, k)

**Performance Table**

Outstanding >90	Acceptable 70	Unacceptable <50
<i>(1) Interpret and solve chemical engineering problems by using techniques from applied mathematics (ABET a, e)</i>		
Students can rigorously formulate mathematical models and translate them into forms appropriate for computation. Students can readily identify problem structure, scale, and complexity.	Students can generally identify modeling paradigms with some errors in formulation and/or translation for computation. Students may have difficulty identifying problem structure, scale, and/or complexity.	Students are unable to formulate models and/or translate them for computation. Students lack the fundamental understanding for problem structure, scale, and/or complexity.
<i>(2) Discriminate between various methods and software to select for characteristics appropriate for specific problem types and structures (ABET a, e, k)</i>		
Students can defend the selection of methods and software based on characteristics such as convergence properties, time complexity, storage complexity, accuracy, and limitations with respect to specific problems.	Students can generally select methods and software based on problem types but lack a working understanding of algorithm analysis such as complexity and convergence results.	Students are unable to select appropriate methods and software for solving specific problem types.
<i>(3) Demonstrate proficiency in numerical analysis by solving chemical engineering problems using MATLAB. (ABET a, e, k)</i>		
Students have a working knowledge of MATLAB. Students can readily produce working code to solve common chemical engineering problems including steady-state and dynamic simulation. Students can readily interpret results and output and demonstrate proficiency in debugging.	Students can generally read and understand MATLAB code but make common mistakes with data structures and function calls. Students make frequent errors in translating problems into code and struggle with interpreting output and debugging.	Students may only superficially understand MATLAB code. Students are unable to translate chemical engineering problems into code.

**Course Grading and Policies:** Course grades will be based on the following overall rubric:

Classroom Participation	5%
Problem Sets	30%
Mid-Term Exam 1	20%
Mid-Term Exam 2	20%
Final Exam	25%
<hr/> Total	<hr/> 100%

Grades will be distributed according to the following guidelines:

A	96-100	Complete Mastery of subject material.
A-	90-95	
B+	88-89	Some mild deficiencies in Mastery of subject material.
B	82-87	
B-	80-82	
C+	77-79	Some deficiencies in understanding the core subject material.
C	72-76	
C-	70-72	
D+	68-69	Serious deficiencies in understanding the core subject material.
D	62-67	
D-	60-61	
F	≤59	Unacceptable understanding of course material.

- All course-related emails to the instructor or the TAs should have the subject “CHEG 3145 Fall 2017”.
- Homework problem sets are due by 11AM, in class, on their respective due date. Physical copies of your solutions are to be submitted. Anything handwritten should be single-sided, legible, and clearly organized.
- Late homework can be turned in for 50% credit up to one week after the due date and 0% thereafter. Late homework will be graded with least priority (you may not get timely feedback).
- Students missing 3 or more homework problem sets will get an incomplete for the course.
- All homework problem sets are to be completed individually. It is encouraged that students discuss problem sets together but each student must turn in their own version.
- Any computer code written must be submitted digitally on HuskyCT in addition to your physical solutions. Please print off your code and submit physical copies as an appendix to your homework solutions.
- All computer code written must contain sufficient commenting including input requirements, documentation of structure and subroutines, and sample output.
- All exams are closed book/closed notes. You will be allowed one self-prepared double-sided hand-written “cheat sheet” or “crib sheet”.

- **Inclement weather** may pose hazardous conditions for commuting. Use your best judgment when conditions are hazardous. Classes may be canceled at the University's or instructor's discretion. Email notification will be given and students are responsible for reviewing the day's lecture materials, available on HuskyCT.
- **Special consideration** will be granted for individuals with unique circumstances at the instructor's discretion. If you feel that your situation requires you to miss problem sets or an exam, please do not hesitate to discuss with the instructor. Situations such as chronic and acute illness, death in the family, mental health, etc. can be accommodated within reason.
- **Final Exam** A note on final exams from the Vice Provost of Academic Affairs and the Associate Dean of Students:

Final exam week for Fall 2017 takes place from Monday, December 11 through Sunday, December 17, 2017. Students are required to be available for their exam during the stated time. If you have a conflict with this time, you must visit the Dean of Students Office to discuss the possibility of rescheduling this exam.

Please note that vacations, previously purchased tickets or reservations, social events, misreading the exam schedule and over-sleeping are not viable excuses for missing a final exam. If you think that your situation warrants permission to reschedule, please contact the Dean of Students Office with any questions. Thank you in advance for your cooperation.

## Tentative Schedule

TUESDAY		THURSDAY	
Aug 29th <u>Introduction</u> 1. Mathematical Modeling 1.1-1.2	1	31st <u>Introduction</u> 1.3-1.4 Structured Programming	2
Sep 5th <b>Problem Set 1 Due</b> <u>Algebraic Equations</u> 2. Linear Systems, 2.1-2.5	3	7th <u>Algebraic Equations</u> 2. Linear Systems, 2.6-2.12	4
12th <b>Problem Set 2 Due</b> <u>Algebraic Equations</u> 2. Linear Systems, 2.13-2.14	5	14th <u>Algebraic Equations</u> 3. Nonlinear Systems, 3.1-3.4	6
19th <b>Problem Set 3 Due</b> <u>Algebraic Equations</u> 3. Nonlinear Systems, 3.5, 3.7-3.8	7	21st <u>Algebraic Equations</u> 3. Nonlinear Systems, 3.9-3.10	8
26th <b>Problem Set 4 Due</b> Review	9	28th <b>Exam 1</b>	
Oct 3rd <u>Differential Equations</u> 4. ODE-IVPs, 4.1-4.2	10	5th <u>Differential Equations</u> 4. ODE-IVPs, 4.2-4.3	11
10th <b>Problem Set 5 Due</b> <u>Differential Equations</u> 4. ODE-IVPs, 4.4-4.6	12	12th <u>Differential Equations</u> 4. Higher-Order ODE-IVPs, 4.7-4.9	13
17th <b>Problem Set 6 Due</b> <u>Differential Equations</u> 5. Dynamical Systems, 5.1-5.3	14	19th <u>Differential Equations</u> 5. Dynamical Systems, 5.3-5.5	15
24th <b>Problem Set 7 Due</b> <u>Differential Equations</u> 5. Dynamical Systems, 5.6-5.7	16	26th <u>Differential Equations</u> 6. ODE-BVPs, 6.1-6.2	17
31st <b>AIChE - No Class</b> <b>Problem Set 8 Due</b>		Nov 2nd <b>Exam 2</b>	

TUESDAY		THURSDAY	
7th	<b>18</b>	9th	<b>19</b>
<u>Differential Equations</u> 6. ODE-BVPs, 6.3		<u>Differential Equations</u> 6. ODE-BVPs,6.4-6.6	
14th	<b>20</b>	16th	<b>21</b>
<b>Problem Set 9 Due</b> <u>Differential Equations</u> 7. PDEs, 7.1-7.2		<u>Differential Equations</u> 7. PDEs, 7.2-7.3	
21st		23rd	
<b>Thanksgiving Break - No Classes</b>		<b>Thanksgiving Break - No Classes</b>	
28th	<b>22</b>	30th	<b>23</b>
<b>Problem Set 10 Due</b> <u>Differential Equations</u> 7. PDEs, 7.4		<u>Differential Equations</u> 7. PDEs, 7.5	
Dec 5th	<b>24</b>	7th	<b>25</b>
<u>Optimization</u>		<b>Problem Set 11 Due</b> Review	
12th		14th	
<b>Finals Week - No Classes</b>		<b>Finals Week - No Classes</b>	