CHBE 2120: Numerical Methods in Chemical Engineering
Instructor: Yoshiaki Kawajiri

Course Objectives:
This course introduces a range of numerical methods for the approximate solution of mathematical equations encountered in chemical engineering. The methods are introduced in a problem specific context, such as the mass and energy balances learned in ChBE 2100. In addition to learning the methods, a focus is made on how the methods can fail, how failure can be diagnosed, and how this can be addressed. Two software packages are used in the course: (i) MATLAB, which is used for programming and visualization, and is learned in CS 1371, and (ii) ASPEN, a graphics based process simulator with built-in chemical properties databases, which is widely used in the chemical process industry.

Learning Outcomes:
By the end of this course, a student should be able to:
1. Formulate a chemical engineering problem as a mathematical model, and select an appropriate solution method.
2. Analyze the accuracy of the numerical solution and identify alternate strategies and methods to achieve greater accuracy when it is needed.
3. Understand the computational requirements of various solution options and use this understanding in the selection of the solution method
4. Select the appropriate software package to perform the numerical solution to a chemical engineering problem.
5. Design experiments using statistical methods, for the purpose of building models and designing chemical processes.
6. Formulate and solve process design problems, based on economic analysis and using mathematical models of chemical processes

Text:
Chapra, S.C., Canale, R. P., "Numerical Methods for Engineers," Sixth edition, McGraw-Hill, 2006.

Prerequisites: ChBE 2100 and CS 1371

Class web site: *T-Square* http://t-square.gatech.edu

Class meeting time: MWF at 8:05-8:55am in L1255 ES&T
Class will occasionally be held in the computer lab, L2230 ES&T.

Teaching assistant: Jungmin Oh, joh77@gatech.edu, 404-894-0643
Ambarish Kulkarni, akulkarni34@gatech.edu, 404-385-7608

Office hours:

Jungmin Oh	Fridays 3:30-5:30 pm in computer lab (L2230 ES&T)
Ambarish Kulkarni	Tuesdays 4:00-6:00pm in computer lab (L2230 ES&T)
Yoshiaki Kawajiri	Thursdays 2:00-4:00 pm, or by appointment, in L1224 ES&T

Open Door Policy by instructor:
In addition to my office hours above, I will try to answer your question as frequently as possible in my office. If my door is open, you are welcome to come in. If my door is closed, I am having lunch, on the phone, or dealing with urgent issues. I appreciate your understanding before deciding if you should knock on my door.

Grading:		
	Exam 1	20%
	Exam 2	20%
	Final Exam	25%
	Quizzes	10%
	Homework	15%
	Project	10%
	Participation: up to 2% bonus	

Participation is strongly encouraged, and amounts to up to 2% extra credit. Participation is defined as answering questions from other students and asking insightful questions in class and on T-Square Forums (see below). Please also note that the full 2% bonus is given only to students who make very active participations both in class and on T-Square Forums (simply attending the class is not considered participation). It is not meant to boost the grades of those on the border line automatically.

Exams

Two exams will be given, in addition to the final exam. All exams will be closed book. You will be allowed to bring to the exam a single 8.5x11" sheet of paper with formulas, algorithms, and other information written on one side only.

Exam 1	October 3 (Wednesday)	6:30pm-8:30pm
Exam 2	October 31 (Wednesday)	6:30pm-8:30pm
Final exam	December 10 (Monday)	8:00am – 10:50pm

If you have any unavoidable conflict, you must let the instructor know in writing two weeks prior to the exam date. Make up exams will be scheduled only for unavoidable conflicts. No make up exam will be given if the conflict was not reported two weeks prior to the exam date at the latest.

Grade Scale:

A: [85, 100]
B: [75, 85)
C: [65, 75)
D: [55, 65)
F: [0, 55)

Quizzes

At least five quizzes will be given during class. The lowest two scores will be dropped in computing the overall quiz grade. The quiz dates will not be announced ahead of time. If

you need to miss class for any reason and you miss a quiz, then you will receive a zero for that quiz.

All quizzes will be given at the beginning of a lecture. You have to arrive before the lecture begins to take a quiz. No make-up quiz will be given for any reason. I understand that some of you may have unavoidable conflicts, and this is why two lowest scored quizzes will be ignored.

Class attendance

Attendance is crucial to learn and complete this course. The past course statistics demonstrate that those with good class attendance records obtain higher grades in quizzes, homework assignments, and exams. Always arrive in time to complete all quizzes, and try to participate in discussions in class.

Note the difference between class attendance and participation (defined above). There is no formal mechanism to include you class attendance directly to your grade. Therefore, it is not necessary to report your leave of absence to the instructor even if you have an occasional unavoidable conflict such as job interviews or jury summons.

If there is any unavoidable event that makes your attendance impossible for a long period of time–such as an illness or injury–please contact the instructor.

Homework

Homework assignments are to be turned in electronically through *T-Square*. The files must be uploaded BEFORE class on the day it is due. (Note: this time will be rigidly enforced by T-Square.)

All MATLAB code must be submitted electronically. The code must be thoroughly commented, and must use indenting within loops. In some cases, a portion of the homework may be submitted on paper, but you always have the option of submitting everything electronically (e.g. scanned in, MS Word, PDF). Any work on paper must be turned in to your instructor *before class* on the day it is due.

You must confirm yourself that your file is submitted on T-Square. Many students forget to click the "submit" button after uploading their files (this is the reason of the problem in 100% of all cases in my experience). You are also able to resubmit your file as many times as you like until the deadline.

In all assignments you must clearly explain your work and the steps taken to obtain the answer, either as comments within the Matlab file, or in a separate document. It is never sufficient to submit only the code.

Failure to staple multi-page paper submission would result in a 30 percent penalty. We will not be responsible for any loss of pages from unstapled submissions.

The homework turned in must be your own work. You may discuss technical concepts relating to the homework with your classmates, but must work the problems and write the code by yourself. Copying directly from another person's homework or exam is a serious violation of the Georgia Tech Honor Code (http://www.honor.gatech.edu/).

Late submission for homework and project

Given zero point.

Communicating with instructors and TA

Students are always encouraged to ask questions. We are always available during office hours. If you have trouble following lectures, please try to see us as soon as possible. The instructor will be happy to help you by giving supplemental practice problems and discussing your study plan.
You are always welcome to ask questions even out of class, but you should choose the most appropriate communication format depending on your situation:

- **T-Square Forums:** All non-personal questions should be posted on T-Square Forums (see below).
- **Appointments with instructor:** For making an individual appointment to discuss personal issues in person with the instructor, please visit https://www.timetrade.com/book/CQ3MC.
- **Email:** Email communications are restricted only to personal issues. Non-personal questions by email will not be responded but directed to T-Square Forums. This is to give the same information to all of you. Please allow at least 24 hours for responses.
- **Phone:** For issues that require immediate attention from the instructor within 24 hours, please call the instructor's office, 404-894-2856. Please leave a voice message if the instructor is unavailable. Please do not try to make an urgent appointment within the same day by email. Email is not the right tool for emergencies.

Forums:

In this course, we use Forums on T-Square as the official communication tool instead of email. You can post any question here (projects, lectures, course schedule, etc). They will be viewed by other students, and it can be helpful to others. We ask you to state your questions clearly in a respectful manner (we may need to skip unclear questions).

Please note that helpful responses to messages posted on the forums will count towards "Participation" (see Grading section).

Questions on Forums will not be responded by the instructor or TA for the first 24 hours. We will wait for other students to respond in the first 24 hours. If nobody answers correctly, the instructor or TA will answer your questions.

Regrading

Requests for regrading of a homework assignment or an exam may be submitted in writing within one week of the day the homework or exam is handed back to the class (regardless of whether or not you attend class that day). You must justify in writing the technical basis for the regrade. If the regarding request is accepted, your entire homework or exam may be regarded (your grade may decrease after regarding). Please do not assume that your grade will always go up after regrading.

To create a fair environment for all students, all deadlines will be strictly enforced. If you experience a personal situation that makes it difficult for you to meet the requirements of this course, please consider contacting the Dean of Students, who can act as an advocate on your behalf (http://www.deanofstudents.gatech.edu/).

How to succeed in this course

- Read the textbook before/after each lecture.
- Come and see the instructor and TA. Ask plenty of questions.
- Check Forums on T-Square as frequently as possible.
- If you find it difficult to follow the lectures, or if you have any other concern, come and see the instructor/TA. We are always happy to help you. Some students need extra practice problems, and we can advise you.
- Do not copy someone else's work. Students caught cheating will be given a zero for the assignment and will be reported to the Dean of Students without any exception.