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Fall 2019

CHE 365-001: Chemical Engineering Computing

Roman S. Voronov

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ChE365 – Chemical Engineering Computing
Fall 2019
Otto H. York Department of Chemical, Biological & Pharmaceutical Engineering
New Jersey Institute of Technology

Course Schedule: W:600PM - 905PM, TIER411
Office Hours: Friday 3:00-5:00 PM, and MTRF after 5pm. Other times by appointment. Skype is possible.
Instructor: Dr. Roman S. Voronov, Assistant Professor
Instructor Contact: Tiernan Hall 378, 1.973.642.4762 (voicemail=slow), rvoronov@njit.edu (fast). Note, please avoid sending internal messages through 3rd party platforms like Moodle or Canvas.
Instructor Webpage: http://chemicaleng.njit.edu/people/rvoronov.php

Teaching Assistant: Anne Tong and Danh Nguyen
TA Contact: anh.tong@njit.edu
danh.t.nguyen@njit.edu

Please add ChE365 in the subject of your emails

Catalog Description: https://catalog.njit.edu/search/?P=CHE%20365

Specific goals for the course

a. The student will be able to

1. Master basic programming proficiency

2. Describe and interpret error and convergence

3. Solve Root searching problems using Bracketing and Open Methods, while assessing the trade-offs between them

4. Apply Optimization methods in order to search for maxima or minima of a function.

5. Represent and solve a system of linear equations in matrix form

6. Fit data using Linear Regression

7. Integrate functions Numerically

8. Differentiate functions Numerically

9. Solve Ordinary Differential Equations Numerically

10. Utilize advanced engineering software packages

11. Work on group exercises and apply a range of numerical methods to evaluate solutions to chemical engineering problems

12. Self-acquire Advanced Engineering Software Skills

13. Communicate Project Results in a Technical Writing Report Format

b. This course explicitly addresses the following student ABET outcomes: 1, 3, 5, 7

Textbooks: Required –
1) Applied Numerical Methods with MATLAB for Engineers and Scientists / Edition 4 by Steven Chapra. ISBN-13: 978-0073397962; ISBN-10: 0073397962. Alternatively, you may be able to get away with using the cheaper international or 3rd editions, at your own risk.

Note: Students may optionally purchase the electronic version of this book:
Connect Access Card for Applied Numerical Methods with MATLAB for Engineers and Scientists by Chapra, 4th edition, ISBN: 9781259547669

2) You already have the electronic copy of this book through NJIT libraries, so do NOT need to buy the hard copy (unless you really want to). Introduction to Chemical Engineering Computing 2nd Edition by Bruce A. Finlayson. ISBN-13: 978-1118888315; ISBN-10: 1118888316.

Recommended/Alternative Resources – 1) Numerical Methods for Chemical Engineers Using Excel, VBA, and MATLAB by Victor J. Law. ISBN-13: 9781466575349; 2) Numerical Methods for Engineers - 7th edition ISBN13: 9780073397924; ISBN10: 007339792X

Required Software: Latest versions of COMSOL, Matlab, MS Office, Adobe Reader (all can be downloaded from NJIT IST webpage). Student Mall labs and ChE department PC lab have most of the software. Please see Highlander Pipeline for Matlab tutorial and example programs.

Clickers: Required – we will use them to take some of the quizzes.

Grading (curved at the end of the course, if needed):
HOMEWORK (HW) — 5%
LABORATORY* – 25%
QUIZES – 15%
MIDTERM – 20%
INDIVIDUAL PROJECT — 15%
FINAL — 20%

*This course will implement an "active learning" environment. Therefore, a significant portion of the grade will depend on interactive assignments during class. Furthermore, the Laboratory grade for each chapter will depend on the homework grade as follows: LAB GRADE = IN-CLASS ASSIGNMENT GRADE * CORRESPONDING HOMEWORK GRADE. In other words, if you don't turn in a homework, you will get a zero for the corresponding lab as well; if you get a 50% on the homework, your lab grade will divided by half; and so on.

Grade Cut-offs
A = Above 90%
B+ = 80-89%
B = 70-79%
C+ = 65-69%

C = 60-64%
D = 50-59%
F = below 50%

Homework will be assigned through Moodle: http://moodle.njit.edu. Please check these sites and your email often. Most of the homework, quizzes and solutions will be on these sites, as well important course announcements.

There may be a gray area between each two letter grades in the final distribution, so that two students getting similar weighted average, at the border of grade categories, could get different letter grades. If you are in one of these gray areas, whether you get the higher or lower grade depends on whether your performance has been improving or declining over the course period and on your overall class participation (attendance/discussion etc.).

Important University Dates (Add/Drop/Refund/Last Day to Withdraw/Recess/Finals):
http://www.njit.edu/registrar/calendars/
http://www.njit.edu/registrar/exams/finalexams.php

Make-up sessions — If classes are cancelled due to inclement weather, students will be asked to attend make-up session(s) on a Saturday (TBA).

Class Attendance: Experience shows that students who do not regularly attend class typically perform poorly in the course. In addition, examples are worked out during the lectures. These examples are may not be posted online. Students are responsible for all material covered in class.

Office Hours Attendance: This time is for you to come and seek help in case you don't understand the material, have an English problem, or are concerned about your grade. Coming to office hours shows that you care about learning and positively affects both your performance and evaluation. Do not wait until the very end to do this!

Seating Chart: The instructor reserves the right to assign seating during the class lecture.

NJIT Honor Code: The NJIT honor code is being upheld on all issues related to the course. Students are expected to be familiar with the code and conduct themselves accordingly. Any violations will be brought to the immediate attention of the Dean of Students.

Academic integrity: Academic Integrity is the cornerstone of higher education and is central to the ideals of this course and the university. Cheating is strictly prohibited and devalues the degree that you are working on. As a member of the NJIT community, it is your responsibility to protect your educational investment by knowing and following the academic code of integrity policy that is found at: http://www5.njit.edu/policies/sites/policies/files/academic-integrity-code.pdf.

Please note that it is my professional obligation and responsibility to report any academic misconduct to the Dean of Students Office. Any student found in violation of the code by cheating, plagiarizing or using any online software inappropriately will result in disciplinary action. This may include a failing grade of F, and/or suspension or dismissal from the university. If you have any questions about the code of Academic Integrity, please contact the Dean of Students Office at dos@njit.edu.

A VERY *ROUGH* AND *PRELIMINARY* SCHEDULE FOR THE SEMESTER:

Lecture #	Date	Computing Method
1	09/04	INTRO TO COMPUTERS & CHE MODELING
2	09/11	CH 2-3: CHE COMPUTING FUNDAMENTALS
3	09/18	CH 4: ROUND OFF AND TRUNCATION ERRORS, CONVERGENCE
4	09/25	CH 5: ROOTS BRACKETTING METHODS
5	10/02	CH 6: ROOTS OPEN METHODS
6	10/09	CH 7: OPTIMIZATION
7	10/16	CH8-9: LINEAR SYSTEMS
8	10/23	CH14: CURVE FITTING
9	10/30	**MIDTERM (NOTE THAT THE EXACT DATE MAY CHANGE)**
11	11/06	CH17: INTERPOLATION
12	11/13	AICHE CONFERENCE (NO CLASS → WILL MAKE UP)
13	11/20	CH 19: NUMERICAL INTEGRATION
14	11/27	FRIDAY CLASSES MEET
15	12/04	CH 21: NUMERICAL DIFFERENTIATION
16	12/11	CH 22: ORDINARY DIFFERENTIAL EQUATIONS – INITIAL VALUE PROBLEMS
17	TBA	**FINAL**

Policies and Expectations about Exams/Grades

- The course letter grade will be assigned and **rounded** automatically by Excel (no emotions attached). The assigned letter grade is FINAL without subject to negotiation!
- Any excuses used to drop missed assignments or exams must first be documented with the Dean of Students.
- Students have to plan, study and do well in exams/HW if they want to get a good grade in this class. Instructor will NOT change letter grades to accommodate any special circumstances (unless excused by the Dean of Students). The student will get the letter grade he/she deserves.
- Students can dispute the assignment and exam scores within a week following the announcement of the score. Students **cannot** dispute their prior exams or assignments after one week or at the end of the semester! Furthermore, upon requesting grade review the student accepts the possibility of instructor both **removing points**, as well as giving points, in case grading mistakes are found.
- **Student handwriting must be legible in order to receive points.**
- **The graded exams must be returned within a week to be saved for the department course assessment initiative.**
- Students will get 0 for not showing up to quizzes, laboratory, exams, or any other course activity. If a student misses an exam due to extreme circumstances (such as a medical problem or a death in the family), he/she needs to notify the instructor via email **before** the beginning of the exam, and provide proof of the circumstance to the Dean of Student's office. Only in this case of official approval from the Dean of Student's office, may a make-up be given. When a student invokes extenuating circumstances for any reason (late withdrawal from a course, request for a make-up exam, request for an Incomplete grade) the student will be sent to the Dean of Students Office. The Dean of Students will be making the determination of whether extenuating circumstances exist or not and will be notifying the instructor accordingly. Instructors will never request or

accept medical or other documents from students; such documents need to be submitted by the student to the Dean of Students. Except for cases determined by law, an instructor is not required to accommodate student requests even when extenuating circumstances are certified by the Dean of Students; however, all efforts should be made to ensure a student-friendly environment.

- Extra credit may be assigned during the semester, at the discretion of the instructor. There will be no make-ups, extra credit, or any additional projects/assignments given beyond the semester's completion.
- **If cheat sheets are allowed on the exam, these must be hand-written (not typed or photocopied). They also cannot contain computer code, or homework solutions.**
- **When writing code, you may not "simplify" your assignment if all of your input data happens to fall within a single case scenario. Your code should be general enough to handle ALL possible input.**
- **During laboratory exercises, students may not leave if finished early. Instead, they are to assume TA roles and walk around (without computers) to help their classmates complete the assignment.**
- **If multiple students turn in identical (or very similar) code/assignment/exam, a single grade will be SHARED between those students.**
- If you need accommodations due to a disability please contact the Associate Director of Disability Support Services, Fenster Hall Room 260 to discuss your specific needs.   A Letter of Accommodation Eligibility from the Disability Support Services office authorizing your accommodations will be required.

Most important: Have lots of fun!