**ChE365 – Chemical Engineering Computing**
**Fall 2024**
**Otto H. York Department of Chemical & Materials Engineering**
**New Jersey Institute of Technology**

**Course Schedule**: Wednesdays 6:00 PM - 10:05 PM at CKB G-08.
**Zoom/Office Hours:**  Wednesday 4:00-5:00 PM. Other times by appointment.  Note, you *must* let me know ahead of time if you plan on joining an online session, otherwise I won't be expecting you.
**Instructor:** Dr. Roman Voronov, Associate Professor
**Instructor Contact:** Tiernan Hall 378, 1.973.642.4762 (voicemail=slow), rvoronov@njit.edu (fast). Please include the course number and problem number your question is about in the subject of your email. Note, please avoid sending internal messages through 3rd party platforms like Moodle or Canvas.
**Instructor Webpage:** http://chemicaleng.njit.edu/people/rvoronov.php

**Join the Department's Linked in Profile and Group for networking opportunities**:
https://www.linkedin.com/in/njitcme/
https://www.linkedin.com/groups/8907579/

**Teaching Assistant:**  Haq, Muhtasim <mah239@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:**
1) Applied Numerical Methods with MATLAB for Engineers and Scientists / Edition 5 by Steven Chapra. ISBN10: 126416260X | ISBN13: 9781264162604. Alternatively, you may be able to get away with using the cheaper international or older editions, at your own risk. https://www.mheducation.com/highered/product/applied-numerical-methods-matlab-engineers-scientists-chapra/M9781264162604.html Or, you may optionally purchase the electronic version of this book.

Recommended/Alternative Resources
1) free MATLAB textbook (see video description) about numerical methods in chemical engineering with supporting YouTube lecture videos: https://www.youtube.com/watch?v=OUPgLw56-p0&list=PLRihodfxzBsVb_xaas2pufgNCxt8oOjSs

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 2$^{nd}$ Edition by Bruce A. Finlayson. ISBN-13: 978-1118888315; ISBN-10: 1118888316.

3) 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

4) Website with lots of Matlab examples: http://matlab.cheme.cmu.edu/

**Required Software**: Latest versions of **Matlab (must be installed prior to the first-class period!)**, COMSOL, 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.

Mathworks Grader: Students are required to create a free account at https://grader.mathworks.com/ and register for the Che365 course there.

Grading (curved at the end of the course, if needed):
HOMEWORK (HW) — 5%
QUIZES – 15%
PROJECT — 10%
LABS:

| # | GROUP CONTRIBUTION | INDIVIDUAL CONTRIBUTION |
|---|---|---|
| 1 | 5.00% | 0.00% |

| | | |
|---|---|---|
| 2 | 4.50% | 0.50% |
| 3 | 4.00% | 1.00% |
| 4 | 3.50% | 1.50% |
| 5 | 3.00% | 2.00% |
| 6 | 0.00% | 7.50% |
| 7 | 2.50% | 2.50% |
| 8 | 2.00% | 3.00% |
| 9 | 1.50% | 3.50% |
| 10 | 1.00% | 4.00% |
| 11 | 0.50% | 4.50% |
| 12 | 0.00% | 5.00% |
| 13 | 0.00% | 7.50% |

This course will implement an "active learning" environment.  Therefore, a portion of the grade will depend on interactive assignments during class (i.e., "Labs").  Hence, your participation in class work will be graded.  In the *group* format you are allowed to talk to your groupmates only, while in the *individual* mode you may only ask questions from the TA or the instructor.   The labs may be either computer- or paper-based. In other words, you may be asked to write and/or debug code on paper (without computer access).

A portion of your *group* lab grade will also depend on how your groupmates grade your contribution.  The groups will be up to the instructor.

Grade Cut-offs

| Percent | Grades |
|---|---|
| >= 90% | A |
| >= 85% | B+ |
| >= 80% | B |
| >= 75% | C+ |
| >= 70% | C |
| >= 60% | D |
| < 60% | F |

Homework and exams will be assigned through Canvas:  https://canvas.njit.edu/ – Please check this site and your email often.  Most of the homework, quizzes and solutions will be on this site, as well as 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:** Students must be present in class to receive any credit on the quizzes, labs, assignments or tests that occurred during it. Also, 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.

**Online Synchronous Delivery**: If the class is to meet via video conferencing (e.g., Webex, Zoom, or similar) software. Students must keep their webcams ON at all times. NO audio or video recording is allowed. Nonoffending virtual backgrounds are allowed to maintain privacy. The use of offending backgrounds is not allowed and will be punished.

**Cell phones and other electronic devices:** must be turned off during both lectures and exams, unless specifically permitted by the instructor. For example, the use of personal computers or tablet devices for attending the video conferencing lectures is allowed.

**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:**

| Class #-Date | Computing Method | LAB # |
|---|---|---|
| 1-Sept 4 | INTRO TO COMPUTERS & CHE MODELING | x |
| 2-Sept 11 | CH 2-3: CHE COMPUTING FUNDAMENTALS | x |
| 3-Sept 18 | CH 4: ROUND OFF AND TRUNCATION ERRORS, CONVERGENCE | 1 |
| 4-Sept 25 | CH 5: ROOTS BRACKETTING METHODS | 2 |
| 5-Oct 2 | CH 6: ROOTS OPEN METHODS | 3 |

| 6-Oct 9 | CH 7: OPTIMIZATION | 4 |
|---|---|---|
| 7-Oct 16 | CH8-9: LINEAR SYSTEMS | 5 |
| 8-Oct 23 | PUTTING IT ALL TOGETHER | 6 |
| x-Oct 30 | AICHE CONFERENCE (NO CLASS) | x |
| 10-Nov 6 | CH14: CURVE FITTING | 7 |
| 11-Nov 13 | CH17: INTERPOLATION | 8 |
| 12-Nov 20 | CH 19-20: NUMERICAL INTEGRATION | 9 |
| x-Nov 27 | FRIDAY CLASSES MEET | x |
| 13-Nov 27 | CH 21: NUMERICAL DIFFERENTIATION | 11 |
| 14-Dec 4 | CH 22: ORDINARY DIFFERENTIAL EQUATIONS – INITIAL VALUE PROBLEMS | 12 |
| 15-Dec 11 | ADVANCED SOFTWARE / PROJECTS | x |
| 16-Dec 18 | PUTTING IT ALL TOGETHER | 13 |

**Policies and Expectations about Exams/Grades**

- Absolutely no late work is accepted unless stated otherwise by the course instructor
- 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 by 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 grade prior exams or assignments after the one week or after the course grades have been issued! Furthermore, upon requesting a grade review the student accepts the possibility of instructor **removing points** in case grading mistakes are found. All disputes must be directed to the course instructor (and not to the TA) via email.
- **Student handwriting must be legible in order to receive points.**
- **The graded paper exams and assignments must be returned to the instructor 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.**
- **If any of in-class assignments or laboratories are due after class, students must be present during the entire class of the lab or assignment in order to receive any credit for it.   In other worse, students may not complete in-class labs or assignments outside of class, unless explicitly allowed to do so by the course instructor.**
- **Even though homework is assigned through Canvas, students must still bring a hard copy of their solutions to class and show it to the TA to receive credit.**
- **Computer codes submitted for both labs and exams must run without errors to receive partial credit.**
- **During laboratory exercises, students may not leave if they finish early. Instead, they should sit quietly until the end of the class, unless they are explicitly allowed to 'check out' and leave by the instructor.  Specifically, to leave early, students need to 'check out' with the TA by showing the grade earned prior to leaving so that it can be recorded.  By leaving early students agree that the recorded grade will be their final grade, which cannot be improved after they have left the class.  Leaving without 'checking out' may trigger a cheating investigation and *will* result in lost credit for the assignment.  This policy is intended to prevent cheating.**
- **During the *group* laboratory exercises, students may not communicate with anyone outside of their group.**
- **During the *individual* laboratory exercises, students may not communicate with anyone besides the instructor or the TA.**
- **Students may NOT seek help from someone outside of the class on any of the in-class laboratory exercises, homework assignments, quizzes tests or projects.**
- **Students may NOT use course materials from the previous semesters, unless such materials have been explicitly shared with them by the instructor.**
- **Students may NOT use code from online resources, unless explicitly allowed to do so by the course instructor.**
- **Students may NOT post course materials to external resources, such as Chegg.com and others, even after they have finished the course.**
- **Students may NOT share course materials with other students or persons, even after course completion.  Doing so may result in penalties to the grade that has already been earned.**
- **If multiple students turn in identical (or very similar) code/assignment/exam, this is considered to be a violation and the case will be turned over to the Dean of Students for further examination.  In class group labs do not fall under this policy.**
- **Any homework, individual labs not finished in class, and take-home exams must be done *individually*.**
- **-There seems to be some misunderstanding that it is possible to keep working after the deadline, because the instructors and the TA to stay and help students debug their code after class.  However, your grade is your best attempt that was submitted BEFORE the announced deadline (which is also listed as the 'due' date on Canvas).  Although the platform allows you to keep working on the code after the deadline AND shows the most recent grade (even if its officially 'late') in the**

**gradebook, only 'on-time' scores will be considered. Also, unfortunately, there is no way I can get Canvas to take the best attempt, as it only cares about the last attempt. So, if there is any inconsistency in your grading, please email us and we will correct it.**

- **Please start setting up your ProctorU screen recording ahead of the class start-time. I will try my best to have it available about 5-10 minutes ahead of time. You do NOT need to wait until the lab formally starts to turn on your screen recording. Furthermore, 99% of the ProctorU issues are fixed by restarting the browser and going through the setup process from scratch. So try that a few times before calling for help.**

- 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.

- *NJIT policy requires that all midterm and final exams must be proctored, regardless of delivery mode, in order to increase academic integrity. Note that this does not apply to essay or authentic based assessments. Effective beginning Fall semester 2019, students registered for a fully online course section (e.g., online or Hyflex mode) must be given the option to take their exam in a completely online format, with appropriate proctoring.*

- Class Recordings: Class sessions may be recorded by the instructor. These recordings shall only be used as an educational resource and are not to be distributed or used outside of this class. Information on how to access recorded lectures will be made available by your instructor. Any recordings that contain identifiable information about students will not be used beyond this semester.

- Class Recording Etiquette: Students are expected to respect their fellow students' privacy and freedom to learn without disruption. Students are not allowed to capture or reproduce anyone's name, image, or voice without permission. They must be polite and respectful in the online chat. Informal chat is okay, but typing is restricted to things that one would say out loud in front of the entire class. Students must always conduct themselves on their webcam video as they would in person in a classroom.

- Eating and drinking in class is subject to the instructor's approval.

- Course assignments and labs may be proctored via 3rd party services, such as ProctorU+, which may implement human and/or AI proctoring, or a combination thereof.

- Absolutely no artificial intelligence of any kind (e.g., ChatGPT) is allowed in this course without the explicit permission of the instructor.


**Most important:** Have lots of fun!