14:155:307 – Computational Methods in Chemical Engineering (Spring 2025)

Lectures Monday/Thursday 10:20-11:40 AM in Engineering C-233

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Textbooks
1. [official] Chapra and Canale, "Numerical Methods for Engineers", 8th edition (2021), McGraw-Hill
2. [supplementary] Riggs, "Computational Methods for Chemical Engineers", (2020), Ferret Publishing

Course description
This course introduces students to numerical methods for solving a variety of problems in the context of chemical engineering. Students will learn general and transferrable computational principles, best practices, and strategies for approaching chemical engineering problems computationally (and debugging said approaches). Students will learn the theoretical and mathematical foundations for these numerical methods and gain hands-on experience in implementing these methods in both MATLAB and Python, as well as an understanding of advantages or motivation for using one language over another.

Learning objectives
Students will learn to use MATLAB and Python to perform numerical calculations, write and run scripts and functions, solve algebraic and differential equations numerically, and perform optimization and regression. Students will learn how to apply this computational toolset to solve complex chemical engineering problems.

Software
Please install MATLAB and check your access to Google Colab as soon as possible.
(1) MATLAB: Download the version of MATLAB provided through the official Rutgers software portal (software.rutgers.edu). You will need to log in using your Rutgers credentials in order to download the installer.
(2) Python: We will use Google Colab (colab.research.google.com), which allows you to write and execute Python from within your browser. You should be able to access this with your ScarletMail account.

Assessment / Grading

Homework	35%
Quizzes	25%
Midterm exam	20%
Final exam	20%

Homeworks
Homework assignments will be due 11:59PM on their designated due date (Fridays). Each completed problem set should be submitted by uploading a file to Canvas. Students are encouraged to work together on problem sets, but each student must submit their own work (see Academic Integrity). Late homework will be deducted 10% per day for first two days past its deadline, and 20% per day for three days late and beyond. Unsubmitted homework will receive a grade of zero. Solutions to problem sets will be posted on Canvas once submissions have been received from all students.

Getting Help with Code
When seeking help with code-related issues, students must provide the following:
1. A screenshot or copy of the code exactly as it was run
2. The output and any error message that is produced
3. Their interpretation of the error message, if there is one
4. A description of what they have already tried on their own

Following these steps helps you develop your own debugging skills and helps the instructor and TA more effectively answer your question. Requests must have this information in order to be answered.

Commenting Requirements
All code submissions must include clear and concise comments that:

1. Explain the overall purpose of the script/function at the beginning
2. Document each major step or block of code
3. Explain any non-obvious calculations or procedures
4. Define key variables and their units

Comments help both you and the graders understand your work. Code submitted without adequate commenting will lose points. Simply running your code correctly is not enough—it is also important to communicate your intentions to anyone who may reference or modify your code after you write it.

External Resources & AI Tools
You are welcome to use external resources including AI tools, Stack Overflow, online tutorials, or other resources to help you learn. If you use approaches that differ from what is taught in class on your homework, you must note your sources in your comments, be able to explain your solution, and be prepared to justify your work and approach on a closed-resource quiz or exam.

Attendance Policy
Attendance is not mandatory, but strongly encouraged. Absences due to religious observances will be excused. Please let me know in writing at least two days in advance so that we may accommodate for any conflicts with assignments or exams.

Ethics & Academic Integrity
Students are expected to be familiar with and to follow the University's policy on academic integrity, which can be found at http://academicintegrity.rutgers.edu. Engineering is a profession demanding a high level of integrity and responsibility in collaborative environments. Students are encouraged to work together on problem sets, review course materials together, and learn from one another. However, cheating, plagiarizing, or misrepresenting another individual's work as one's own will not be tolerated. Assignments or exams in violation of this policy will be reported and given a grade of zero.

Learning Accommodations

Rutgers University is committed to creating an inclusive and safe learning environment for all students. Students with disabilities are welcome to request accommodations through the Office of Disability Services (ODS). You can contact ODS at 848-445-6800 or via email at dsoffice@echo.rutgers.edu. Please submit requests to ODS as early in the term as possible, as accommodations are not retroactive. Letters of accommodation and arrangement of accommodations can be discussed in private during office hours or by special appointment.

Course Schedule

Week	**Dates** (M,Th)	**Topics**	**HW Due** (Fri 11:59PM)
1	1/23	Course introduction, Intro to MATLAB & Python, Best Practices	
2	1/27 1/30	Continue Intro to MATLAB & Python, Best Practices, Plotting and Visualization	HW 1
3	2/3 2/6	Numerical differentiation & integration, Polynomial Approximations	HW 2
4	2/10 2/13	Single linear and non-linear equations Quiz (2/13)	HW 3
5	2/17	Systems of linear equations	HW 4

	2/20		
6	2/24 2/27	Systems of non-linear equations Quiz (2/27)	HW 5
7	3/3 3/6	Practice Problems	
8	3/10 3/13	Review + Midterm Exam (Th 3/13)	
Spring Break			
9	3/24 3/27	Initial Value Problems	HW 6
10	3/31 4/3	Initial Value Problems Quiz (4/3)	HW 7
11	4/7 4/10	Boundary Value Problems	HW 8
12	4/14 4/17	Optimization Quiz (4/17)	HW 9
13	4/21 4/24	Regression	HW 10
14	4/28 5/1	Practice Problems	
15	5/5	Review for Final Exam	
	5/12	Final Exam (Mon 5/12 8AM-11AM)	