Spring 2021

CHE 490-002: Special Topic - Python Programming for Chemical Engineers

Gennady Gor

1. **ChE 490: ST - Python for Chemical Engineering Calculations**
2. **Credits and contact hours:** 3-0-3 (3 lecture hr/wk - 0 lab hr/wk - 3 course credits)
3. **Course Coordinator or Instructor:** Gennady Gor
4. **Textbook:** not required, class notes will be provided
5. **Specific course information**

    a. **Description:** Modern engineering calculations are hard to imagine without a flexible and efficient programming language. Python is such a language. Python is open source, free, easy to learn, and simple to use. These factors make Python one of the most popular programming languages in the world, highly demanded by employers. The goal of this course is to introduce undergraduate ChemE students to Python, (including NumPy and SciPy) and demonstrate how it can be used for solving a spectrum of chemical engineering problems.

    b. **Prerequisites:** none

    c. **Required, Elective, or Selective Elective** - Elective

6. **Specific goals for the course**
   A student should be able to:

    a. Utilize Python to solve problems within the ChemE curriculum:

        1. Systems of linear and non-linear equations (CPC, Separations)
        2. Initial and boundary value problems (Fluid flow, Heat and Mass, Kinetics)
        3. Integration, differentiation, interpolation, data regression (Thermo)
        4. Optimization (Thermo, Control, Design)

    b. Utilize Python for working on research projects

    c. Utilize Python for solving practical problems in industry

   This course explicitly addresses the following student outcomes: 1

7. **Topics**

    1. Basics of Python
    2. Debugging, Collaboration, Version control
    3. NumPy: working with data
    4. SciPy: integration, optimization, statistics
    5. Application of Python to solve selected problems from ChemE curriculum
    6. Application of Python for experimental and modeling research in ChemE
    7. Industry perspectives (software engineering and chemical engineering)

ChE 490: ST - Python for ChemE Calculations
Synchronous Online Course, Spring 2021

Instructor: Dr. Gennady Gor, Assistant Professor
Office/Lab: 357/321A Tiernan Hall, Phone: 973-596-2944, E-mail: gor@njit.edu
Class: Monday, Wednesday 11:00 AM – 12:20 PM; Room: online, WebEx link
Office Hours: Tuesday, Thursday 3:00 PM – 4:00 PM; Room: online; WebEx link
Additional appointments can be made by email.

Course Description and Requirements

Modern engineering calculations are hard to imagine without a flexible and efficient programming language. Python is such a language. Python is open source, free, easy to learn, and simple to use. These factors make Python one of the most popular programming languages in the world, highly demanded by employers. The goal of this course is to introduce undergraduate ChemE students to Python, (including NumPy and SciPy) and demonstrate how it can be used for solving a spectrum of chemical engineering problems.
Pre-Requisites: the course does not have formal pre-requisites, however it is expected that the students have strong ChemE fundamentals (CPC, Thermo I, Fluid Flow). Additionally strong math background is required (Calculus, Differential Equations).

Course Objectives

Taking this course, a motivated student will learn to:

a. Utilize Python to solve problems within the ChemE curriculum:

   1. Systems of linear and non-linear equations (CPC, Separations)
   2. Initial and boundary value problems (Fluid flow, Heat and Mass, Kinetics)
   3. Integration, differentiation, interpolation, data regression (Thermo)
   4. Optimization (Thermo, Control, Design)

b. Utilize Python for working on research projects

c. Utilize Python for solving practical problems in industry

Learning Materials

Course webpage on Canvas: https://njit.instructure.com/courses/15834. All the updates and homework assignments will be posted on Canvas webpage. It is the students' responsibility to check the course webpage on a regular basis.
Textbook: There is no textbook, all the resources will be provided in the form of slides and lecture notes.
Other Learning Material: Video lectures will be recorded and made available on Canvas or Youtube. Links to additional online resources will be provided.
Hardware: An up-to-date personal computer will be required to participate in class. Any OS will work: MacOS, Windows, or Linux.
Software: Python is free and does not require a license. Installation instruction will be provided.

Course Outline

Class	Date	Topic (preliminary, subject to changes)
1	Jan. 20	Why do we need Python: Motivational Examples.
2	Jan. 25	Python Installation and Environment. Basics: Variables, Types, Strings.
3	Jan. 27	Basics of Python: Math, Boolean, Conditional Statements, Lists, Loops.
4	Feb. 1	Basics of Python: Math, Functions, Working with files.
5	Feb. 3	Basics of Python: Data structures (lists, tuples, dictionaries).
6	Feb. 8	Classes and Objects. Structure of Code. Debugging.
7	Feb. 10	Guest Lecture 1: Software Engineering Perspective on Python
8	Feb. 15	Versions. Collaboration. Git.
9	Feb. 17	NumPy: Array Math, Reading and writing data.
10	Feb. 22	NumPy: Plotting and Curve-fitting. Examples from Thermo.
11	Feb. 24	SciPy: Linear algebra. Examples from CPC.
12	Mar. 1	SciPy: Numerical integration.
13	Mar. 3	SciPy: Optimization. Examples from Thermo.
14	Mar. 8	SciPy: Statistics. Example: working with experimental data.
15	Mar. 10	SciPy: ODE. SymPy. Examples from Heat and Mass.
	Mar. 14-21	Spring recess.
16	Mar. 22	Midterm exam.
17	Mar. 24	CoolProp: Calculations for Thermodynamics.
18	Mar. 29	Guest Lecture 2: Materials Science Perspective on Python
19	Mar. 31	Research Example: Molecular thermodynamics.
20	Apr. 5	Research Example: Monte Carlo method.
21	Apr. 7	Research Example: Gas adsorption models.
22	Apr. 12	Research Example: Evolution of aerosols.
23	Apr. 14	Working with data. Pandas.
24	Apr. 19	Guest Lecture 3: Chemical Engineering Perspective on Python
25	Apr. 21	Python and Excel.
26	Apr. 26	Interfacing Python with C++
27	Apr. 28	Guest Lecture 4: Data Science Perspective on Python
28	May 3	Final project discussions

Guest Lectures

In order to bring the industry perspective to this course several guest lectures will be given by the lecturers working full time in industry:

- Guest Lecture 1: Speaker – Michael Pliskin (MS, Computer Science, Engineering Manager at Google) Software Engineering Perspective on Python
- Guest Lecture 2: Speaker – Jonghun Lee (Ph.D. Chemistry, Research Scientist at Colgate-Palmolive) Materials Science Perspective on Python
- Guest Lecture 3: Speaker – Christopher Rasmussen (Ph.D. Chemical Engineering, Senior Scientist at Zymergen, Inc.) Chemical Engineering Perspective on Python
- Guest Lecture 4: Speaker – TBD, Data Science Perspective on Python

Assessment and Grading

Homework: Homework assignments will be given regularly. The assignments will be posted on Canvas. The homework (including reading, watching video lectures, and problems assignments) must be completed by 11:59PM a day before the next class, unless otherwise is explicitly stated. Late assignments will be accepted with a penalty of 20% for each day (full or partial) it is late. If the solution for assigned problem was posted or discussed in class, late assignment will not be accepted. The homework assignment will be of two types: individual and team assignments.
Quizzes: Regular quizzes will be given based on the homework material, including both concepts and problems. The quizzes will not be announced in advance, so please be prepared to have a quiz during every class. No make-up quizzes will be allowed. All quizzes will be closed book with no material allowed. The quizzes will often take place at the beginning of the class, so being on time is strongly encouraged. Online quizzes will be proctored using the Respondus and Lockdown Browser and other tools used by NJIT, see https://ist.njit.edu/respondus. Late quizzes will not be accepted.
In-class activities: Students will need to participate in regular in-class activities, which will be mostly Python exercises and problem sets. Work on in-class activities is individual, and any cooperation will be considered as violation of honors code, unless team work is explicitly stated in the assignment. Late in-class activities will be accepted with a penalty of 20% for each day (full or partial) it is late.
Weights: The weights for each of the quizzes, homework, and in-class activities will be 0.5%, 1% or 1.5% of the total grade.
Exams: There will be two exams: one midterm and the final exam. The final exam will be cumulative. The exams will be project-based. Each student will get an individual project which will include solving problems and require writing a report in the form of a detailed narrative. After the report is submitted, each student will have to defend their report orally. The defense will include a set of questions on the details of the solution, as well as concept questions related to the project. The weight of the oral defense can be up to 50% of the exam grade. The defense will take place using a WebEx video call with the instructor. Each project defense will be recorded.

Homeworks Quizzes In-class activities	45%
Midterm Exam/Project	25%
Final Exam/Project	30%
	100%

Percent	Grades
$\geq 90\%$	A
$\geq 85\%$	B+
$\geq 80\%$	B
$\geq 75\%$	C+
$\geq 70\%$	C
$\geq 60\%$	D
$< 60\%$	F

Important Dates

- Midterm exam: March 22, 2021
- Final exam: between May 7 and 13, 2021
- Withdraw Deadline: April 5, 2021

Policies

Academic Integrity

- A student should be familiar with the University Policy on Academic Integrity
- Any violations of academic integrity will be reported to the Dean of Students
- Any collaboration is prohibited unless explicitly stated in the assignment
- When collaborations are allowed they include discussion, but not exchange of the code
- If a team assignment assumes team work on the code, the authors of different parts of the code should be clearly stated
- Copying or adapting code which is not yours is plagiarism
- Copying code from others (other students, or sources on Internet) is cheating
- If you are using pieces of code from the course materials provided by instructor, a comment should be added where the code comes from
- Students cannot share any of the course materials (including assignments), with anyone outside the ChE 490 class, or post any of the materials on the Internet

Special Needs

If you need accommodations due to a disability please contact Chantonette Lyles, 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.

Lectures

- This is synchronous online class, thus attendance is required and will be recorded. Students who do not attend a class cannot earn the points for in-class activities.
- Cameras should be ON during the classes.
- The classes start at 11:00, and the students must be in class by that time. Being late to class may have consequences for the grade, since many of the classes will start from quizzes.
- Electronic devices other than laptops/desktops used for coding (such as tablets, cell-phones etc.) are not permitted during the classes. No audio or video recording is allowed.
- Cellphones should be turned off during both regular classes and exams and not allowed under any circumstances.
- No eating any time during the classes.

Course materials, office hours and correspondence

- The course Canvas page is the main platform for delivering information about the course. All relevant course materials and assignments will be posted on Canvas, so a student should check it regularly.
- The students have to upload a professional-looking head shot for their Canvas profile.
- All the communications should be done via email (not Canvas), emails will be responded within 24 hours.

- E-mail correspondence is intended only for quick questions. Questions which require a detailed discussion should be discussed during the Office Hours.
- All correspondence should be conducted in a professional style, using formal English.
- To assure quick response to your emails, please add "ChE 490" in the subject of your emails.
- The instructor reserves the right not to respond to emails if the email does not have a greeting or a signature.

Exams, Quizzes, Homeworks and Grades

- A letter grade is based on the final score, calculated using an Excel spreadsheet in accordance with the Tables given in this syllabus. The assigned letter grade is final and cannot be negotiated.
- A student can dispute the exam scores within a week after the announcement of the score. Exam scores can be disputed during the official Office Hours, not during class time or via email.
- Students will get zero for not coming to quizzes, exams, or any other course activity.
- If students miss an exam due to extreme circumstances (such as a medical problem), they need to notify the instructor via email before the beginning of the exam, and bring proof of the circumstance to the Dean of Student's office. Only in the case of official approval from the Dean of Student's office, a make-up exam can be given.
- If a student misses a quiz or an in-class activity due to a legitimate reason (absence approved by the Dean of Students), the student has to take this quiz/in-class activity within a week after being back, during the Office Hours.
- If a student does not take the missed quiz/in-class activity within a week, the student gets zero for this assignment.

Honors Section

In addition to the regular section, and honors section will be offered. Up to 50% of the homework problem assignments, and both exam projects for the honors section will be different compared to the regular section.