1. **ChE 365 - Chemical Engineering Computing**
2. **Credits and contact hours:** 2-2-3 (2 lecture hr/wk - 2 lab hr/wk - 3 course credits)
3. **Course Coordinator or Instructor:** Gennady Gor
4. **Textbook:** Applied Numerical Methods with Python for Engineers and Scientists, 1st Edition, Steven Chapra and David Clough, ISBN10: 1266651497, ISBN13: 9781266651496.
   Note that hands-on programming experience on the level of CS115 is required (it is a pre-requisite). The course will use Python programming language, prior knowledge of which is not required, but would certainly help. The course will include the basic Python training. The main Python learning materials are the video lectures recorded by the instructor and available on his YouTube channel
   Online videos: https://www.youtube.com/playlist?list=PLWx-kn1Xf12a77HKLCtZn4E2cjjjoL8N8
5. **Specific course information**
   a. **Description:** Introduction to basic concepts of computational methods for solving chemical engineering problems and performing process simulations. Topics include common numerical techniques encountered in chemical engineering, for the solution of linear and nonlinear algebraic equations and ordinary differential equations, differentiation/integration, optimization and interpolation/regression of data. Students will be exposed to modern computational software and commercial chemical processes simulators.
   b. **Prerequisites:** ChE 370, CS 115. **Co-requisites:** ChE 360.
   c. **Required, Elective, or Selective Elective** - Required
6. **Specific goals for the course**
   a. A student should 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 outcomes: 1, 3, 5, 7

ChE 365: Chemical Engineering Computing
Spring 2023

Instructor: Dr. Gennady Gor, Associate Professor, https://people.njit.edu/faculty/gor
Office/Lab: 357/321A Tiernan Hall, Phone: 973-596-2944, E-mail: gor@njit.edu
Teaching Assistant: Santiago Flores Roman, Ph.D. student, E-mail: saf5@njit.edu;

Class: Monday, Wednesday, 11:30 AM - 01:35 PM; Room: Tiernan Hall 411
Office Hours: TBD; Room: 373 Tiernan Hall
Additional appointments can be made by email.
Course Web Page: https://njit.instructure.com/courses/27252

Course Description and Requirements

Introduction to basic concepts of computational methods for solving chemical engineering problems and performing process simulations. Topics include common numerical techniques encountered in chemical engineering, for the solution of linear and nonlinear algebraic equations and ordinary differential equations, differentiation/integration, optimization and interpolation/regression of data. Students will be exposed to modern computational software and commercial chemical processes simulators.
Pre-Requisites: ChE 370, CS 115. **Co-requisites:** ChE 360.

Course Objectives

Taking this course, a student should 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

Learning Materials

Textbook Required: Applied Numerical Methods with Python for Engineers and Scientists, 1st Edition, Steven Chapra and David Clough, ISBN10: 1266651497, ISBN13: 9781266651496.
Other Learning Material: The textbook is the main source for preparing for classes and reading the textbook before each class is necessary. Additional materials will be posted on Canvas https://njit.instructure.com/courses/27252
Note that hands-on programming experience on the level of CS115 is required (it is a pre-requisite). The course will use Python programming language, prior knowledge of which is not required, but would certainly help. The course will include the basic Python training. The main Python learning materials are the video lectures recorded by the instructor and available on his YouTube channel
Online videos: https://www.youtube.com/playlist?list=PLWx-kn1Xf12a77HKLCtZn4E2cjjjoL8N8
Computer: Students have to bring their laptops to every class. The laptops' batteries have to be charged, as power outlets may not necessarily be available. In-class activities and quizzes will require use of laptop computers. In-class use of computers at times other than for in-class activities or quizzes is not permitted.
OS: Any OS will work: Linux, Windows or MacOS, as long as it supports the necessary software.
Software: Python 3 and Anaconda should be installed. Respondus and LockDown Browser should be installed and functioning.

Course Outline

Class	Date	Topic (preliminary, subject to changes)
1	Jan. 18	Mathematical Modeling in Chemical Engineering
2	Jan. 23	Analytical and Numerical Methods for Solving ChemE Problems
3	Jan. 25	Straight-Line Linear Regression
4	Jan. 30	Use of Linear Regression and Linearization
5	Feb. 1	Polynomial Interpolation: Newton Polynomials
6	Feb. 6	Polynomial Interpolation: Lagrange Polynomials
7	Feb. 8	Linear Algebraic Equations
8	Feb. 13	Basics of Matrix Algebra
9	Feb. 15	Root Finding. Bracketing Methods: Graphical and Incremental Search
10	Feb. 20	Root Finding. Bracketing Methods: Bisection and Regula Falsi
11	Feb. 22	Root Finding. Open Methods: Newton-Raphson, Fixed Point Iteration
12	Feb. 27	Root Finding. Open Methods: Wegstein and Modified Secant Method
13	Mar. 1	Root Finding. Brent's Method
14	Mar. 6	Optimization. Single Variable.
15	Mar. 8	Optimization. Multivariable.
	Mar. 13	*Spring Break.*
	Mar. 15	*Spring Break.*
16	Mar. 20	**Midterm Exam.**
17	Mar. 22	Numerical Integration: Trapezoidal Rule and Newton-Cotes Formulas
18	Mar. 27	Numerical Integration: Simpson 1/3 and 3/8
19	Mar. 29	Numerical Integration of Functions
20	Apr. 3	Binary Numbers
21	Apr. 5	Roundoff and Truncation Errors
22	Apr. 10	Roundoff and Truncation Errors
23	Apr. 12	Numerical Differentiation
24	Apr. 17	Initial Value Problems: Euler's Method and Improvements
25	Apr. 19	Initial Value Problems: Runge-Kutta Methods
26	Apr. 24	Initial Value Problems: Systems of Equations
27	Apr. 26	Boundary Value Problems
28	May. 1	Boundary Value Problems for Non-Linear ODEs
	May. 5	Final exams begin
	May. 11	Final exams end

Important Dates

- Midterm exam: March 20, 2023
- Final exam: between May 5 and 11, 2023
- Withdraw Deadline: April 3, 2023