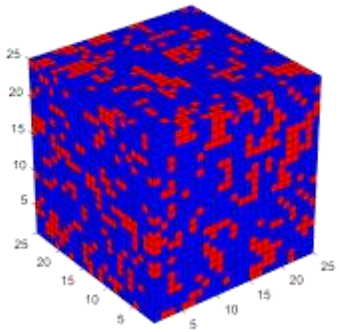
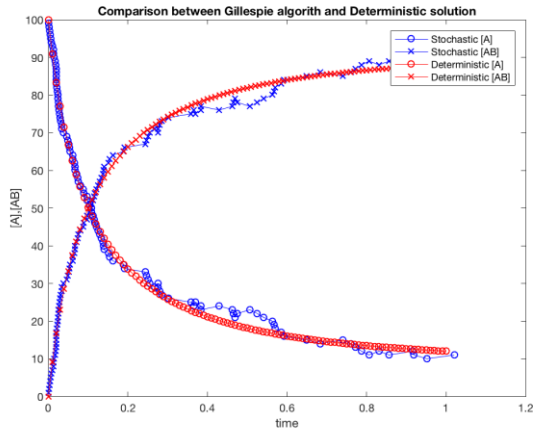
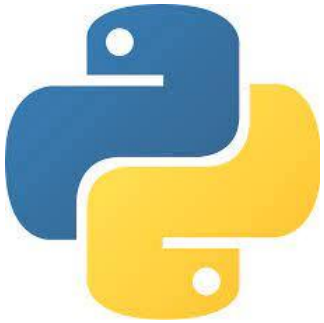
# WELCOME TO CHEM260

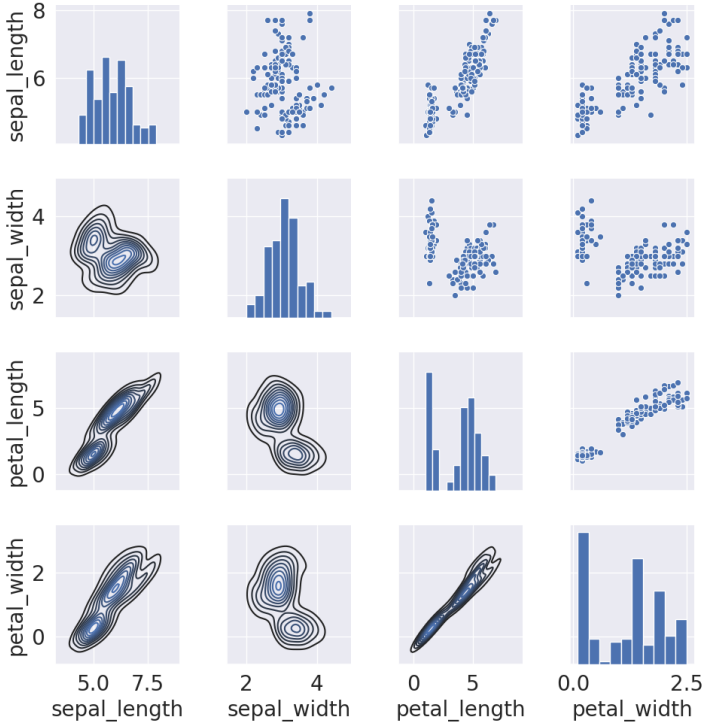


matplotlib

pandas






seaborn

NumPy

# About me

- Contact:

  **Email:** ssukenik@ucmerced.edu (subject line should have **CHEM260**)

  **Slack:** More details today

  **Office hours:** after class or by appointment

- Research topic: Protein biophysics – disordered protein

- History with coding: Never formally learned to code

- Why this course?

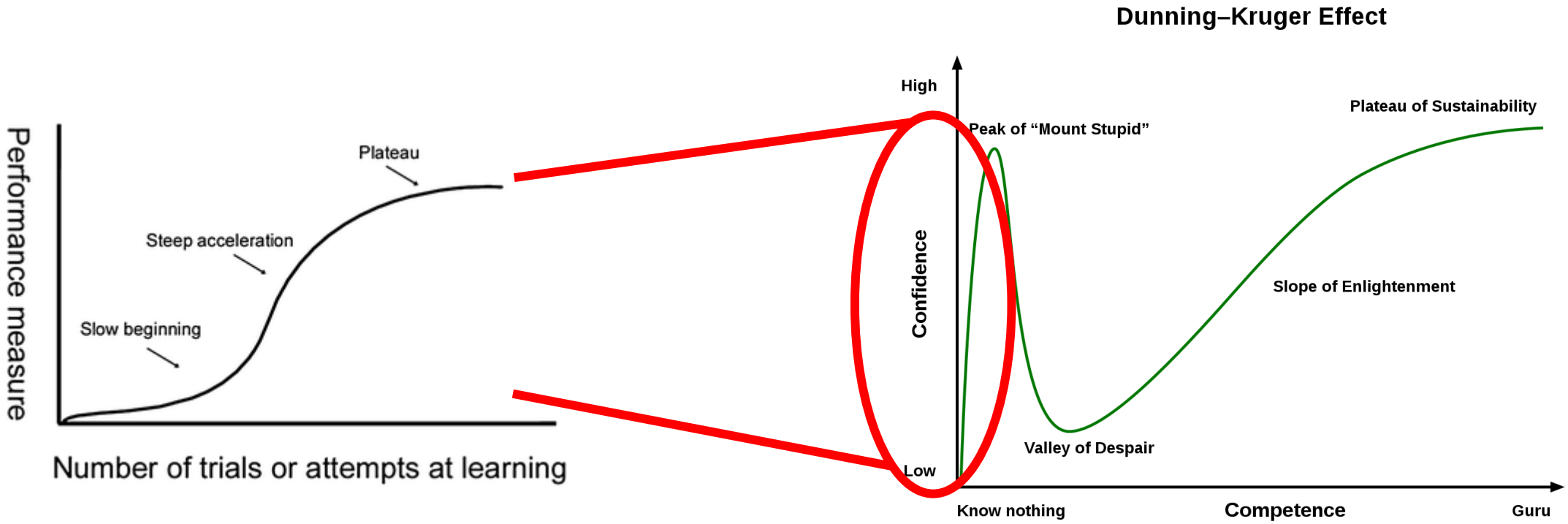
# Let’s do a quick round of introduction

- Name
- Grad program, lab, and year
- Brief description of your research
- Previous programming experience
- One thing you hope to learn

# What pre-requisites are needed?

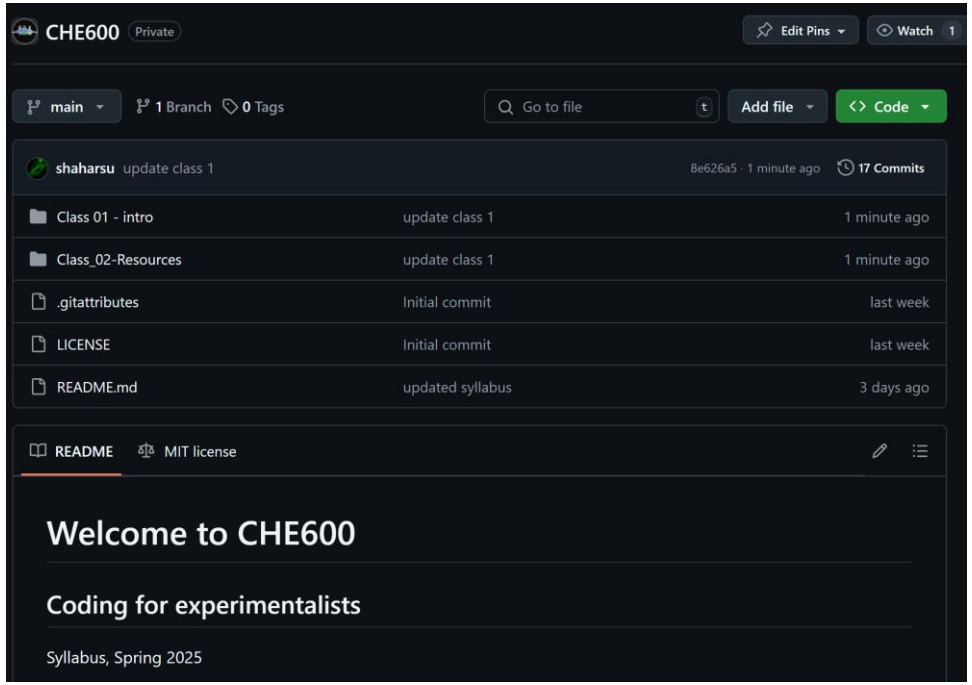
- **WHAT IS NOT NEEDED:**
  - **Programming experience**
  - **Any specific scientific background**
- What is needed:
  - Access to a computer
  - Will power (in lieu of programming knowledge)
  - Effort
  - Creativity/thinking outside the box
  - The ability to google/use chatGPT

# What should you expect from this course?




**This course will give you the basics –**
**but you will need to continue on your own to become truly proficient**

# How will it work?




- For the first time, this course will use GitHub
- http://github.com/sukeniklab/CHE600
- Each class a worksheet will be posted to the repository - No need to print it out!
- You will work from these worksheets individually
- I will project my screen, explain the assignments and answer questions
- You can follow me or work independently – your choice!
- Pacing is tricky – we'll figure it out!

# What will the course cover?

Weeks 1-3

Linux and bash

- Working in bash / Command line environment
- Basic linux utils and sed/awk
- Command line scripting

Weeks 4-6

Python

- Vanilla python basics
- Numpy and pandas
- Data visualization w/matplotlib and seaborn
- Object oriented programming

Weeks 7-13

Algorithms and modeling

- All w/python
- Optimization (curve fitting)
- Integration methods
- Monte Carlo methods
- Agent-based modelling
- Machine learning

Last week – work and presentation of individual projects

# Syllabus

| Date | Unit | Class | Topics |
|---|---|---|---|
| 1/14 | Intro | 1 | Introduction, syllabus, course expectations |
| 1/16 | Resources | 2 | Accessing the server, google/AI coding resources |
| 1/21,1/23 | Linux I | 3-4 | Linux commands for files & directories, pipes, text editors, slicing & dicing files, system commands. Introduction to Bash programming; for loops & if statements |
| 1/28,1/30 | Linux II | 5-6 | Bash variables, Data processing with sed and awk |
| 2/4,2/6 | Python I | 7-8 | Introduction to Python<br>Python overview—using the Spyder IDE<br>Python control flow, data types, and variable scoping<br>Python functions and modules, molecular dynamics program |
| 2/11,2/13 | Python II | 9-10 | Numpy and Matplotlib |
| 2/18,2/20 | Python III | 11-12 | Dataframes with pandas, Optimization using SciPy |
| 2/25,2/27 | Modelling I | 13-14 | Models I – game of life |
| 3/4,3/6 | Modelling II | 15-16 | Models II – master equations, numerical integration |
| 3/11,3/13 | **Spring break** | | |
| 3/18,3/20 | Application I | 17-18 | Python Object Oriented programming (Classes) |
| 3/25,3/27 | Application II | 19-20 | Database accession and parsing (REST and other tools) |
| 4/1,4/3 | ML I | 21-22 | Machine learning basics – *de novo* protein sequence generation |
| 4/8, 4/10 | ML II | 23-24 | Machine learning – *de novo* protein structure design |
| 4/15, 4/17 | ML III | 25-27 | Machine learning SMILES notation |
| 4/22, 4/24 | Projects | 26-27 | Final Project presentations |

# Class assignments

- Every week we focus on one topic, and get assigned tasks related to the topica
- Tasks must be finished the same week
- If you did not finish class assignments – it is your responsibility to complete them.
- Many (but not all) classes will require submission. This is done through a Blackboard submission link.
- Class work represents 20% of the final grade.

# Homework assignments

- At the conclusion of selected topics you will get a homework assignment
- Usually there will be two weeks to finish these
- Remember that at the same time the class moves on!
- Submission through Blackboard
- Homework assignments are to be completed individually
- Homework assignments are 40% of your grade.

# Final project

- There is no final. Instead each student will present a final project
- Ideas for the final project should be your own
- look for some experiment, idea, or concept that you encountered during your research that can be modelled
- The project and its scope needs to be approved by me to ensure it is sufficient and not too difficult.
- Grades will be based on the difficulty of the problem, the feasibility of the approach, the execution, and the presentation.
- The final project is 40% of your grade.

# Grading

| Activity | Number | Percentage of Final Grade |
|---|---|---|
| Class activity | ~ 14 | 20% |
| Homework submissions | ~ 6 | 40% |
| Final Project | 1 | 40% |
| Total | | 100% |

| Grade | % of total points achieved |
|---|---|
| A (A-, A, or A+) | Over 90% |
| B (B-, B, or B+) | Over 80% |
| C (C-, C, or C+) | Over 70% |
| D (D-, D, or D+) | Over 60% |

# What do I expect from you?

- Communication
- Honesty
- Effort

# What can you expect from me?

- Communication
- Clarity
- Individual attention and support

# Next class:

- Thursday, 1/16, 12:30 PM in LSC 215
- What's the plan?
    1. We'll talk about available resources
        1. Google
        2. ChatGPT
        3. Online resources
        4. Textbooks?
    2. We'll all log on to the server
    3. We'll introduce the linux operating system
    4. We'll discuss filesystem and directory structure

# What now?

- In the time left in class (if any) we will:

    1. Create a slack account for easy and fast communication – link on GitHub
    2. Try to login to the linux shell (see instructions in class 1 folder on github)