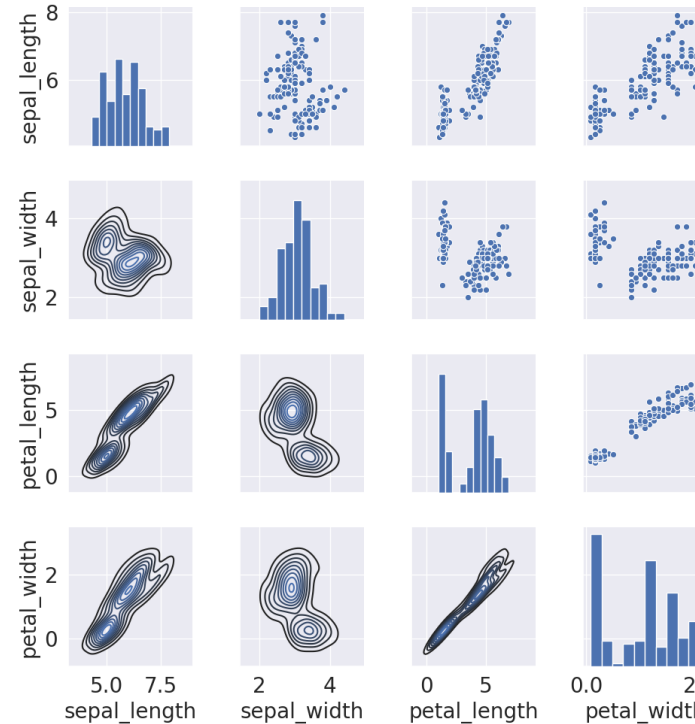
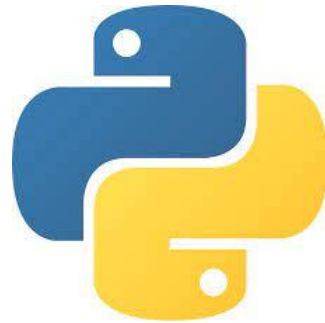
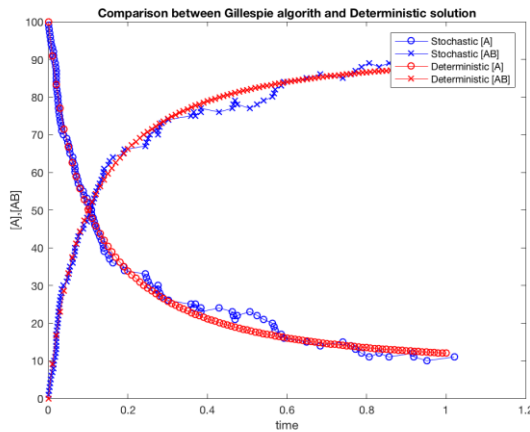
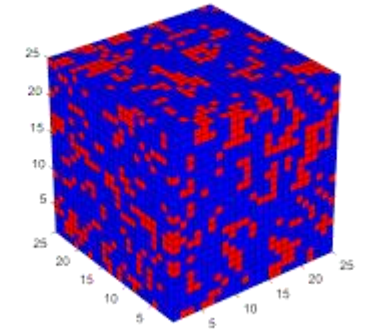




WELCOME TO CHE600

matplotlib

pandas



NumPy

About me

- Contact:
 - Email:** ssuikenik@syr.edu (subject line should have **CHE600**)
 - Slack:** More details over blackboard announcements
 - Office hours:** after class or by appointment
- Research topic: Protein biophysics – disordered protein
- History with coding: Never formally learned to code
- Why this course?

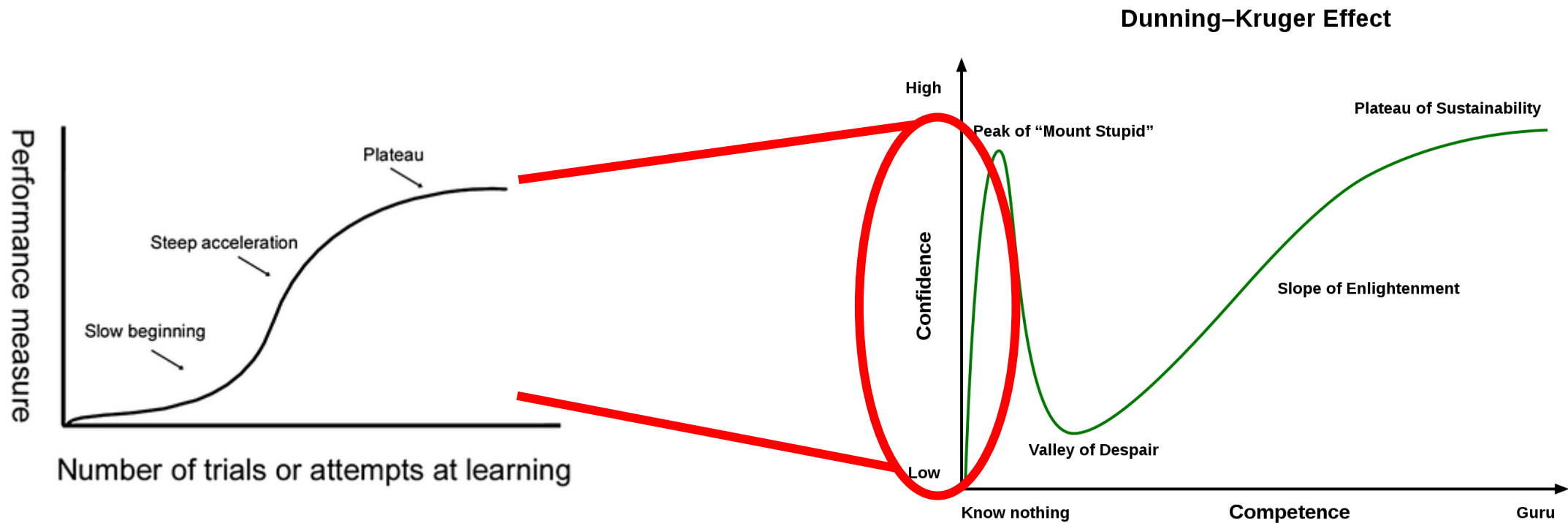
Let's do a quick round of introduction

- 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

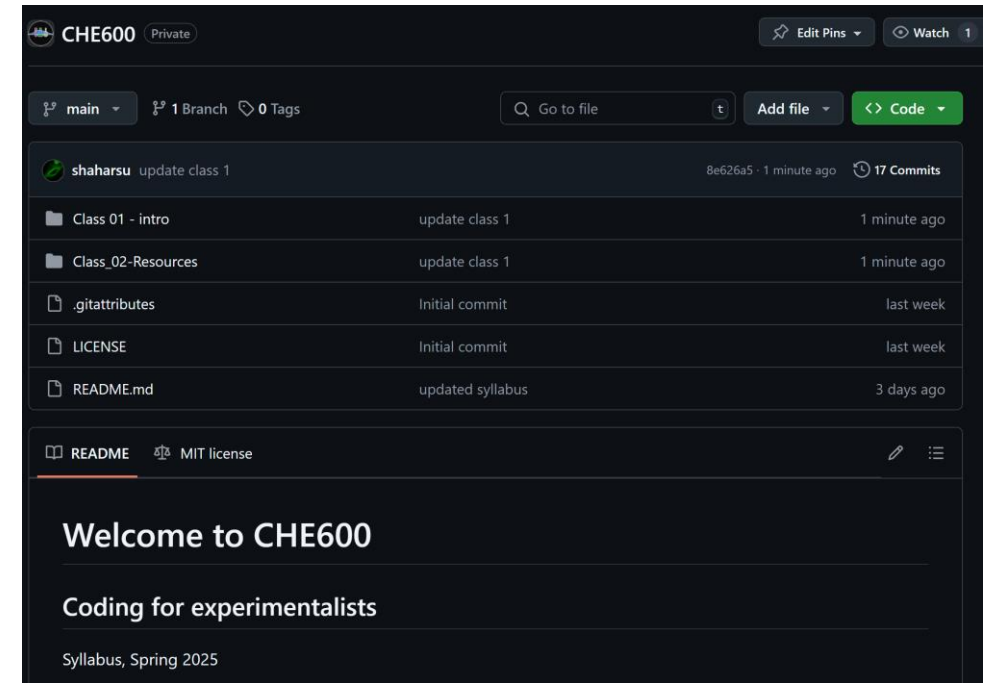
What should you expect from this course?



**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 will have a worksheet posted to GitHub - No need to print it out!
- You will work from these worksheets individually
- Before individual works start, 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 Python overview—using the Spyder IDE Python control flow, data types, and variable scoping 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 – <i>de novo</i> protein sequence generation
4/8, 4/10	ML II	23-24	Machine learning – <i>de novo</i> 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

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%

Class activity

- Every week we focus on one topic, and get assigned tasks related to the topic
- 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 submissions

- 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.

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?
 - We'll talk about available resources
 1. Google
 2. ChatGPT
 3. Online resources
 4. Textbooks?
 - We'll all log on to the server
 - We'll introduce the linux operating system
 - 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)