CHEM 600: Coding for Experimentalists

Syllabus, Spring 2025

Note: details of the syllabus may change as the semester progresses

Class sessions: Tuesdays and Thursdays, 12:30-1:50 PM, LSC 215

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 – *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