Mathematics for Chemistry
CHEM 1000 - Fall 2020

Lecture: M, W, F - 3:25-4:15 343 Alumni Hall (if we meet in person)
Recitation: W 4:30-5:20, (*online*)
Office Hours - TBD by poll and Online - http://doodle.com/geoffhutchison

> "The goal of teaching should not be to help the students learn how to memorize and spit out information under academic pressure.
>
> The purpose of teaching is to inspire the desire for learning in them and make them able to think, understand, and question."
> *- Richard Feynman - 1965 Nobel Prize in Physics*

Overview: How does one calculate the concentration of chemical reactants and products as a function of time? Where do molecular orbitals get their shape? How does Fourier transform spectroscopy work? Mathematical tools are essential across chemistry. In this class, we will survey the most important mathematical methods for chemists and illustrate applications to problems from across the chemical field.

Learning Objectives: After finishing the course, students should be able to apply mathematical tools to common problems in physical and analytical chemistry, including solving ordinary and partial differential equations, performing Fourier transforms, calculating differentials, solving integrals, optimizing functions, working with complex numbers, vectors, matrices, and eigenvalues. *Phew, that's a lot*. Students should be able to solve basic chemistry-related mathematical problems using the Python programming language and use Jupyter notebooks.

Readings:

Straub, J.E. *Mathematical Methods for Chemists*; © John E. Straub, 2020
http://sites.bu.edu/straub/mathematical-methods-for-molecular-science/

This is an eBook for which there is **no charge**. A copy of the eBook and its license agreement are in Canvas. A print version can be available for about $30; let the instructor know if you are interested.

Reference texts:

Mortimer, R.G. Mathematics for Physical Chemistry, 4th ed.; Elsevier, 2013. Available as an eBook in the Pitt Library. Search on the title in PITTCat+ at https://pitt.edu/libraries.

D. A. McQuarrie. Mathematics for Physical Chemistry; University Science Books, 2008. Available on reserve in the Chemistry Library.

Barrante, J.R. Applied Mathematics for Physical Chemistry, 3rd ed.; Pearson/Prentice Hall, 2004. Available on reserve in the Chemistry Library.

Grading:

Homework & In-Class Exercises:	100 pts
Piazza / Participation:	100 pts
Exams: (4 total - 100 pts each)	400 pts

Participation: Class participation entails both engagement in the class in the form of questions and also performance on in-class exercises. In-class discussion and questions are strongly encouraged. We will use a discussion forum on piazza.com for pre-class quiz/polls, questions, answers, etc. **You can post anonymous questions.**

Find our class signup link at: https://piazza.com/pitt/fall2020/chem1000

Flex@Pitt

1. Course will be delivered in classroom under "Guarded Risk" posture and remotely under "Elevated" or "High Risk" posture.
2. Under Guarded Risk posture in-person interactive activities include live synchronous lectures and recitations. These activities will be available to students participating remotely.
3. When the instructor is not physically present in the classroom the instructor will be available via a monitor when teaching remotely.
4. Sessions conducted synchronously will be recorded for asynchronous viewing and posted on Canvas. If you miss a synchronous class or recitation, you should post questions to the Piazza discussion forum.
5. This class will use Canvas for course documents, Zoom for synchronous meetings, Panopto for recorded lectures, Piazza for course discussions, and JupyterHub for computational notebooks.
6. All class materials will be available via Canvas, including links to Piazza discussion, links for Zoom sessions, and links to Jupyter computational notebooks connected each activity / topic.
    1. Office hours and recitations will be held as outlined in the syllabus. Office hours and recitations will be the same regardless of risk posture. Students may make online appointments via Doodle (http://doodle.com/geoffhutchison) if the timing of office hours conflicts with other classes / activities.
7. Grades will be assigned as outlined in the syllabus for Guarded posture. Adjustments made during Elevated or High Risk postures and grades are to offer flexible deadlines for homework and exams as appropriate. Please contact me if adjustments are needed.
8. Any change in mode of instruction, or other course adjustments, will be announced prominently on Canvas and Piazza.

Jupyter:

We will use Jupyter, an online platform for computational notebooks, graphing, etc. through Pitt's Center for Research Computing. Links for all materials will be posted through Canvas. If you are so inclined, you can use other services to run Python and Jupyter, but this is not necessary.

Help / Tutoring: Between the TA and the instructor, there are ample resources if you need help. Post questions to Piazza, ask questions in class and in recitation. Like many STEM courses, the material builds up over the course of the semester. If you're confused, unclear, or otherwise unsure, please ask for help early and often. It counts for participation in the course, and not be held against you - it's how we learn.

If needed, both the TA and the instructor are available for one-on-one sessions. Please ask to set up an appointment.

Homework*:* We will have a series of take-home problems throughout the course. These assignments are designed to stimulate critical thinking about facts and concepts covered in class. *Your work will be evaluated on effort in addition to accuracy*. If you work in a group, please indicate everyone involved - discussions are encouraged, but all work that you turn in should be your work.

Academic Integrity: Students in the course are expected to comply with the University of Pittsburgh's Policy on Academic Integrity. If you are not aware of the specifics, you may obtain these guidelines from the CAS Dean's Office or on the web at www.cfo.pitt.edu/policies/policy/02/02-03-02.html Violations of these guidelines can result in a zero for the assignment or failure of the course.

> To be completely clear, it is reasonable (and encouraged) to search online and/or work with your classmates to develop ideas for approaching each assignment. However, you should never copy code from another source. Put another way, each assignment you submit for credit must show that you understand how to solve the problem.

***Disability Resources*:** If you have a disability for which you are or may be requesting an accommodation, please contact the Office of Disability Resources and Services, 216 William Pitt Union (412-624-7890) as early as possible in the term.

Title IX:

> "No person in the United States shall, on the basis of sex, be excluded from participation in, be denied the benefits of, or be subjected to discrimination under any education program or activity receiving Federal financial assistance."

As a professor I am a mandatory reporter, and I am required to report violations of Title IX that I observe or am made aware of to the Title IX office (https://www.titleix.pitt.edu/). Title IX violations include, but are not limited to, sexual harassment, sexual violence and verbal or sexual abuse. Within the classroom, behavior in violation might appear as: suggestive jokes or innuendos, inappropriate touching, and unwanted sexual behavior or advances, but my capacity and obligation to report does not end at the classroom.

Inclusion: We support an inclusive, equitable, and open learning environment in which individual differences and opinions are understood, respected, and appreciated. We expect that students, TAs, and faculty will promote an atmosphere of respect for all members of the class. Expressions or actions that disparage a person's or race, ethnicity, nationality, political opinions, culture, gender, gender identity / expression, religion, sexual orientation, age, disability, or marital, parental, or veteran status are contrary to the mission of this course and will not be tolerated.

If you encounter any issue, with other students or the TA, please contact the instructor. For an incident involving the instructor, please contact the Department of Chemistry and Pitt's Office of Diversity and Inclusion.

Copyright: Much of the material in this course is covered under a "Creative Commons NoCommercial Attribution" license. That means, you can use it yourself for free, but you ***cannot*** publish it on a commercial service (*cough, cough* Chegg). Suffice to say that doing your own work is important, and extracting answers off a website won't help you to learn the material.

Chem 1000 - Fall 2020

Date		Likely Topic
Week 1	August 19	Intro / Basic Math Review
	August 21	Ch. 1 - Functions, coordinate systems (skip 1.2.5 on cylindrical coords)
Week 2	August 24	Ch. 2 - Complex numbers and logarithms - skip 2.1.5, C2, D2
	August 26	Ch. 2
	August 28	Ch. 3 - Derivatives - skip 3.3.2, 3.3.3, A3, B3
Week 3	August 31	Ch. 3
	September 2	Ch. 4 - Vectors - skip 4.2.3
	September 4	Ch 4 & Review
Week 4	September 7	**Labor Day (No Class)**
	September 9	**Examlet (1, 2, 3)**
	September 11	Ch 5 - Scalar and Vector operations (do 5.1, 5.2.3, 5.2.4, 5.2.5, A5 only)
Week 5	September 14	Ch 5
	September 16	Ch 6 - Optimizing / extrema of functions - skip A6 and B6
	September 18	Ch 6
Week 6	September 21	Ch 6
	September 23	Ch 7 - Sequences, series - skip C7
	September 25	Ch 7
Week 7	September 28	Ch 7
	September 30	**Examlet (4, 5, 6)**
	October 2	Ch 8 - Integration - skip A8, B8, C8, D8.2
Week 8	October 5	Ch 8
	October 7	Ch 8
	October 9	Ch 9 - Probability and statistics
Week 9	October 12	Ch 9
	October 14	(no class)
	October 16	Linear regression, data science (readings to be posted online)
Week 10	October 19	Review
	October 21	**Examlet (7, 8 , 9)**
	October 23	Ch 10 - First order Diff Eq - skip 10.2.2, 10.2.3, A10
Week 11	October 26	Ch 10
	October 28	Ch 11 - Second order Diff Eq. - (do 11.1, 11.2, 11.3, A11, skip the rest)

Date		Likely Topic
	October 30	Ch 11
Week 12	November 2	Ch 11
	November 4	Ch 12 - Examples of partial diff. eq.
	November 6	Ch 12
Week 13	November 9	Ch 13 - Fourier series & Fourier transforms
	November 11	Ch 14 - Matrices and matrix algebra
	November 13	Ch 14
Week 13	November 16	Ch 15 - Eigenvalues & eigenvectors
	November 18	Ch 15
	November 20	Final review / end of classes
Thanksgiving		
Take-Home Final		