



CHEM 3PC3

F2024

Rodrigo A. Vargas-Hernández
vargashr@mcmaster.ca



Housekeeping

Class Schedule	Monday & Thursday 12:30PM - 1:20PM Tuesday 1:30PM - 2:20PM
Location	ABB 163
Tutorial Schedule	Tuesday 12:30 PM – 1:20 PM
Location	KTH B132
Office Hours	Thursday 4:00 PM
Location	TBD (probably ABB 266)

Course Overview and Assessment*

Week	Dates	Topic
1	Sept. 3-6	Univariate Calculus and Series: Thermodynamic, heat capacity and integration
2	Sept. 9-13	
3	Sept. 16-20	
4	Sept. 23-27	Multivariate Calculus: Fundamental Equations of Thermodynamics
5	Sept. 30 – Oct. 4	
6	Oct. 7-11	Linear Algebra: Simple and complex equilibrium
7	Oct. 14-20	
	TBD	Fall break. No classes this week!!
8	Oct. 21-25	Midterm exam
9	Oct. 28 - Nov. 1	
10	Nov. 4-8	More Linear Algebra: Equilibrium and steady state solutions
11	Nov. 11-15	
12	Nov. 18-22	Orbitals and decay to equilibrium: Eigenvalues and eigenvectors
13	Nov. 25-29	
14	Dec. 2-5	
	Before Dec 10	
		Regression and classification: 1. Linear regression 2. Neural Networks 3. Classification
		Final exam

*dates could change during the term

Week structure

Week	Topic	*tentative
Monday	Theory Lecture	
Tuesday		
Thursday	Programming Lecture	



*working on the AV2L :/

<https://chemai-lab.github.io/Math4Chem/intro.html>

Tutorials

Tutorial Schedule	Tuesday 12:30 PM – 1:20 PM
Location	KTH B132



Alexandre de Camargo

Goals:

1. Answer **YOUR** questions.
2. HELP you understand the content.
3. Coding and math exercises.

Evaluation

Assessment Method	Weight
Four Avenue Quizzes (dates TBD)	20%
2 Python assignments (dates TBD)	20%
Mid-Term Exam	25%
Final Exam	35%
Total	100%

If your final exam's mark is higher, I will give you that mark!

Python Assignments

I believe that in today's job market one of the most underrated skills is the ability to work with different people.

- You will work in groups of 2 (3).
- Submission will be a *.ipynb* file deployable in GoogleColab.
- The teams will be randomly assigned this week when enrollment is final.

Books and additional resources.

Books:

- Applied mathematics for Physical Chemistry,
James R. Barrante.
- Mathematics for Physical Chemistry,
Donald A. McQuarrie.
- Physical Chemistry,
Ira N. Levine.
- Linear Algebra with applications,
Gareth Williams.

Other resources

- Use the internet.
 - YouTube.
 - <https://chem.libretexts.org/>
 - <https://stackoverflow.com/>
- Notes from prev. years
will be provided.

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- The Matrix Cookbook,
<http://matrixcookbook.com>

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Course and Learning Objectives

At the end of the course, the student will have elementary algebra, calculus, and programming skills tailored to model chemical systems.

Academic Integrity in the era of Generative AI

As a researcher in the field of machine learning and AI, I recognize the significant potential of these modern tools to enhance the learning process. I support their responsible use, with the understanding that the author who submits the work is ultimately accountable for its content and any potential repercussions.

In this course, where the primary objective is to develop students' mathematical and coding skills, it is essential to ensure that all work reflects genuine analysis and understanding.

The instructor and TA will be vigilant in identifying any instances of **"copy-paste" answers**, particularly those that appear to be generated by AI without sufficient student comprehension. If the instructor or TA suspects that an answer has been directly copied from a chatbot, the student will be required to explain their reasoning. **Responses such as "this is what ChatGPT told me" will not be tolerated. Based on the explanation provided, appropriate consequences may be determined.**

Use these amazing tools but do not take them for granted

Why should Chemist develop some Math and Programming skills?

