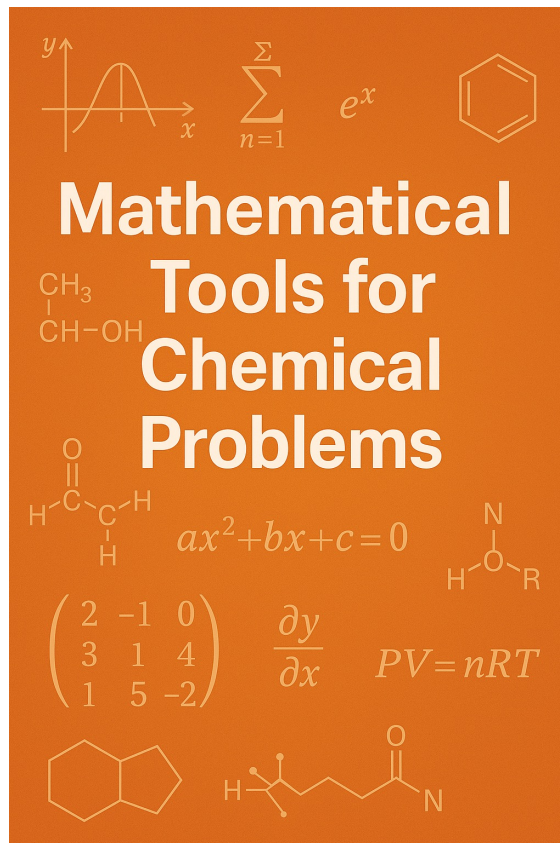


# CHEM 3PC3 F2025

Rodrigo A. Vargas-Hernández  
vargashr@mcmaster.ca

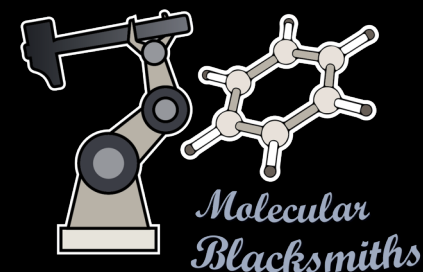




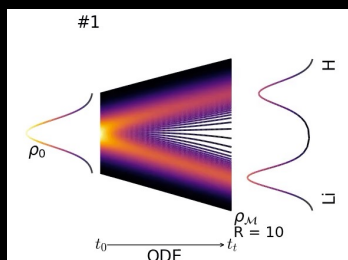
GenAI for Quantum Science



**Chem.AI**  
**Lab**



AI for Materials



- How much can ML models learn?
- Can we improve physical models?
- Do pre-trained ML models work?

## Housekeeping

<b>Class Schedule</b>	<b>Tuesday 9:30AM - 10:20AM</b> <b>Thursday 8:30AM - 10:20AM</b>
<b>Location</b>	<b>ETB 227</b>
<b>Tutorial Schedule</b>	Tuesday 1:30 PM – 1:20 PM
<b>Location</b>	HH 102
<b>Office Hours</b>	TBD
<b>Location</b>	TBD (probably ABB 266)

# Course Overview and Assessment\*

Week	Dates	Topic	Book	Chapter
1	Sept. 2-4	Univariate Calculus and Series:	PC	1
2	Sept. 9-11	Thermodynamic, heat capacity and integration	MPC	1,2
3	Sept. 16-18	Multivariate Calculus:	PC	2,3
4	Sept. 23-25	Fundamental Equations of Thermodynamics	AMPC	4,7
			MPC	12
5	Sept. 30 – Oct. 2	Linear Algebra:	LAWA	1
6	Oct. 7-9	Simple and complex equilibrium	PC	4
7	<b>Oct. 13-19</b>	<b>Fall break. No classes this week!!</b>		<b>None</b>
	<b>TBD</b>	<b>Midterm exam</b>		
8	Oct. 21-23	More Linear Algebra:	LAWA	2,3
9	Oct. 28-30	Equilibrium and steady state solutions	PC	9
10	Nov. 4-6	Orbitals and decay to equilibrium:	MPC	16
11	Nov. 11-13	Eigenvalues and eigenvectors	MPC	19
12	Nov. 18-20	Regression and classification:	LAWA	7
13	Nov. 25-27	1. Linear regression	NMSE	7
14	Dec. 2-4	2. Neural Networks	Class notes	None
		3. Classification		
	<b>TBD</b>	<b>Final exam</b>		

\*dates could change during the term

## Week structure

Week	Topic
Tuesday	Theory/Math Lecture
Thursday	Theory/Math + Programming Lecture



\*link will be posted in AV2L :/

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

# Tutorials

Tutorial Schedule	Tuesday 1:30 PM – 1:20 PM
Location	HH 102



Alexandre de Camargo

## Goals:

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

## 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!**

With great power comes great responsibility

# 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.
- STUDENT1\_SURNAME1\_STUDENT1\_ID\_STUDENT2\_SURNAME2\_STUDENT1\_ID\_QUIZ\_NUMBER.ipynb  
(e.g., SMITH\_001234567\_JUAN\_001234098\_QUIZ\_2.ipynb).



## 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.
- Mathematics for Quantum Chemistry, Jay Martin Anderson.
- Numerical Methods for Scientists and Engineers, R. W. Hamming.

### Other resources

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

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Donald A. McQuarrie.
- Physical Chemistry,  
Ira N. Levine.
- Linear Algebra with applications,  
Gareth Williams.
- The Matrix Cookbook,  
<http://matrixcookbook.com>

### Other resources

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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**