Syllabus

CHEM 2PC3: Mathematical Tools for Chemical Problems

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Meeting Times/Location:

Lecture:
PC-155 9:30 – 10:20 (MoTh)
PC-155 10:30 – 11:20 (Tu)
ABB-271 11:30 – 12:20 (Fr) [Tutorial]

Office Hours: 10:30-12:30 MoTh; 11:30-12:30 Tu

Overview:

The purpose of this course is to provide students with the mathematical tools that are needed for further study in chemistry. The emphasis is on techniques from calculus (limits, differentiation, integration, differential equations, Taylor series, line integrals, etc.) and linear algebra (linear equations, basis sets, eigenvalues and eigenvectors, linear regression, etc.). The second purpose of this course—which sounds different but really is not—is to elucidate the mathematical framework of chemical thermodynamics and kinetics.

Course Materials:

In lieu of a mandatory textbook, we will post numerous free online resources on the web. Please check the Avenue to Learn site frequently.


This book is good, and modestly priced by the standards of university textbooks. The late Prof. MacQuarrie was the best writer of physical chemistry texts in his generation, and his texts are usually gems. I will not follow the text closely, but the problems are very valuable practice, and it is a very useful reference. You may be able to find a cheap copy www.bookfinder.com.

Teaching Assistant:

The teaching assistant for this course is David Kim, kimt33@mcmaster.ca.

Course Outline:

1. Simple thermodynamic changes in one variable. Univariate calculus including series expansions.
Objectives:
The goal of this course is to teach you how to solve chemical problems using mathematical tools. As such, the course is very “problem-oriented.” (This is old-fashioned “problem-based learning.”) A more ambitious, but more important, goal is teach you how to take a chemical problem, rewrite it in mathematical language, solve the mathematical problem, and then extract chemical insight from the mathematical solution. Even though the emphasis of the course is on mathematical problem-solving, by studying these tools in context you will learn about many different aspects of chemistry, with emphasis on thermodynamics and kinetics.

This year, for the first time, we will be adding a “mathematical software” component. The goal is to familiarize you with how to solve “real problems” that are too complicated to solve by hand, using a computer. This will also introduce you to the rudiments of computer programming in Python.

Tutorials:
In tutorial, we typically start with a brief overview of the previous week’s lectures. Then we will present material related to computational methods (the computational component of the course is entirely presented in the tutorial and assignments) and answer any questions that may arise. In addition to the scheduled tutorial, we will schedule optional tutorials and problem help sessions. We will try to adapt them to meet your needs.

Assessment:

20%  10 “weekly” quizzes. These are really short assignments, administered through Avenue to Learn. They are due each Friday, by 11:59 pm.

20%  3 “monthly” assignments. These in-depth assignments are designed to add to your mastery of the material and teach you the rudiments of computer programming and scientific computation. (Feb. 1, Feb. 29, March 28. Due by 11:59 pm.)

25%  1 mid-term examination. (March 9)

35%  1 final examination. (to be scheduled by registrar)

Disclaimer:
The instructor and university reserve the right to modify elements of the course during the term. The university may change the dates and deadlines for any or all courses in extreme circumstances. If either type of modification becomes necessary, reasonable notice and communication with the students will be given with explanation and the opportunity to comment on changes. It is the responsibility of the student to check their McMaster email and course websites weekly during the term and to note any changes.

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