Mathematics for Chemistry

Lecture: Mon, Wed, Fri 11-11:50 AM, 154 Chevron
Recitation: Mon 12-12:50 PM, 132 Chevron

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Course Description: How does one calculate the concentration of a reactant as a function of time, given the kinetic rate constant and initial concentration? How does Fourier transform spectroscopy work? How does the energy of a chemical reaction change as a function of pressure and temperature? Where do molecular orbitals come from? Mathematical methods are essential tools to answer these and many other questions for example in physical chemistry, biophysics, and analytical chemistry. In this class we will survey the most important mathematical methods for chemists and their applications to physical chemistry and related fields.

Course Learning Objectives: After finishing this course, students will be able to choose and apply mathematical tools to tackle some common problems in physical chemistry, such as solving simple ordinary differential equations, performing Fourier transforms, calculating differentials, solving multiple integrals, operating with vectors, matrices, determinants, and eigenvalue equations. Students will be able to solve basic chemistry-related mathematical problems using the Mathematica computer algebra system.

Course Expectations & Requirements:

- Course participants are expected to have a working knowledge of the material from Calculus I+II, as taught at Pitt (single-variable differentiation, integration, and basic vector algebra).
- This course will require weekly problem sets to be turned in and graded. You will find that a thorough understanding of each problem set will help you master the concepts.
- Three 50-minute exams will be given. A non-cumulative final exam will also be required.
- Our classes will involve hands-on worksheets to summarize key ideas/results and to practice new material. You will find that participating in the in-class exercises will help you master the concepts.
- Students will be expected to prepare course material as indicated in reading assignments.
- Important announcements will be made via e-mail; you will be expected to check your Pitt account regularly (at least once every day).
- It is your responsibility to obtain copies of the handouts from the lecturer and to ask your peers for written notes, should you miss class.

Grading: 25% Problem Sets, 25% Exam 1, 25% Exam 2, 25% Exam 3 (Final)

CHEM 1000 **Fall Term, 2018**

Tentative Syllabus

Dates of Lectures				Topic(s)
Week 1:	1/7	1/9	1/11	Complex Numbers
Week 2:	1/14	1/16	1/18	Ordinary Differential Equations
Week 3:	--[1)]	1/23	1/25	Ordinary Differential Equations
Week 4:	1/28	1/30	2/1	Initial Value Conditions
Week 5:	**2/4**	2/6	2/8	Systems of Equations
Week 6:	2/11	2/13	2/15	Vectors
Week 7:	2/18	2/20	2/22	Matrices and Operators
Week 8:	2/25	2/27	3/1	Matrix Eigenvalue Equations
Week 9:	3/4	3/6	3/8	Partial Derivatives
	Spring Recess			
Week 10:	3/18	3/20	3/22	Partial Derivatives and Differentials
Week 11:	**3/25**[2)]	3/27	3/29	Differentials and Line Integrals
Week 12:	4/1	4/3	4/5	Line Integrals and Multiple Integrals
Week 13:	4/8	4/10	4/12	Multiple Integrals
Week 14:	4/15	4/17	4/19	Fourier Transforms, Basis Sets & Series Expansions
Week 15:	**4/22 – 4/27 (date TBA)**			Final Exam Week

1) MLK Day.
2) Take-home exams due.
Exam dates shown in bold.
Please note that final grades will be due by 5/1 at 11:59 PM.

Required Textbook

"Mathematics for Physical Chemistry", 4th Ed., by Robert G. Mortimer, ISBN 978-0124158092. An electronic copy of the 3rd Edition is available via the Pitt library (see CourseWeb -> Resources for a link). Should you decide to work with the 3rd edition, it is your responsibility to obtain a

Required Software

Top Hat: Students are required to sign up for an account on www.tophat.com. This class will use Top Hat to perform in-class activities.

Supplementary Books & Resources

"Mathematics for Physical Chemistry" by Donald A. McQuarrie, 1st Edition, University Science Books, 2008 (ISBN-9: 1891389564, ISBN-13: 978-1891389566).

"Mathematical Methods for Physicists, Seventh Edition: A Comprehensive Guide" by George B. Arfken and Hans J. Weber, 7th Edition, Academic Press, 2012 (ISBN-10: 0123846544, ISBN-13: 978-0123846549).

"Mathematical Methods for Scientists and Engineers" by Donald A. McQuarrie, University Science Books, 2003 (ISBN-9: 1891389246, ISBN-13: 978-1891389245). A reserve copy is available at the Engineering Library.

Mathematica 10.0 for Students, available for download from https://my.pitt.edu/portal/server.pt/community/software_downloads/872. Also available for use in campus computing labs.

"Mathematica®: A Problem-Centered Approach" by Roozbeh Hazrat, Springer London, 2010 (ISBN 978-1-84996-250-6). An electronic copy can be accessed from the campus network via http://link.springer.com/book/10.1007/978-1-84996-251-3.

"Mathematica in Action" by Stan Wagon, 3rd Edition, Springer New York, 2010 (ISBN 978-0-387-75366-9). An electronic copy can be accessed from the campus network via http://link.springer.com/book/10.1007/978-0-387-75477-2.

Assignments

Reading

Preparing the material from the textbook for each class is essential, so we can use the classes for hands-on exercises and discussion.

- The lectures will be there to summarize important results from the textbook, to clarify, discuss, and to work through examples.
- There will be pre-lecture assignments testing the reading assignments. These will be part of your homework grade (graded for completeness).
- I will ask for your questions at the beginning of each lecture, so we can discuss these together.

Problem sets

New assignments will be posted regularly. You will typically have one week to complete the homework set.

- Homework problems will be graded.
- Late submissions will be not be accepted.
- Solutions to selected problems will be posted after the homework due date.

In-class exercises

- Learning math is most interesting and rewarding when applied to real chemistry problems.
- We will therefore spend as much time as possible with *real-life examples and exercises* (team and individual), going through questions together, and discussing the concepts.

Exams

Each exam will focus on material covered after the preceding exam. More details on coverage for each exam and allow tools will be outlined in class at least a week before the exam. If you miss an exam, you will be assigned a score of zero, unless the non-attendance is due to a serious illness or extreme emergency. In the latter case the other exams will be appropriately averaged to determine your score. Make-up exams will not be given. *It is your responsibility to inform the instructor ahead of time in writing if you will not be able to attend an exam or, if this is a result of an unforeseen illness or event, to provide the instructor with a doctor's note or equivalent documentation within 5 days of your absence.* Exam dates are marked in bold on the tentative syllabus. All three exams will be 50 minutes and non-cumulative (but note that topics in mathematics are highly interrelated, so that understanding of a previous topic is often required to master a new concept).

Grades

Grades will be assigned according to the following scale:

A+ 100-97.5%	A 97.4-92.5%	A- 92.4-87.5%
B+ 87.4%-82.5%	B 82.4%-77.5%	B- 77.4-72.5%
C+ 72.4%-67.5%	C 67.4-62.5%	C- 62.4-57.5%
D+ 57.4-52.5%	D 52.4-47.5%	D- 47.4-42.5%

F 42.4% and below		

If necessary (e.g. when the class average is exceptionally low), the grades will be assigned on a curve.

University Policies:

Academic Integrity

Students in this course will be expected to comply with the University of Pittsburgh's Policy on Academic Integrity. Any student suspected of violating this obligation for any reason during the semester will be required to participate in the procedural process, initiated at the instructor level, as outlined in the University Guidelines on Academic Integrity. This may include, but is not limited to, the confiscation of the examination of any individual suspected of violating University Policy. Furthermore, no student may bring any unauthorized materials to an exam, including dictionaries and programmable calculators.

Disability Services

If you have a disability that requires special testing accommodations or other classroom modifications, you need to notify both the instructor and Disability Resources and Services no later than the second week of the term. You may be asked to provide documentation of your disability to determine the appropriateness of accommodations. To notify Disability Resources and Services, call (412) 648-7890 (Voice or TTD) to schedule an appointment. The Disability Resources and Services office is located in 140 William Pitt Union on the Oakland campus.

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Statement on Classroom Recording

To ensure the free and open discussion of ideas, students may not record classroom lectures, discussion and/or activities without the advance written permission of the instructor, and any such recording properly approved in advance can be used solely for the student's own private use.