Mathematics of Chemistry: Techniques & Applications (CHEM-UA 140)

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Class Time & Location: Tuesday, Thursday: 6:20 – 7:35 pm

125 W 4th Street, Room C-13

Course Description and philosophy: Advanced work in chemistry, including upper division courses such as Quantum Mechanics and Spectroscopy, Advanced Biochemistry, Physical Chemistry Laboratory, or Thermodynamics and Kinetics, as well as graduate coursework and advanced research in physical or materials chemistry tracks, often requires mathematical concepts beyond those taught in introductory calculus courses. This course will provide you with the mathematical foundations you need to progress into these advanced areas of chemistry. Course topics will include a brief review of calculus I and calculus II, and then it will move forward to cover new topics including algebra of complex numbers, vectors and matrices, calculus of several variables, basis expansions and integral transforms, ordinary differential equations, partial differential equations, and an introduction to group theory. Rather than presenting these topics in a highly theoretical manner, however, they will be conveyed through the vehicle of and in the context of actual applications to real chemical problems. Concepts are enforced through in-class problem solving as well as weekly problem sets. You will be encouraged to apply both analytical techniques as well as numerical tools available in packages such as Matlab or Mathematica, and high-level programming languages such as Python.

Course goals: By the end of the course, you should be able to solve succinctly stated mathematical problems. You should also be able to translate a complex chemical problem into an appropriate mathematical formulation and apply the techniques, both analytical and numerical, learned in the course to solve the problem.

Prerequisites: Calculus I and II or equivalent.

Textbook: *Mathematical Methods in the Physical Sciences, Third Edition* by Mary L. Boas, published by John Wiley & Sons (2006), Additional recommended (but not required) textbook: *Essential calculus: Early Transcendentals* (2012) by James Stewart, published by Brooks/Cole Cengage Learning.

Grading: The grading will be as follows: The two midterms will count for 25% each, and the final for another 25%. Weekly problem sets will count for 5% of your grade, quizzes 15%, and class participation for 5%. Science and math courses cannot be taken as "spectator sports". The only way to learn the material is to solve problems, both in class and on your own. This is the rationalization for the grading scheme outlined above.

Teaching Assistant: The teaching assistant for this course is (clinical) Professor Dubravko Sabo. He will be in charge of the weekly recitation and will substitute in for me on a few occasions when I will be out of town. Although I will be working together with the TA throughout the course, the person ultimately responsible for the content of the course and the grading is me. Therefore, please do NOT go badgering the TA about issues/concerns that you should be discussing with me.

APPROXIMATE TIMELINE:

<u>Week 1: Brief review of calculus I and II (no assigned reading)</u>

Lecture 1:

- Functions of one variable.
- Rules of differentiation.

Lecture 2:

- Techniques for integration.

*Problem set 1 assigned.

<u>Week 2 (Complex numbers and linear algebra (Reading: Chapters 2, 3.1-3.6):</u>

Lecture 3:

- Algebra of complex numbers

Lecture 4:

- Introduction to vectors and matrices, Dirac notation

Example application: Atomic coordinates in molecules.

*Problem set 1 due.

*Problem set 2 assigned.

Week 3: Linear Algebra (Reading: 3.7-3.11)

Lecture 5:

- Basic vector and matrix operations in Dirac notation

Lecture 6:

- Linear dependence and linear independence
- Basis vectors and expansions
- Introducing the eigenvalue problem

Example application: Electron spin matrices.

*Problem set 2 due.

*Problem set 3 assigned.

Week 4: Linear algebra, functions of several variables (Reading 3.12-3.14, 4.1-4.4)

Lecture 7:

- Eigenvalues and matrix diagonalization

Lecture 8:

- Introduction to functions of several variables

Example application: Thermodynamic state functions.

*Problem set 3 due.

*Problem set 4 assigned.

Week 5: Calculus of several variables (Reading: 4.5-4.12)

Lecture 9:

- Rules of partial differentiation.
- Maximization and minimization of functions in several dimensions.
- Contour plots and isosurfaces.

Lecture 10:

- Numerical methods for function optimization

Example application: Optimization of error functions for machine learning.

*****Problem set 4 due**.**

Week 6: Calculus of Several Variables: (Reading Chapter 5)

Lecture 11:

- Double and triple integrals
- Changing variables in multidimensional integrals

Lecture 12:

- Changing variables and the Jacobian factor
- Special coordinate transformations:
    1. Polar coordinates
    2. Cylindrical coordinates
    3. Spherical coordinates

Example application: s and p hydrogenic orbitals

*Midterm examination on weeks 1-5.

*Problem set 5 assigned.

Week 7: Calculus of many variables, basis sets (Reading: Supplementary material)

Lecture 13: Integrals of very high dimension

- Analytically solvable examples
- Introduction to Monte Carlo methods

Lecture 14:

- Introduction to basis set expansions
- Dirac delta functions

Example application: Maxwell-Boltzmann distribution of an ideal gas

*Problem set 5 due.

*Problem set 6 assigned.

Week 8: Basis sets, integral transforms, ODEs (Reading: 7.1-7.5, 8.1-8.6)

Lecture 15:

- Linear Hermitian operators and basis sets
- The Fourier basis and Fourier expansions
- Fourier transforms

Lecture 16:

- First-order separable equations
- Types of second-order differential equations

Example application: Chemical kinetics – first and second-order rate laws.

*Problem set 6 due.

*Problem set 7 assigned.

Week 9: Ordinary differential equations (Reading: 8.7-8.12, 12.1)

Lecture 17:

- Power-series solutions

Lecture 18:

- Laplace transforms and the solutions of ODEs

Example application: The classical harmonic oscillator and bond vibrations

*Problem set 7 due.

Week 10: ODEs and Partial differential eqns. (Reading: 13.1-13.8, Supplemental)

Lecture 19:

- Numerical methods for ordinary differential equations
    1. Single equations
    2. Systems of equations

Lecture 20:

- Spatial PDEs and boundary conditions
- Laplace and Poisson equations
- Solution by separation of variables (start)

Example application: Electrostatics

*Midterm examination on Weeks 6-9

*Problem set 8 assigned.

Week 11: Partial differential equations (Reading: Supplemental)

Lecture 21:

- Solution by separation of variables (finish).
- Green's function methods.
- Basis-set expansion and matrix methods.

Lecture 22:

- Spatio-temporal PDEs
- Boundary and initial conditions
- The diffusion equation
- The Schrödinger equation and the eigenvalue problem.

Example application: Particle in a three-dimensional box

*Problem set 8 due.

*Problem set 9 assigned.

<u>Week 12: Partial differential equations (Reading: 13.9, Supplemental)</u>

Lecture 23:

- Solution by integral transforms
- Numerical operator splitting methods

Lecture 24:

- Systems of coupled PDEs and self-consistent problems

Example application: Chemical reactive scattering

*Problem set 9 due.

*Problem set 10 assigned

<u>Week 13: Probability and statistics (Reading: Chapter 15)</u>

Lecture 25:

- Random variables
- Probabilities and probability distribution functions
- Linear regression

Lecture 26:

- Sampling probability distribution functions
- Introduction to Monte Carlo methods

Example application: Linear regression for the Arrhenius law

<u>Week 14: Introduction to Group Theory (Supplemental reading)</u>

Lecture 27:

- Review of set theory
- Transformations and symmetry elements
- Representations

Lecture 28:

- Point groups and molecules
- Space groups and crystals

Example application: Molecular crystal structures.

*Problem set 10 due.

Week 15:

*Final examination: Cumulative.