

Syllabus of CHEM-761 (Graduate Students)
Computational Chemistry and Biochemistry: Theories and Applications
(Spring 2018)

Instructor: Rui Sun
Office: Bilger 245B
Phone: (808) 956-3207
Email: ruisun@hawaii.edu

Lectures: **Tuesday 12:00 (noon) – 1:15 AM in Bilger 341C**
Thursday 12:00 (noon) – 1:15 AM in Bilger 242

Office Hours: Thursday 2:00 – 4:00 PM in Bilger 245B or by appointment.

Textbook: *Computer Simulation of Liquids*, M.P Allen and D. J. Tildesley, 2nd Edition, ISBN-13: 978-0198803201, ISBN-10: 0198803206
There is a previous edition of this book that is free on line. Handouts will be provided for some of the lectures.

Prerequisites: Physical Chemistry or Physical Biochemistry (300 level, C or better)
Physics (200 level, C or better)
Calculus (200 level, C or better)
Programming experience is not required
An override request is required for undergraduate students to enroll
Access to computer

Learning Outcomes: This course is to learn to the theories and applications of computational studies of the biophysics processes. Further, it should introduce you to use computers to mathematically model a system of interest and to process the data. When you finish this course, you should be able to model a biophysical system, and convert it into a relevant computer program. You are also expected to simulate and check the computer program, make sense of the output files, and present the data.

Specifically:

- **Write a computer program**
- Understand the basics concepts of statistical mechanics
- Understand the theories behind molecular dynamics simulations
- Analyze and visualize the computational data
- Be capable of reading research that involves computational studies

Course Outline:

The following topics will be covered:

- **Basic computer programming:** This is not a computer science course about writing a computer program, so we'll learn and use only the features that we'll need. We will use a programming language called *Fortran*. While not so elegant or brief as languages like Mathematica or MathCAD, Fortran is quite easy to use (much easier than, say, C++, and almost as easy as Matlab); and more importantly, anybody with basic understanding of one program language (FORTRAN in this class), will be able to learn C, C++, Basic, Visual Basic, Java, Pascal, Matlab, Simulink, Mathematica, Maple, MathCAD can very quickly.
- Introduction to simulation methods
- Statistical mechanics
- Molecular dynamics simulation
- Monte Carlo simulation
- Free energy calculation
- Data Visualization

Assessments:

The learning outcomes will be assessed through homework, midterms, and a final project, with bonus points from quizzes. There will be NO final exam.

Method of Assessments	Total Points
Homework	44
Midterm Exam 1	20
Midterm Exam 2	20
Final Project	20
Quizzes	16

1. Homework (44 pts) – Homework will be assigned almost weekly (11 in total) and you will be given a about week to finish it. Homework is deducted by 25% every 24 hours past the deadline. You can discuss the homework with other students; however, assignments must be finished and submitted independently. **Most of the homework will involve computer programing.**

2. Midterm Exams (40 pts) – There will be two midterm exams (20 pts each). Exam questions will be based on the reading assignment and class content. The dates of the midterms are to be announced. Both midterms will be closed-book exams.

Students who miss an exam due to medical reasons or university obligations will be given a make-up exam up until **one week after the date of the missed exam**, if they are able to provide a proper documentation proof. After that period, if the student has not contacted me and arranged a make-up, you will receive zero credit for that exam.

3. Final Project (20) – There will be one final project by the end of the semester. Again, you can discuss the final project with other students; however, the project report must be finished and submitted independently.

4. Quizzes (16) – There will be eight quizzes (2 points for each quiz) throughout the semester. The dates of the quizzes will NOT be announced in prior because they also serve as taking attendance.

Grading Scheme: You will get partial credits for a reasonable attempt at each assessment. The sum of all the above will determine your final score, for which letter grades will be assigned (**A:** 88 pts or above; **B:** 73 ~ 87 pts; **C:** 60 ~ 72 pts; **F:** 60 pts or below).

Special Conditions: Any student who feels he/she may need an accommodation based on the impact of a disability is invited to contact me privately. I would be happy to work with you, and the KOKUA Program (Office for Students with Disabilities) to ensure reasonable accommodations in my course. KOKUA can be reached at (808) 956-7511 or (808) 956-7612 (voice/text) in room 013 of the Queen Lili'uokalani Center for Student Services.

Academic Honesty: It is the aim of the University to foster a spirit of complete honesty and high standard of integrity. Any attempt of cheating and plagiarism is regarded by the faculty and administration as a **most serious offense** and renders the offenders liable to serious consequences, possibly suspension. <http://www.catalog.hawaii.edu/about-uh/campus-policies1.htm>

Syllabus of CHEM-761 (Undergraduate Students)
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