Molecular Modeling Methods

CHBE 476 and ENCH648P

Tuesday & Thursday, 12:30-1:45 pm
EGR 1104
Spring 2015

Instructor: Prof. Jeffery B. Klauda
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Course Description

Statistical mechanics will be introduced to give the fundamental background for atomic to mesoscale molecular modeling. Classical atomic-level simulations methods (Monte Carlo and Molecular Dynamics) and the procedures to develop intra- and intermolecular potentials will be covered. This course will also discuss the theory and application of coarse-grained molecular simulations, mesoscale simulations and other modern simulation techniques. A broad range of applications will be included throughout the semester, e.g., phase behavior of small molecules, kinetics, and biophysics. Prerequisite: CHBE 302 or equivalent.

Course Objectives for Students

- Understand the advantages and limitations of molecular simulation methods.
- Understand how to relate properties at the atomic or molecular level to macroscopic properties via statistical thermodynamics.
- Critically analyze the scientific work by other researchers in molecular modeling.
- Improve communication skills by classroom discussion, problem solving, and written assignments.
- *Graduate Students*: Directly apply molecular modeling principles to their research.

Required Course Readings

Textbook

- S.I. Sandler. (2011). *An Introduction to Applied Statistical Thermodynamics*. USA: John Wiley & Sons, Inc. ISBN: 978-0-470-91347-5

Useful Websites

- www.charmming.org
- www.charmm-gui.org
- www.charmm.org
- www.ks.uiuc.edu/Research/namd/
- www.etomica.org/
- polymer.bu.edu/vmd/

Computer Software

The use of computer software is essential in this course. Mathematical software (MATLAB/Excel) will be helpful in material covered for the statistical mechanics portion of the course. Most of the course will involve the use of simulation software, e.g., CHARMM and NAMD. CHARMM will only be accessible on XSEDE resources, but NAMD can be used on a personal computer under Windows and on terpconnect and XSEDE.

Lecture

The lecture time will consist of an overview of the topics given in the course calendar for that day. Students are expected to read the material to be covered the day before class. The lecture time will also consist of in-class problem solving activities. Some lecture periods will consist of in-class demonstrations that involve the use of a computer. Personal laptops or those shared between students is recommended.

Class Participation

Students will be expected to participate in class and during group problem solving activities. Solutions to these problems will be discussed and presented by students. Everyone is expected throughout the semester to contribute to these discussions. Dr. Klauda will determine the grade for class participation based on the student's involvement.

Homework

Homework problems will be assigned regularly and will be graded. These will consist of problems that only require pencil and paper to those that require software to run simulations. You are allowed to help each other on the homework problems but **each person must turn in their own work**. Homework that is copied from another student is in violation the university's Code of Academic Integrity. Similarly, you are not allowed to use the publisher's solution manual or those from previous students.

Midterm Exam

There will only be one midterm exam (**March 10)**. The midterm exam will only cover the material listed on the course calendar and is *OPEN* book and calculator. The exam for undergraduates and graduates will be different.

Scientific Critique

Each student will critically review a scientific journal article that involves molecular simulation. Details on this assignment will be given later, but it will consist of an oral presentation that introduces and critically reviews the article. A written response to a set of general questions will also be graded.

Term Projects

The focus of the term projects will be different for the undergraduates and graduate students and will be in lieu of a final exam. Undergraduates will work as a team on a project of their choice (see Dr. Klauda for ideas). Graduate students are expected to work on a project that involves molecular modeling methods related to their own research. A proposal of groups and a short description of your project is due April 1st. Students **must** meet with Dr. Klauda twice before the final to ensure decent progress on the project. A short 5 page, single spaced report not including graphs and tables is due the date of the final exam. The student(s) will also present their work to the class on the date of the final exam.

Computer Accounts

Small computing accounts may be setup for students on the High Performance Computing Cluster (HPCC) at OIT. Details will be given later in the semester.

Grading Summary

Homework	30%
Midterm	25%
Scientific Critique	15%
Term Project	20%
Class participation	10%

Class Policies

Absences from class: If you must miss class for any reason, I strongly recommend that you ask a classmate for any notes, handouts, or announcements you may have missed. In addition, please notify me as far in advance as possible if you know that you are going to miss class for a university-approved reason, so that we can discuss any necessary arrangements. Please see the Undergraduate Catalog's description of university-approved reasons for absence (http://www.umd.edu/catalog) and our Department's policy http://www.chbe.umd.edu/policies/index.html.

Academic integrity: The University of Maryland, College Park has a nationally recognized Code of Academic Integrity, administered by the Student Honor Council. This code sets standards for academic integrity at Maryland for all undergraduate and graduate students. As a student you are responsible for upholding these standards for this course. It is very important for you to be aware of the definitions and consequences of cheating, fabrication, facilitation, and plagiarism. For more information on the Code of Academic Integrity or the Student Honor Council, please visit http://www.shc.umd.edu and our Department's policy http://www.chbe.umd.edu/undergraduate/policies. Violations of the code will not be tolerated in this class.

Accommodations for students with disabilities: In order to receive accommodations, students with learning disabilities must provide a written request and documents from the University of Maryland Disability Support Services (http://counseling.umd.edu/DSS). Please submit any requests by **February 9**.

Cell phones: Please keep cell phones and other communicative devices silent and out of sight during class. Text messaging is not allowed during class and will be reflected in the class participation grade.

Inclement weather: In the event of inclement weather, I will comply with the University's decision regarding whether classes are going to be held or not. Any assignments due on the day of a cancellation will be due instead at the next class meeting.

Late Homework: These items are due at the designated time stated on each assignment. Email submissions will not be accepted, unless approved by myself. The penalty for lateness without a university-approved reason for absence on the due date is half credit up to 24 hours late and no credit after 24 hours.

Make-ups: Exams, critiques and term projects are considered Major Grading Events (see Departmental policy) and may only be made up if you are absent for a documented, university-approved reason.

Religious observation: If you will miss class on the day of an exam or on the date that an assignment is due because of a religious observation that is not officially recognized by the university, you must contact me **at least 2 weeks before your anticipated absence** in order to discuss alternative dates for the exam or assignment.

ELMS (www.elms.umd.edu): On ELMS, I will post this syllabus, assignments, and any major changes to the course calendar. In addition, I may sometimes post handouts utilized in class and links to useful web sites. You will also be able to access your grades via ELMS.

CourseEvalUM (www.courseevalum.umd.edu): Your participation in the evaluation of courses through CourseEvalUM is a responsibility you hold as a student member of our academic community. Your feedback is confidential and important to the improvement of teaching and learning at the University as well as to the tenure and promotion process. By completing all of your evaluations each semester, you will have the privilege of accessing online, at Testudo, the evaluation reports for the thousands of courses for which 70% or more students submitted their evaluations.

Course Calendar

Note: Students should read the chapter associated with the lecture PRIOR to class. Homework (HW) assignment dates are tentatively listed; due dates will be listed on the assignment.

Day	Date	Topic	Chapter/Section	HW
Tue	Jan 27	Introduction to Molecular Modeling Review of Classical Thermodynamics	In Class Notes	
Thr	Jan 29	Statistical Mechanical Ensembles	Ch. 1-2	
Tue	Feb 3	Ideal Gases: Monotonic & Energy Fluctuations	Ch. 3.1-3.5	
Thr	Feb 5	Ideal Gases: Diatomic and Polyatomic	Ch. 4	#1
Tue	Feb 10	*No Class (Biophysical Society Meeting)*		
Thr	Feb 12	Other Ensembles & Applications	Ch. 6	
Tue	Feb 17	Chemical Equilibrium	Ch. 5	#2
Thr	Feb 19	Imperfect Gases	Ch. 7-8	
Tue	Feb 24	Distribution Functions and Real Liquids	Ch. 11	#3
Thr	Feb 26	Modeling Molecule Interactions for Simulations Introduction to Intra- & Intermolecular Potentials	In Class Notes	
Tue	Mar 3	Complexity of Molecular Force Fields Case Study	In Class Notes	
Thr	Mar 5	Introduction to Molecular Dynamics/Monte Carlo, Relations to Statistical Mechanics, and Periodicity	In Class Notes	
Tue	Mar 10	**MIDTERM**	All Previous Material	
Thr	Mar 12	Long-range Forces Statistical Errors Molecular Dynamics		
Tue	Mar 17	*Spring Break*		
Thr	Mar 19	*Spring Break*		
Tue	Mar 24	*No Class (ACS Meeting)*		
Thr	Mar 26	*No Class (ACS Meeting)*		
Tue	Mar 31	Molecular Dynamics Theory & Application Simple Web-based Examples	In Class Notes	
Thr	Apr 2	Crash Lecture on Linux/UNIX Operating Systems Setting up and Running a Simple Simulation	In-class examples	
Tue	Apr 7	Analysis of Simulation Data	In-class examples	
Thr	Apr 9	Overview of Computing Clusters and Visualization of Simulation Data	In-class examples	#4
Tue	Apr 14	Setting up and Running Biological Simulations	In-class examples CHARMM-GUI.org	
Thr	Apr 16	**Student Journal Article Critiques**	Student Lectures	
Tue	Apr 21	**Student Journal Article Critiques**	Student Lectures	
Thr	Apr 23	Analysis of Biological Simulations	In-class examples	#5
Tue	Apr 28	Biological Membrane Simulations	CHARMM-GUI.org	
Thr	Apr 30	Complex Biological Simulations	Bionanotech (VMD)	#6
Tue	May 5	Monte Carlo Methods	In Class Notes	#7
Thr	May 7	Conformational Space, Docking & Protein Structure Prediction/Refinement	In Class Notes	
Tue	May 12	Advanced Atomic-level Simulation Techniques Replica-exchange/SGLD	In Class Notes	
Tues	May 19	**Student Projects (1:30-3:30 am)**		