The University of Ottawa - Winter 2020

CHEMISTRY 4390
Introduction to Molecular Simulation and Statistical Mechanics

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Course Web: http://titan.chem.uottawa.ca/teaching.htm

Lectures: Tuesdays 17:30 – 20:30 MNT 142

Textbook: None. Lecture slides and extended lecture notes made available on-line.

Grading Scheme:
40% assignments
25% midterm exam (in-class)
35% final exam

Prerequisites: Chemistry 2330/2730 or equivalent. 3140/3540 recommended.

Course Description: This course provides a practical introduction to modern molecular simulation techniques that are widely used as tools in chemical research. More specifically, classical molecular dynamics and Monte Carlo simulation methods are discussed. The necessary statistical mechanics required to understand and properly interpret the molecular simulations and link the results to measured bulk properties are also be introduced. Lectures and assignments include hands-on exercises where simulations are setup, performed, and analyzed by the students with software packages in common usage by researchers. An introduction to modern scientific computing environments and the Linux operating system is also provided.

Important Notes:

1) Due to the hands-on nature of the course, the lectures are held in the computer labs. We ask that students only use the internet during class for purposes required for the course. For example, please refrain from accessing Facebook, e-mail, etc as it is distracting to other students. Additionally, we ask that students not text in class. If you have an urgent message that you need to respond to, please leave the room.

2) The class notes and extended lecture notes may be modified as the course progresses. The most up-to-date versions are always posted on the course website. Use the most recent versions for study. The in-class lecture notes do not include all details taught. Refer to the extended lecture notes to more details.

3) If for any reason you need to hand in an assignment late, please tell Woo ahead of time (an e-mail will be sufficient) such that possible accommodations can be made. Marks will be deducted from late assignments (~20% per day).

4) Lectures where hands-on computational tasks are taught and students perform exercises are very important. The skills taught in these lectures are required for completing the assignments. These should be considered as a "lab" component of the course.

5) Some assignments will require the use of a spreadsheet (e.g. Excel) for calculations. The Excel sheet can be handed in as 'supporting material' for the assignment, but all discussion, final answers, and figures must be put in the hard copy, Word or PDF document.

6) Hard copies of assignments are preferred, but assignments can be handed in electronically. When doing this, do not send in individual scanned copies of individual pages. Please hand in a single word or PDF file. Supplementary files, such as spreadsheets can be handed in separately.

Course Outline

1. **Introduction**
   - Motivation: relating microscopic molecular properties to macroscopic / thermodynamic behavior of bulk systems. Molecular dynamics and Monte Carlo simulations can be used to model macroscopic scale experiment;
   - Introduction to scientific computing and using the Linux operating system.

2. **Empirical Force Field Models**
   - Modeling the potential energy surface of non-reactive systems;
   - Inter- and intra-molecular force fields: design and choice of force fields, calculation of the force field parameters using quantum chemistry.

3. **Classical Mechanics for many-molecule systems**
   - Newton's equations of motion for many-molecule systems;
   - Analytical solution of Newton's equations for simple systems;
   - Numerical solution of Newton's equations, finite-difference method;
   - The Verlet and leapfrog time progression algorithms;
   - The concept of trajectory for a many-particle system

4. **Introduction to Statistical Mechanics**
   - Basic concepts of probability theory;
   - The concept of partition function and ensemble in statistical mechanics: a quantum mechanical approach;
   - Thermodynamic properties: energy, temperature, pressure, entropy, free energy, fluctuations in these quantities in microscopic systems;
   - Statistical mechanics in classical mechanics language.

5. **Molecular Dynamics (MD) Simulations**
   - Periodic boundary conditions: simulating "infinite" bulk systems with a finite number of molecules. Simulating bulk phases, surfaces, and nanoparticles;
   - Short-range van der Waals forces: truncation of potentials;
   - Long-range electrostatic forces: Ewald summations;
   - Including the effect of the environment in molecular simulations: thermostats and barostats;
   - Determining thermodynamic averages from molecular dynamics trajectories: Multiple time origins and maximizing sample size and statistical averaging.

6. **Applications of Molecular Dynamics Simulations**
   - Characterizing the microscopic structure of phases; radial distribution functions;
   - Dynamics of molecules from MD; mean-square displacements, velocity autocorrelations, diffusion coefficients;
   - Applications of MD to materials science and biological systems with the DL_POLY and AMBER molecular dynamics software packages

7. **Monte Carlo (MC) Simulation Methods and Applications**
   - Principles of Monte Carlo methods: Importance sampling, microscopic reversibility;
   - Advantage and disadvantages of Monte Carlos simulations in comparison to MD simulations;
   - Simulations in different ensembles with MC.