WESTERN UNIVERSITY
DEPARTMENT OF CHEMISTRY

CHEM 9564Y-Molecular Simulations
September 2013-March 2014

COURSE OUTLINE

Instructor Dr. Styliani Constas, Room 071-Chemistry Building, ext. 86338

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Lecture times two hours/week. Lecture times, TBA; Starting date: TBA; Room TBA.

Office hours Monday, Wednesday 12:00-2:30 pm or by appointment

Website http://owl.uwo.ca/

Course Textbook Lecture Notes provided by the Instructor;

Classic books to strengthen or develop the background in statistical mechanics and molecular simulations are:

- "Computer simulation of liquids" by M. P. Allen and D. J. Tildesley;
- "Molecular Dynamics Simulation, Elementary Methods" by J.M. Haile.
- "Physical Chemistry: Statistical Mechanics" by Horia Metiu;
- "Introduction to Statistical Mechanics" by T. Hill;
- "Statistical Mechanics" by D. McQuarrie;

All books are on reserve in the library. The primary material of the course consists of: references to parallel material in various books available in the library which will be made during the course, your lecture notes, material distributed in the class and your work on the assignments.

General description The first part of the course deals with molecular dynamics (MD) methodologies, setting-up and performance of simulations using MD methods. The second part of the course deals with Monte Carlo (MC) methods and sampling of rare events such as transition states of chemical reactions that take place in condensed phase (solutions), conformations changes of macromolecules such as polymers, polypeptides, proteins; nucleation processes in the condensed phase. The objective of the course is for students to learn about the molecular dynamics methods hidden in a black-box simulation package and develop a critical understanding of how to set-up simulations. This goal will be achieved by learning details about the methodologies of Molecular Dynamics and presenting examples where Molecular Dynamics may produce artifacts. How

to present the MD methodologies in an article will be also practiced. The expectation of the course is the students to be able to understand certain molecular dynamics and Monte Carlo methods, their limitations and the parameters of the simulations. Practical applications will be done with GROMACS simulation software and VMD visualization package.

Course Evaluation 3 assignments (45 % of the final mark); Assignment questions may be based on search of the current literature (for instance why certain simulation techniques are applied to particular systems and comparisons between methods), and critical questions on methodologies; Mid-term presentation of a project (25 %) and final presentation on a project (30%).

Project The project may be related to simulations in one's research field and the topic has to be in the field of statistical mechanics or molecular simulations. The topic may involve discussion of certain molecular dynamics methods used in the literature. It is important to present a critical discussion in your presentation. The midterm and final examinations will be based on a 20 min class presentation and 10 min for questions asked by the instructor and audience. The oral presentation will worth 55 %; responses to the questions of audience and instructor 45 %.

Accessibility

Please contact the course instructor if you require material in an alternate format or if you require any other arrangements to make this course more accessible to you. You may also wish to contact Services for Students with Disabilities (SSD) at 661-2111 x 82147 for any specific question regarding an accommodation.

Course Outline

1. Examples of uses of computer simulations in material science and biological systems. Role of statistical mechanics. Ensemble average of properties and postulates of statistical mechanics; Time average; Ensemble average; Liouville equation; quantum statistical mechanics (5 h).

2. Basic steps in simulations. Periodic boundary conditions. (1 h)

3. Basic Algorithms of Molecular Dynamics (leap-frog; Verlet, velocity-Verlet and other variations); Advanced Molecular Dynamics to speed up simulations in biological systems. (2 h)

4. Basic Algorithms of Monte Carlo. (2 h)

5. Treatment of intermolecular interactions; truncation of interactions; Ewald summation. treatment of interactions in biological systems such as proteins; bi-lipid membranes. (1 h)

6. Ensembles used in molecular dynamics (canonical ensemble, isobaric ensemble). (1 h)
7. Treatment of slow processes such as conformational changes of macromolecules. Replica Exchange Molecular Dynamics. (1 h)
8. Computation of properties to characterize the structure; radial distribution functions. (1 h)
9. Computation of diffusion coefficients. (1 h)
10. Sampling methods: Umbrella sampling. (2 h)
11. Blue moon ensemble. (2.5 h)
12. Transition path sampling. (2.5 h)
13. Order parameters; reaction coordinates. (1 h)
14. Time correlation functions. (1 h)
15. Fluctuation dissipation theorem. (1 h)
16. Rates of reactions and of conformational changes of macromolecules. (2 h)
17. Algorithms for the computations of reaction rates. (2 h)
18. Familiarization with GROMACS simulations package; perform molecular dynamics simulations. Learning of how to report the computational methodology and understand the computational molecular dynamics and Monte Carlo literature pertaining to biological systems and material science topics. (3h)