Course Outline

Proposed course name: Computer methods in chemistry
Course number: Chem 3300G
Planned: Winter 2020

Instructor: Mikko Karttunen
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Web: WebOwl

Schedule:
- Lectures: Monday, Wednesday, Friday, 10:30–11:20 am, PAB 117
- Labs: Monday, 6:00–9:00 pm, SH 1310
Office hours: By appointment
Teaching Assistant: TBA

Target audience: Graduate students in Chemistry. This course should also be of interest for students in Applied Mathematics, Physics, Chemical Engineering, Pharmaceutical Science, and related, interested in computational modeling, molecular visualization and data analysis. In addition to students working in computational modeling, the course is useful for anyone interested in the practical aspects of modern simulations. The data analysis and visualization parts are also applicable to analysis / visualization of experimental data.

Pre-requisites: Chemistry 2272F, 2281G, 2283G, 2384B. Unless you have either the requisites for this course or written special permission from your Dean to enroll in it, you may be removed from this course and it will be deleted from your record. This decision may not be appealed. You will receive no adjustment to your fees in the event that you are dropped from the course for failing to have the necessary prerequisites.

Topics: To aim of this course is to familiarize the student with modern methods and methodology in computational chemistry. Emphasis is put on direct hands-on experience using production-quality molecular dynamics software (see below). The course provides a broad overview of the common methods in the framework of molecular modeling and, importantly, how to relate the data to experiments. Simulations of proteins, lipid bilayers and solvation of organic molecules will be performed. The course will be a balanced treatment of modeling, data analysis, visualization and relation to experimentally observable / measurable phenomena.

Special: There will be reading material every week. The material is based on current topics in materials and biomaterials modeling. From this material, the students will have to prepare presentations as will be discussed during the first meeting.

Material: Lecture notes and material provided during lectures.

Practical requirements:
- Installation of Gromacs (version 2018.6) is required. This means: either the ability to install it on your own personal laptop or having access to Gromacs otherwise (that access must be available during labs). For installation on your own computer: Works easily if
your operating system is either Windows 10, Linux, or OSX. Detailed instructions will be provided during the first lecture / labs. About Gromacs: Gromacs is one of the world’s most popular and fastest molecular simulation software and available freely (open source) at www.gromacs.org

- **VMD.** VMD (Visual Molecular Dynamics) is a powerful tool for analysis and visualization of molecules. It is freely available at http://www.ks.uiuc.edu/Research/vmd/. VMD is available for all common operating systems.
- **Python installation.** Some python programming is included in the course. Python is available for all common operating systems at www.python.org
- **Plotting program like grace, gnuplot, Matlab, etc.**

**Helpful reference / background material (not required):**

- D. Frenkel & B. Smit: Understanding molecular simulation - from algorithms to application M.P Allen & D.J. Tildesley: Computer simulations of liquids
- D. Rapaport: The Art of Molecular Simulation
- A.R. Leach: Molecular Modeling

**Evaluation:** Tentative plan: Assignments (25%), Reports / presentations (25%), Final project (50%)

**The fine print - University guidelines on various issues:**

The UWO Senate Academic Handbook has specified that the following points should be added to all course outlines:

**A. Prerequisites:**

**B. Medical/Compassionate Excuses:** Students missing work for valid medical or other reasons are governed by the regulations https://studentservices.uwo.ca/secure/index.cfm

**C. Student Accessibility Services (SAS):** Western is committed to achieving barrier-free accessibility for all its members, including graduate students. As part of this commitment, Western provides a variety of services devoted to promoting, advocating, and accommodating persons with disabilities in their respective graduate program. Graduate students with disabilities (for example, chronic illnesses, mental health conditions, mobility impairments) are encouraged to register with Student Accessibility Services, a confidential service designed to support graduate and undergraduate students through their academic program. With the appropriate documentation, the student will work with both SAS and their graduate programs (normally their Graduate Chair and/or Course instructor) to ensure that appropriate academic accommodations to program requirements are arranged. These accommodations include individual counselling, alternative formatted literature, accessible campus transportation, learning strategy instruction, writing exams and assistive technology instruction.

For more information, see http://www.sdc.uwo.ca/ssd/
E. **Academic Offences:** Scholastic offences are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at the following Web site: http://www.uwo.ca/univsec/handbook/appeals/scholastic discipline undergrad.pdf

F. **Plagiarism:** All required papers may be subject to submission for textual similarity review to the commercial plagiarism detection software under license to the University for the detection of plagiarism. All papers submitted for such checking will be included as source documents in the reference database for the purpose of detecting plagiarism of papers subsequently submitted to the system. Use of the service is subject to the licensing agreement, currently between The University of Western Ontario and Turnitin.com (http://www.turnitin.com).

G. **Support Services:** Support is available from the Registrar: http://www.registrar.uwo.ca, via the university students council (http://westernusc.ca/services/) and at Student Development Services (http://www.sdc.uwo.ca/).

H. **Mental or Emotional Health:** Students who are in emotional/mental distress should refer to Mental Health@Western http://www.uwo.ca/uwocom/mentalhealth/ for a complete list of options about how to obtain help.