

CHM 1485: Topics in Statistical Mechanics: The Foundations of Molecular Simulation

Course Syllabus: Winter 2024

I CONTACTS

INSTRUCTOR:

Name: Jeremy Schofield

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Office: Lash Miller, Room 420E

Classes: Wednesdays, 1 – 3 p.m., UC-69

Office hours: By appointment.

II COURSE OVERVIEW

COURSE DESCRIPTION:

The foundational principles of numerical solutions of structural and dynamical properties of many body systems will be presented.

PREREQUISITE COURSES:

This course assumes you have a basic understanding of statistical mechanics.

III TOPICS

1. Review
 - Classical Mechanics
 - Ensembles
 2. Numerical integration and importance sampling
 - Quadrature
 - Monte Carlo
 - Error Analysis
 3. Applications of the Monte Carlo Method
 - Umbrella Sampling
 - Parallel Tempering
 4. Molecular Dynamics
 - Basic integration schemes
 - Stability and symplectic properties
 - Higher order schemes
 5. Advanced Topics
 - Hybrid Monte Carlo
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IV EVALUATION/GRADING SCHEME

- **Marked problem sets:** Four in total worth a total of 70% of the final mark
- **Short literature report (3500 words) or simulation project:** 30% of final mark.

V COURSE POLICIES

- We will strive to answer all communications such as emails in a 24-hour period.
- The University of Toronto is committed to equity, human rights and respect for diversity. All members of the learning environment in this course should strive to create an atmosphere of mutual respect where all members of our community can express themselves, engage with each other, and respect one another's differences. U of T does not condone discrimination or harassment against any persons or communities.
- All work for the course must be submitted using Quercus.
- Normal University procedures should be followed to signal course absences and request make-up tests or exemptions from exams.

VI TECHNOLOGY REQUIREMENTS

This course requires the use of computers, and of course sometimes things can go wrong when using them. You are responsible for ensuring that you maintain regular backup copies of your files, use antivirus software (if using your own computer), and schedule enough time when completing an assignment to allow for delays due to technical difficulties. Computer viruses, crashed hard drives, broken printers, lost or corrupted files, incompatible file formats, and similar mishaps are common issues when using technology, and are not acceptable grounds for a deadline extension.

VII INSTITUTIONAL POLICIES AND SUPPORT

ACADEMIC INTEGRITY

On Academic Integrity:

Academic integrity is essential to the pursuit of learning and scholarship in a university, and to ensuring that a degree from the University of Toronto is a strong signal of each student's individual academic achievement. As a result, the University treats cases of cheating and plagiarism very seriously. The University of Toronto's Code of Behaviour on Academic Matters (<https://governingcouncil.utoronto.ca/secretariat/policies/code-behaviour-academic-matters-july->

[1-2019](#)) outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences. Potential offences include, but are not limited to:

In assignments:

1. Using someone else's ideas or words without appropriate acknowledgement.
2. Submitting your own work in more than one course without the permission of the instructor.
3. Making up sources or facts.
4. Obtaining or providing unauthorized assistance on any assignment.

On tests and exams:

1. Using or possessing unauthorized aids.
2. Looking at someone else's answers during an exam or test.
3. Misrepresenting your identity.

In academic work:

1. Falsifying institutional documents or grades.
2. Falsifying or altering any documentation required by the University.

Please note that the use of websites (such as Chegg.com or the course discussion board) to post questions or to post/access answers to questions is an academic offence under the University of Toronto's Code of Behaviour on Academic Matters. Alleged instances of this nature are forwarded to the Faculty of Arts & Science Student Academic Integrity office.

All suspected cases of academic dishonesty will be investigated following procedures outlined in the Code of Behaviour on Academic Matters. If you have questions or concerns about what constitutes appropriate academic behaviour or appropriate research and citation methods, you are expected to seek out additional information on academic integrity from your instructor or from other institutional resources (see <https://www.academicintegrity.utoronto.ca/>).

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This course, including your participation, will be recorded on video and will be available to students in the course for viewing remotely and after each session.

Course videos and materials belong to your instructor, the University, and/or other sources depending on the specific facts of each situation and are protected by copyright. Do not download, copy, or share any course or student materials or videos without the explicit permission of the instructor.

ACCESSIBILITY NEEDS

Students with diverse learning styles and needs are welcome in this course. The University of

Toronto is committed to accessibility: if you require accommodations for a disability, or have any other accessibility concerns about the course, please contact [Accessibility Services](#) as soon as possible.

ACCOMMODATIONS FOR RELIGIOUS OBSERVANCES

Following the University's policies, reasonable accommodations will be made for students who observe religious holy days that coincide with the due date/time of an assignment, tutorial, class or laboratory session. Students must inform the instructor before the session/assignment date to arrange accommodations.

ADDITIONAL SERVICES and SUPPORT

The following are some important links to help you with academic and/or technical service and support

- General student services and resources at [Student Life](#)
- Full library service through [University of Toronto Libraries](#)
- Resources on conducting online research through [University Libraries Research](#)
- Resources on academic support from the [Academic Success Centre](#)
- Learner support at the [Writing Centre](#)
- Information for [Technical Support/Quercus Support](#)

ACKNOWLEDGEMENT OF TRADITIONAL LANDS

We wish to acknowledge this land on which the University of Toronto operates. For thousands of years, it has been the traditional land of the Huron-Wendat, the Seneca and, most recently, the Mississaugas of the Credit River. Today, this meeting place is still the home to many Indigenous people from across Turtle Island and we are grateful to have the opportunity to work on this land.