

General Course Information

CHEM 438

Molecular dynamics

0.125 EFTS 15 Points
First Semester 2023

Description

This course is about modelling the behaviour of macromolecular systems (e.g. biomacromolecules such as proteins or supramolecular assemblies such as metal-organic-framework materials), using molecular dynamics. The topics covered by this course are:

- Force fields and equations of motion
- Controlling temperature, pressure, volume within simulations
- Practical considerations when running molecular dynamics simulations
- Assessing how well simulations match experiment

Timetable

Workshops: One hour per week. Details to be confirmed on 'My Timetable' and the Web.

Students should note that this course involves a high degree of self-guided learning. Students will be given course material and assignment instructions in advance and must come to workshops prepared with questions on the assignment material. The first workshop will be a course intro.

Course Coordinator

Associate Professor Deborah Crittenden, School of Physical and Chemical Sciences, BT Room 326, ext 95217
email: deborah.crittenden@canterbury.ac.nz

Assessment

Assignments: 3 assignments worth 100% in total, comprising a mixture of written work and oral presentations.

Prerequisites

P: 300-L CHEM or BCHM

Web-based resources

All learning resources for this course will be available via the University of Canterbury's *Learn* web site -- <http://learn.canterbury.ac.nz/>.

Goal of the Course

The goal of this course is for students to understand how molecular dynamics simulations work, how to meaningfully generate and analyse molecular dynamics data, and be able to critically assess molecular dynamics results presented in the literature.

Learning Outcomes

As a student in this course I will develop the ability to:

- Define what is meant by the terms “force field” and “equations of motion” and describe the relationship between them in the context of performing molecular dynamics simulations
- Perform all of the steps of a molecular dynamics simulation for a simple model system
- Explain how differences in the force field affect the outcome of molecular dynamics trajectories
- Explain how differences in initial conditions (displacements and velocities) affect the outcome of molecular dynamics trajectories
- Explain how the choice of time step affects the accuracy of a simulation
- Recognise how these basic steps can be generalized to simulate systems of arbitrary size and complexity
- Describe the additional complications that arise in larger systems (e.g. controlling pressure, volume, temperature for all atoms) and how they are controlled for within molecular dynamics simulations
- Describe the information required to set up and initiate molecular dynamics simulations on larger systems
- Describe the types of data that are produced during MD simulations and how they can be meaningfully analysed
- Critique the scientific literature in the light of the knowledge I have gained from the above learning outcomes.

Transferable Skill Register

As a student in this course I will develop the following skills:

- Critical analysis of the scientific literature.
- Numeracy: being able to translate equations into simulation processes
- Presentation: the ability to explain what you have learned to a scientifically literate audience
- Writing: the ability to explain yourself clearly and logically in writing.

Summary of the Course Content

The topics covered by this course are:

MOLECULAR DYNAMICS FUNDAMENTALS

(4 workshops)

In this part of the course, you will complete your first assignment: constructing your own molecular dynamics trajectory for an oscillating diatomic molecule and exploring how the results change if you change the input parameters.

MOLECULAR DYNAMICS PRINCIPLES

(4 workshops)

In this part of the course, you will complete your second assignment: summarizing and explaining all of the additional information required to meaningfully run and analyse molecular dynamics simulations on more realistic chemical and biochemical systems.

MOLECULAR DYNAMICS APPLICATIONS

(4 workshops)

In this part of the course, you will choose a scientific article from the literature that presents both experimental and molecular dynamics results and critically assess the match between the two, i.e. how well/appropriately the MD simulations predict and/or explain experiment.

GENERAL INFORMATION | TE KIMI MŌHIOHIO 2023

Policy on 'Dishonest Practice' | Ngā Takahitanga me ngā Tinihanga

The University has strict guidelines regarding 'dishonest practice' and 'breach of instructions' in relation to the completion and submission of examinable material. In cases where dishonest practice is involved in tests or other work submitted for credit, a department may choose to not mark such work – see the online guidelines in relation to ['Academic Integrity'](#).

The School of Physical and Chemical Sciences upholds this policy. It considers plagiarism, collusion, copying and ghost writing – all detailed below – to be unacceptable and dishonest practices:

- **Plagiarism | Tārua Whānako** is the presentation of any material (text, data or figures, on any medium including computer files) from any other source without clear and adequate acknowledgement of the source. Note that the use of **AI generative tools such as ChatGPT** for assessment work is *strictly forbidden*, except where the lecturer concerned has specifically granted approval.
- **Collusion** is the presentation of work performed in whole, or in part, in conjunction with another person or persons, but submitted as if it has been completed by the named author alone. This interpretation is not intended to discourage students from having discussions about how to approach an assigned task and incorporating general ideas that come from those discussions into their own individual submissions, but acknowledgement is necessary.
- **Copying** is the use of material (in any medium, including computer files) produced by another person or persons with or without their knowledge and approval. **This includes copying of the lab reports (raw data may be shared within the group if permitted or required by the experiment) – data analysis and interpretation of obtained results MUST be performed individually.**
- **Ghost writing** is the use of other person(s) (whether with or without payment) to prepare all or part of an item of work submitted for assessment.

Special consideration of assessment | Ngā Pairuri Motuhake

'[Special Consideration](#)' (previously termed 'Aegrotat Application') for an item of assessment is for students who have covered the work involved but have been prevented from demonstrating their knowledge or skills at the time of the assessment due to unforeseen circumstances, whether illness, injury, bereavement, car crash or any other extenuating circumstance *beyond one's control*. Special Consideration for a test/exam may be because a student has not sat it or has done so with impaired performance. Applications can be submitted via the above link and must be made **no later than five working days after the assessment due date**. Note that special consideration is **not available for items worth less than 10% of the overall course mark**. In the case of illness or injury, medical consultation should normally have taken place either shortly before or within 24 hours after the due date for the required work or test/examination.

Note that you may be required to sit a special exam or your grade may not be changed if there is insufficient evidence of your performance from other invigilated assessment items in the course. **You have the right to appeal any decision.**

It is important to understand that Special Consideration is only available *where course work has been covered*, and the inability to demonstrate this fully is both *no longer possible* AND is due to *unexpected circumstances beyond one's control*. Thus Special Consideration is **NOT available for:**

- essays, assignments or quizzes where an extension of time is available to complete the assessment item (see below for the process to involved);
- missed lectures during the semester;
- experiencing examination anxiety;
- having several examinations or assessments close together;
- known impairment, such as chronic illness (medical or psychological), injury or disability unless medical evidence confirms that the circumstances were exacerbated, despite appropriate management, at the time of assessment;
- mistaking the date or time of an examination (this is a circumstance one can control!);
- failing to turn up to an examination or test because of sleeping in (a circumstance as above!);
- where applications are repeatedly made for the same or similar reason, then the application may be declined on the grounds that the reason is not unexpected;
- where the application is made at the time of the assessment but the supporting documentation is received significantly after this date or after the date results are released; or
- the application is made following the release of results (unless under exceptional circumstances).

Extensions of deadlines | Tononga Wā Āpiti

Where an extension may be granted for an assessment item, this will be decided by application to the course coordinator and/or the lecturer concerned.

Late withdrawal from a course

If you are prevented by extenuating circumstances from completing the course after the final date for withdrawing from the course, you may apply for special consideration for late discontinuation. For details on special consideration, or to make an application, refer to the Examinations Office website <http://www.canterbury.ac.nz/exams/>. Applications must be submitted **within five days** of the end of the main examination period for the semester.

Missing of tests | Te Matangaro i ngā Whakamātautau

In rare cases a student will not be able to sit a test. In such cases, the student should consult with the course coordinator to arrange alternative procedures. **This must be done well in advance of the set date for the test.**

Past tests and exams

Past tests can be found on our [Chemistry Undergraduate](#) website. Past exams can be found on the [Library website](#).

Submission of reports and assignments

Reports (including lab reports) and assignments should be handed in on time. Extensions will be granted only in exceptional circumstances (such as illness or bereavement). If an extension is required, as early as possible you should request it from the lecturer concerned.

Note: If you do not submit an assignment for assessment, you will be allotted zero marks, which will affect your final result. You should ensure that you pick up marked assignments and keep them until the end of the course as evidence that the work was completed and marked in the case that either is disputed. To guard against accidental loss, it would be prudent to keep photocopies or electronic copies of anything submitted.

Late Work

Acceptance of late work for assessment will be at the discretion of the course coordinator and/or the lecturer concerned. If your assessment is likely to be late, please contact the relevant of these people **before the assessment is due**. Never assume that an extension will be automatically granted – some courses have the policy of no late work being accepted. A commonly exercised policy is to deduct 10% of the total marks for each day that the work is late, where weekends and public holidays also count as such days.

Marks and Grades | Taumata Ako

The following numbers should be considered as a guide to the expected grades under normal circumstances. The School reserves the right to adjust mark/grade conversions, if necessary.

Grade:	A+	A	A–	B+	B	B–	C+	C	C–	D	E
Minimum mark %:	90	85	80	75	70	65	60	55	50	40	0

Reconsideration of Grades: Students should, in the first instance, speak to the course co-ordinator about their marks. If they cannot reach an agreeable solution, or have questions about their grade in a course, students should then speak to the Coordinator of 400-level studies, [Professor Sarah Masters](#) (phone 369 4229). Students can appeal any decision made on their final grade. You can apply at the Registry for reconsideration of the final grade within four weeks of the date of publication of final results. Be aware that there are time limits for each step of the appeals process.

Students with Disabilities: Students with disabilities should speak with someone at [Equity and Disability Service](#), phone: 369 3334 (or ext. 93334), email: eds@canterbury.ac.nz).

Academic Advice: [Professor Sarah Masters](#) is the coordinator of 400-level chemistry courses. Her interest is in the academic performance and well-being of all such students. Anyone experiencing problems with their chemistry courses or requiring guidance about their 400-level courses should get in contact with Sarah.

Sarah Masters
Coordinator of 400-level Chemistry Courses
School of Physical and Chemical Sciences
February 2023