UNSW Course Outline

MATS6110 Computational Materials Science - 2024

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General Course Information

Course Code : MATS6110
Year : 2024
Term : Term 2
Teaching Period : T2
Is a multi-term course? : No
Faculty : Faculty of Science
Academic Unit : School of Materials Science & Engineering
Delivery Mode : In Person
Delivery Format : Standard
Delivery Location : Kensington
Campus : Sydney
Study Level : Postgraduate
Units of Credit : 6

Useful Links

Handbook Class Timetable

Course Details & Outcomes

Course Description

This course covers the principles and applications of solving material science and engineering problems through computational approaches. Students will have the opportunities to understand how finite elemental analysis, density functional theory and machine learning can be used to

solve problems in the areas of fluid dynamics, electronic properties of advanced materials, and ultimately, de novo predictions of new functional materials.

Course Aims

The course aims to provide the students with the skills to understand and apply common materials modelling software to materials science problems, especially in the area of fluid dynamics, revealing complex structure-property relationships and discoveries of new functional materials. It will prepare the students with essential computational modelling knowledges that are critically needed in material engineering, material physics, as well as machine-learning in material studies.

Relationship to Other Courses

The course is shared the same classes with MATS3006 for weeks 1-5.

Course Learning Outcomes

Course Learning Outcomes
CLO1 : Explain the fundamental principles of various computational modelling techniques (solid modelling, computational fluid dynamics, density functional theory and machine learning).
CLO2 : Use commercial software to solve real problems in materials science and engineering
CLO3 : Choose an appropriate computational method for solving a range of problems in materials science and engineering
CLO4 : Explain the role of computational modelling in current research in materials science and engineering by referencing to the latest literatures in the field.

Course Learning Outcomes	Assessment Item
CLO1 : Explain the fundamental principles of various computational modelling techniques (solid modelling, computational fluid dynamics, density functional theory and machine learning).	• Mid-term Test • Group Activity Report • Assignment 1 • Literature Review Assignment
CLO2 : Use commercial software to solve real problems in materials science and engineering	• Mid-term Test • Assignment 1
CLO3 : Choose an appropriate computational method for solving a range of problems in materials science and engineering	• Mid-term Test • Assignment 1
CLO4 : Explain the role of computational modelling in current research in materials science and engineering by referencing to the latest literatures in the field.	• Group Activity Report • Literature Review Assignment • Assignment 1

Learning and Teaching Technologies

Echo 360 | Moodle - Learning Management System

Learning and Teaching in this course

Lectures: The core concepts will be taught in lectures, students will have access to the lectures notes
before class for annotation during the lecture. Students will be engaged in the learning process through class discussions and problem-solving questions independently and working together with
partners and groups.
Tutorials: Tutorials will consolidate the students learning of the core concepts through short-

answer
and problem-solving questions. Students will have the chance to work collaboratively in class and
independently outside of class. Real world examples of the concepts will engage the students in the
learning processing by connecting theory to practice.

Additional Course Information

The purpose of this course is to provide students with the tools required for computational modelling
for technological and professional materials applications. The course covers two main pillars of modern
material modelling techniques, the finite element analysis and density functional theory, with the applications of later in machine-learning and AI-driven material discoveries. The use of computational
as a part of materials engineering design is emphasised.

Assessments

Assessment Structure

Assessment Item	Weight	Relevant Dates
Mid-term Test Assessment Format: Individual	30%	Start Date: week 5 Due Date: week 5
Group Activity Report Assessment Format: Group	25%	
Assignment 1 Assessment Format: Individual	20%	Start Date: Not Applicable Due Date: Not Applicable
Literature Review Assignment Assessment Format: Individual	25%	Start Date: Not Applicable Due Date: Not Applicable

Assessment Details

Mid-term Test

Assessment Overview

You will complete a test that covers the CFD part of the course. It consists of a theoretical and a practical part, both being open-book.
The 100-min theoretical part includes short-answer and calculation questions.
The 90-min practical test is conducted in the computer lab to solve a complex CFD problem

using software packages.

The mid-term test is typically run in Week 5.

Feedback: Solutions and marked tests will be provided two weeks after submission.

Course Learning Outcomes

- CLO1 : Explain the fundamental principles of various computational modelling techniques (solid modelling, computational fluid dynamics, density functional theory and machine learning).
- CLO2 : Use commercial software to solve real problems in materials science and engineering
- CLO3 : Choose an appropriate computational method for solving a range of problems in materials science and engineering

Detailed Assessment Description

The FEA part will be examined. The exam will be 2 hours duration held in
week 5. It assesses understanding of the FE theory learnt in the course. The exam will be close book.

Assessment Length

2 hours

Assignment submission Turnitin type

Not Applicable

Hurdle rules

Students who fail to achieve a score of at least 40% for the exam component (i.e., mid- session exam), but achieve a final mark >50% for the course, will be
awarded a UF (Unsatisfactory Fail) for the course.

Group Activity Report

Assessment Overview

Using the knowledge learned from the lectures and information gathered from your own literature search, you will work in groups of 2 to select a topic of interest and prepare a short research proposal that could form the basis of Masters research project. A list of potential topics and detailed expectations for the report will be given during the lectures. The assessment is to be submitted at the end of week 11.

Feedback will be given two weeks after submission of the assignment and take the form of the

mark for the assignment, overall comments on how the class performed, any common areas that were not answered correctly. Additionally, personal feedback and how each student performed may be given.

Course Learning Outcomes

- CLO1 : Explain the fundamental principles of various computational modelling techniques (solid modelling, computational fluid dynamics, density functional theory and machine learning).
- CLO4 : Explain the role of computational modelling in current research in materials science and engineering by referencing to the latest literatures in the field.

Assignment 1

Assessment Overview

You will develop analytical solutions, using finite element theory, to basic mechanical loading problems. You will also use ANSYS FE software to numerically solve a complex mechanical loading problem involving a range of materials.

The assignment will be distributed in Week 7 and submitted in Week 10.

Feedback will be given two weeks after submission, including the solutions and your marked assignment with comments.

Course Learning Outcomes

- CLO1 : Explain the fundamental principles of various computational modelling techniques (solid modelling, computational fluid dynamics, density functional theory and machine learning).
- CLO2 : Use commercial software to solve real problems in materials science and engineering
- CLO3 : Choose an appropriate computational method for solving a range of problems in materials science and engineering
- CLO4 : Explain the role of computational modelling in current research in materials science and engineering by referencing to the latest literatures in the field.

Detailed Assessment Description

Lab practice assignment: You will use the ANSYS software to perform your lab practice assignment on finite element modelling
Practice Assignment 1: You will develop analytical solutions, using finite element theory, to basic mechanical loading problem.

Assignment submission Turnitin type

Not Applicable

Literature Review Assignment

Assessment Overview

You will be asked to undertake a review of recently published literature that is relevant to one of the topics that is covered in the second half of the course. You will write a report in 500-1000 words that summarizes the main findings from your literature review. The assessment is to be submitted at the end of week 10, and will be peer-reviewed by other students. The final mark for this assessment will consist of 50% from the course convenor and 50% from the peer assessment.

Feedback will be given two weeks after submission of the assignment and take the form of the mark for the assignment, overall comments on how the class performed, any common areas that were not answered correctly. Additionally, personal feedback and how each student performed may be given.

Course Learning Outcomes

- CLO1 : Explain the fundamental principles of various computational modelling techniques (solid modelling, computational fluid dynamics, density functional theory and machine learning).
- CLO4 : Explain the role of computational modelling in current research in materials science and engineering by referencing to the latest literatures in the field.

Assignment submission Turnitin type

Not Applicable

General Assessment Information

Lab practice and assignment 1:

- Lab practice assignment (12.5%): You will use the ANSYS software to perform your lab practice assignment on finite element modelling. Due date by end of online labs
- Practice Assignment (12.5%): You will develop analytical solutions, using finite element theory, to basic mechanical loading problem. Due date weeek 5

Mid-term exam (25%)

- The exam will be 2 hours duration held in week 5. It assesses understanding of the FE theory learnt in the course. The exam will be close book

Assignment 2

- Group project – Mini Research Proposal (25%). Due date week 10
- Individual literature review (25%). Due date week 11.

Grading Basis

Standard

Requirements to pass course

Students who fail to achieve a score of at least 40% for the overall exam component but achieve a final mark >50% for the course, will be awarded a UF (Unsatisfactory Fail) for the course

Course Schedule

Teaching Week/Module	Activity Type	Content
Week 1 : 27 May - 2 June	Blended	Topics • Revision of elastic theory • Finite element modelling Bar and beam elements, the stiffness method Activity • Lecture exercises • Lab practice
Week 2 : 3 June - 9 June	Blended	Topics • Stiffness methods for connected springs Activity • Lecture exercises • Lab practice • Assignment 1 handed out
Week 3 : 10 June - 16 June	Blended	Topics • Principle of virtual work Activity • Lecture exercises • Lab practice
Week 4 : 17 June - 23 June	Blended	Topics • Principle of virtual work 4-noded rectangular element
Week 5 : 24 June - 30 June	Blended	Topics • Tutorial and revision of FEA Mid-term exam Activity • Lab practice Assignment due • Assignment 1 due
Week 7 : 8 July - 14 July	Blended	Topics • Computational Modelling from First Principles • Structure-Property Relationships from DFT Activity • Assignment 2 and 3 (individual and group assignments) handed out
Week 8 : 15 July - 21 July	Blended	Topics • High-Throughput Computational Material Science and Machine-Learnings
Week 9 : 22 July - 28 July	Blended	Topics • Student Presentation
Week 10 : 29 July - 4 August	Blended	Topics • Student Presentation

Attendance Requirements

Students are strongly encouraged to attend all classes and review lecture recordings.

Course Resources

Recommended Resources

- E. Kreyzig, “Advanced Engineering Mathematics”
- R. F. Cooke, “Finite Element Modelling for Stress Analysis”
- O.C. Zienkiewicz, R.L. Taylor, J.Z. Zhu, “Finite Element Method – Its Basis and Fundamentals (6th Edition)” (Available online)
- J. Fish, T. Belytschko, “A First Course in Finite Elements” (Available online)

Staff Details

Position	Name	Email	Location	Phone	Availability	Equitable Learning Services Contact	Primary Contact
Convenor	Jack Yang				Online by appointment	Yes	Yes

Other Useful Information

Academic Information

Upon your enrolment at UNSW, you share responsibility with us for maintaining a safe, harmonious and tolerant University environment.

You are required to:

- Comply with the University’s conditions of enrolment.
- Act responsibly, ethically, safely and with integrity.
- Observe standards of equity and respect in dealing with every member of the UNSW community.
- Engage in lawful behaviour.
- Use and care for University resources in a responsible and appropriate manner.
- Maintain the University’s reputation and good standing.

For more information, visit the UNSW Student Code of Conduct Website.

Academic Honesty and Plagarism

Referencing is a way of acknowledging the sources of information that you use to research your assignments. You need to provide a reference whenever you draw on someone else's words, ideas or research. Not referencing other people's work can constitute plagiarism.
Further information about referencing styles can be located at https://student.unsw.edu.au/

referencing

Academic integrity is fundamental to success at university. Academic integrity can be defined as a commitment to six fundamental values in academic pursuits: honesty, trust, fairness, respect, responsibility and courage. At UNSW, this means that your work must be your own, and others' ideas should be appropriately acknowledged. If you don't follow these rules, plagiarism may be detected in your work.
Further information about academic integrity, plagiarism and the use of AI in assessments can be located at:

- The Current Students site,
- The ELISE training site, and
- The Use of AI for assessments site.

The Student Conduct and Integrity Unit provides further resources to assist you to understand your conduct obligations as a student: https://student.unsw.edu.au/conduct

Submission of Assessment Tasks

Penalty for Late Submissions

UNSW has a standard late submission penalty of:

- 5% per day,
- for all assessments where a penalty applies,
- capped at five days (120 hours) from the assessment deadline, after which a student cannot submit an assessment, and
- no permitted variation.

Any variations to the above will be explicitly stated in the Course Outline for a given course or assessment task.

Students are expected to manage their time to meet deadlines and to request extensions as early as possible before the deadline.

Special Consideration

If circumstances prevent you from attending/completing an assessment task, you must officially apply for special consideration, usually within 3 days of the sitting date/due date. You can apply by logging onto myUNSW and following the link in the My Student Profile Tab. Medical documentation or other documentation explaining your absence must be submitted with your application. Once your application has been assessed, you will be contacted via your student

email address to be advised of the official outcome and any actions that need to be taken from there. For more information about special consideration, please visit: https://student.unsw.edu.au/special-consideration

Important note: UNSW has a "fit to sit/submit" rule, which means that if you sit an exam or submit a piece of assessment, you are declaring yourself fit to do so and cannot later apply for Special Consideration. This is to ensure that if you feel unwell or are faced with significant circumstances beyond your control that affect your ability to study, you do not sit an examination or submit an assessment that does not reflect your best performance. Instead, you should apply for Special Consideration as soon as you realise you are not well enough or are otherwise unable to sit or submit an assessment.

Faculty-specific Information

Additional support for students

- The Current Students Gateway
- Student Support
- Academic Skills and Support
- Student Wellbeing, Health and Safety
- Equitable Learning Services
- UNSW IT Service Centre
- Science EDI Student Initiatives, Offerings and Guidelines