Course Outline

MATS6110

Computational Materials Science

Materials Science and Engineering

Science

T2, 2020

1. Staff

Position	Name	Email	Consultation times and locations
Course Convenor	Dr Judy Hart	j.hart@unsw.edu.au	Online by appointment
Lecturer	A/Prof. Runyu Yang	r.yang@unsw.edu.au	Online by appointment

2. Course information

Units of credit: 6

Pre-requisite(s): None

Timetable website: http://timetable.unsw.edu.au/2019/MATS6110.html

Teaching times and locations:

Part 1:	**Lecture/Lab ***	**Lecture**	**Lecture/ Tutorial**
Day	Tuesday	Thursday	Friday
Location	Online	Online	Online
Time	10:00-12:00	9:00-11:00	9:00-11:00
Weeks	1-5	1-5	1-5

* All computer labs will be run online.

Part 2:	**Lecture**	**Lecture**
Day	Tuesday	Thursday
Location	Online	Online
Time	10:00-12:00	9:00-11:00
Weeks	7-10	7

2.1 Course summary

This course covers the principles and application of solving materials science problems through computational approaches. Modelling packages such as ANSYS will be used to solve problems in areas of fluid dynamics and the structural properties of advanced materials.

2.2 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 and advanced structural materials.

2.3 Course learning outcomes (CLO)

At the successful completion of this course you (the student) should be able to:

1. Explain the role of computational modelling in current research in materials science and engineering
2. Explain the fundamental principles of various computational modelling techniques (solid modelling, computational fluid dynamics, molecular mechanics and dynamics)
3. Use commercial software to solve real problems in materials science and engineering
4. Choose an appropriate computational method for solving a range of problems in materials science and engineering

2.4 Relationship between course and program learning outcomes and assessments

Course Learning Outcome (CLO)	LO Statement	Program Learning Outcome (PLO)	Related Tasks & Assessment
CLO 1	Explain…	2	Assessment 3
CLO 2	Explain…	2	Mid-term exam Assessment 3 Assessment 4
CLO 3	Use...	3	Assignment 1 Assessment 4
CLO 4	Choose…	1	Assignment 1 Assessment 3 Assessment 4

3. Strategies and approaches to learning

3.1 Learning and teaching activities

(based on UNSW Learning Guidelines)

- *Students are actively engaged in the learning process.*

  It is expected that, in addition to attending classes, students will read, write, discuss, and engage in analysing the course content.

- *Effective learning is supported by a climate of inquiry where students feel appropriately challenged.*

  Students are expected to be challenged by the course content and to challenge their own preconceptions, knowledge, and understanding by questioning information, concepts, and approaches during class and study.

- *Learning is more effective when student's prior experience and knowledge are recognised and built on.*

  Coursework, tutorials, assignments, laboratories, examinations, and other forms of learning and assessment are intended to provide students with the opportunity to cross-reference these activities in a meaningful way with their own experience and knowledge.

- *Students become more engaged in the learning process if they can see the relevance of their studies to professional and disciplinary contexts*

  The course content is designed to incorporate both theoretical and practical concepts, where the latter is intended to be applicable to real-world situations and contexts.

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.

Practical exercises using commercial software to apply the theory learnt in classes to real-world problems will be undertaken. These exercises will be completed either during scheduled computer laboratory classes, or in the student's own time.

3.2 Expectations of students

- Students must attend at least 80% of all classes with the expectation that students only miss classes due to illness or unforeseen circumstances
- Students must read through lecture notes and lab sheets prior to class
- During class, students are expected to engage actively in class discussions
- Students should work through lecture, tutorial and textbook questions
- Students should read through the relevant chapters of the prescribed textbook.
- Students should complete all assessment tasks and submit them on time.
- Students are expected to participate in online discussions through the Moodle page

4. Course schedule and structure

This course consists of 44 hours of class contact hours. You are expected to take an additional 106 hours of non-class contact hours to complete assessments, readings and exam preparation.

Week	Topics	Activity
1	Introduction and Fundamentals of CFD	Lab on ANSYS Workbench
2	Basic CFD discretisation Techniques, FDM and FVM, diffusive and diffusion-convective flow, time discretisation of unsteady state flow, pressure-velocity coupling, Peclet number	Lab on Geometry Assignment 1 handed out
3	Basic CFD solution and analysis, direct and iterative methods, consistence and stability, convergence criteria	Lab on Meshing
4	Practical guideline for CFD simulations, mesh generation, turbulence flow modelling; Applications of CFD modelling	Lab on fluid and particle tracking
5	Tutorial and revision of CFD Mid-term exam	Lab revision Assignment 1 due Mid-term exam
6	**No classes**	
7	Introduction to atomic-scale modelling Interatomic potentials Molecular mechanics calculations	
8	Group activity	
9	Molecular dynamics simulations	
10	Group activity	Assessment 3 due Assessment 4 due

5. Assessment

5.1 Assessment tasks

Assessment task	Description	Weight	Due date
Lab practice and assignment 1	You are required to attend the lab practices and submit the results at the end of the practices. You are required to solve a partial differential equation using finite difference and finite volume methods. You will also need to develop a CFD model using ANSYS FLUENT to solve a typical fluid and heat flow problem in material processing.	10% 15%	Week 5
Mid-term exam:	Theory part: The exam will be 2 hours duration to assess understanding of the CFD theory learnt in the course. Practical part: The exam will be 2 hours duration held in a computer lab and will be open book. It will assess the ability to solve materials problems encountered in design using ANSYS Fluent modelling package	25%	Weeks 5 & 6
Assessment 3:	You will be asked to undertake a review of recent published literature and write a post on an online forum about 2 papers. You will also peer review posts from other students.	25%	Week 12
Assessment 4:	You will undertake a set of numerical problems and practical exercises using commercial software to apply molecular mechanics calculations and molecular dynamics simulations to problems in materials science.	25%	Week 10

Further information

UNSW grading system: https://student.unsw.edu.au/grades

UNSW assessment policy: https://student.unsw.edu.au/assessment

5.2 Assessment criteria and standards

Assessment criteria and standards will be available on the course Moodle page.

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

Please refer to the UNSW guide to grades: https://student.unsw.edu.au/grades

5.3 Submission of assessment tasks

- UNSW operates under a Fit to Sit/ Submit rule for all assessments. If a student wishes to submit an application for special consideration for an exam or assessment, the application must be submitted prior to the start of the exam or before an assessment is submitted. If a student sits the exam/ submits an assignment, they are declaring themselves well enough to do so. Information on this process can be found here: https://student.unsw.edu.au/special-consideration. Medical certificates or other appropriate documents must be included. Students should also advise the lecturer of the situation.
- Unless otherwise specified in the task criteria, all assignments must be uploaded via Moodle prior to the due date for submission.
- Assignments/lab reports submitted after the due date for submission will receive a 10% of maximum grade penalty for every day late, or part thereof.

Students who have a disability that requires some adjustment in their teaching or learning environment are encouraged to discuss their study needs with the course coordinator prior to, or at the commencement of, their course, or with the Equity Officer (Disability) in the Equity and Diversity Unit: https://student.unsw.edu.au/disability. Early notification is essential to enable any necessary adjustments to be made.

5.4. Feedback on assessment

Students will receive feedback on in-class formative laboratory classes prior to the Census date to be able to make an informed decision about continuing the course.

Assignments: 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.

Midsession exams: Students will receive their marked exams indicating what questions were answered correctly and incorrectly. Overall comments and worked solutions may be provided to the class.

Final exam: Students will receive their final mark.

6. Academic integrity, referencing and plagiarism

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.[1] 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 and **plagiarism** can be located at:

[1] International Center for Academic Integrity, 'The Fundamental Values of Academic Integrity', T. Fishman (ed), Clemson University, 2013.

- The *Current Students* site https://student.unsw.edu.au/plagiarism, and
- The *ELISE* training site http://subjectguides.library.unsw.edu.au/elise/presenting

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

7. Readings and resources

- J. Tu, G. H. Yeoh and C. Liu, 'Computational Fluid Dynamics – A Practical Approach' 2nd Ed
- D. Gaskell, 'An Introduction to Transport Phenomena in Materials Engineering'
- J.D. Anderson, 'Computational Fluid Dynamics – The Basics with Applications'
- R. LeSar, 'Introduction to Computational Materials Science'

8. Administrative matters

School Office: Room 137, Building E10 School of Materials Science and Engineering
School Website: http://www.materials.unsw.edu.au/
Faculty Office: Robert Webster Building, Room 128
Faculty Website: http://www.science.unsw.edu.au/

9. Additional support for students

- The Current Students Gateway: https://student.unsw.edu.au/
- Academic Skills and Support: https://student.unsw.edu.au/academic-skills
- Student Wellbeing, Health and Safety: https://student.unsw.edu.au/wellbeing
- Disability Support Services: https://student.unsw.edu.au/disability-services
- UNSW IT Service Centre: https://www.it.unsw.edu.au/students/index.html
- Assessment Implementation Procedure: https://www.gs.unsw.edu.au/policy/documents/assessmentimplementationprocedure.pdf
- Special Consideration: https://student.unsw.edu.au/special-consideration