MSE4119: ADVANCED COMPUTATIONAL METHODS FOR MATERIALS SCIENCE AND ENGINEERS

Effective Term

Semester A 2023/24

Part I Course Overview

Course Title

Advanced Computational Methods for Materials Science and Engineers

Subject Code

MSE - Materials Science and Engineering

Course Number

4119

Academic Unit

Materials Science and Engineering (MSE)

College/School

College of Engineering (EG)

Course Duration

One Semester

Credit Units

3

Level

B1, B2, B3, B4 - Bachelor's Degree

Medium of Instruction

English

Medium of Assessment

English

Prerequisites

MSE3114 Computational Methods for Physicists and Materials Engineers

Precursors

Nil

Equivalent Courses

Nil

Exclusive Courses

MSE6183 Computational Methods for Materials Science

Part II Course Details

Abstract

This class will introduce concepts of computer modeling and simulation in materials science and engineering using both discrete particle (atomic, molecular) systems and continuum fields. Apply statistical mechanics, molecular dynamics, Monte Carlo, mesoscale and continuum methods to study fundamental physical phenomena encountered in the fields of computational materials science, physics, and chemistry. Techniques for statistical sampling, simulation, data analysis and visualization. Applications drawn from a wide range of disciplines to build a broad-based understanding of complex structures and interactions in problems where simulation is on equal-footing with theory and experiment. An individual project or term project allows the development of individual interest.

Course Intended Learning Outcomes (CILOs)

	CILOs	Weighting (if app.)	DEC-A1	DEC-A2	DEC-A3
1	Recognize the importance of simulation and modeling in materials science.	10	x		
2	Demonstrate a few problems in materials science using simulation and modelling tools.	20		x	
3	Identify the key variables that determine the quality and reliability of simulation and modelling.	10	x		
4	Apply basic simulation and modelling tools to solve simple problems in one of the following areas: materials science, physics, chemistry, and life science.	25			x
5	Apply the basic concepts, theories and tools to a discovery oriented project in student's own discipline such as: new materials design, new physics exploration, drug design, etc.	25			x
6	Identify state-of-the-art developments in the relevant area, to form opinions on specific issues and to demonstrate independent problem-solving ability.	10	x		

A1: Attitude
Develop an attitude of discovery/innovation/creativity, as demonstrated by students possessing a strong sense of curiosity, asking questions actively, challenging assumptions or engaging in inquiry together with teachers.

A2: Ability
Develop the ability/skill needed to discover/innovate/create, as demonstrated by students possessing critical thinking skills to assess ideas, acquiring research skills, synthesizing knowledge across disciplines or applying academic knowledge to real-life problems.

A3: Accomplishments
Demonstrate accomplishment of discovery/innovation/creativity through producing /constructing creative works/new artefacts, effective solutions to real-life problems or new processes.

Teaching and Learning Activities (TLAs)

	TLAs	Brief Description	CILO No.	Hours/week (if applicable)
1		Lectures	1, 2, 3, 4	3hrs/wk
2		Tutorials	1, 2, 3, 4	1hr/wk
3		Projects	5, 6	16hrs/4wks(last 4 wks)

Assessment Tasks / Activities (ATs)

	ATs	CILO No.	Weighting (%)	Remarks (e.g. Parameter for GenAI use)
1	Assignments	1, 2, 3, 4	20	performance assessment purpose
2	Project	5, 6	40	Inc. project report and presentation
3	Mid-term Test	1, 2, 3, 4	40	

Continuous Assessment (%)

100

Examination (%)

0

Assessment Rubrics (AR)

Assessment Task

1. Assignments

Criterion

The student completes all assessment tasks/activities and the work demonstrates excellent understanding of the scientific principles and the working mechanisms.

Excellent (A+, A, A-)

High

Good (B+, B, B-)

Significant

Fair (C+, C, C-)

Moderate

Marginal (D)

Basic

Failure (F)

Not reaching marginal level

Assessment Task

2. Mid-term Test

Criterion

He/she can thoroughly identify and explain how the principles are applied to science and technology for solving materials science problems.

Excellent (A+, A, A-)
High

Good (B+, B, B-)
Significant

Fair (C+, C, C-)
Moderate

Marginal (D)
Basic

Failure (F)
Not reaching marginal level

Assessment Task
3. Project

Criterion
The student’s work shows strong evidence of original thinking, supported by a variety of properly documented information sources other than taught materials. He/she is able to communicate ideas effectively and persuasively via written texts and/or oral presentation.

Excellent (A+, A, A-)
High

Good (B+, B, B-)
Significant

Fair (C+, C, C-)
Moderate

Marginal (D)
Basic

Failure (F)
Not reaching marginal level

Part III Other Information

Keyword Syllabus

- Introduction
  Advances in computational methods and tools. Computer-aided design and simulation in multidisciplinary areas including materials science, physics, chemistry, and life science.
- Monte Carlo methods
  History. Applications areas. Use in mathematics. Monte Carlo and random numbers.
- Molecular dynamics simulation
  Areas of Application. Design Constraints. Potentials. Molecular dynamics algorithms.
- Continuum Methods
  Conservation Laws, order parameter, continuum equations, finite difference method for phase transition, dendritic solidification, thermal transport

- Numerical optimization methods
  Conjugate gradient method. Simulated annealing. Genetic algorithms.
- Ab-Initio Calculations (optional)
  First-principles quantum mechanics and density functional theory (DFT) calculations
- Project
  A discovery oriented multidisciplinary project such as new materials design, new physics exploration, or drug design, etc.

Reading List

Compulsory Readings

	Title
1	“Understanding Molecular Simulation: From Algorithms to Applications”, San Diego: Academic Press, 1996.
2	Nikolas Provatas and Ken Elder, Phase-Field Methods in Materials Science and Engineering, 2011
3	Christophe Chipot, Numerical Methods for molecular Dynamics Simulations of Biological Systems, 2010

Additional Readings

	Title
1	K Binder, D W Heermann, “Monte Carlo Simulation in Statistical Physics: An Introduction”, Berlin : Springer-Verlag, 1988. (C0092255)
2	“Monte Carlo method”, http://en.wikipedia.org/wiki/Monte_Carlo_method
3	Alexander K Hartmann, Heiko Rieger, “Optimization Algorithms in Physics”, Berlin: Wiley-VCH, 2002. (QC20.7.C58 H37 2002)
4	David P Landau, Kurt Binder, “A Guide to Monte Carlo Simulations in Statistical Physics”, Cambridge, UK; New York: Cambridge University Press, 2005. (QC174.85.M64 L36 2005)
5	Kurt Binder, “Monte Carlo and Molecular Dynamics Simulations in Polymer Science [electronic resource]”, New York: Oxford University Press, 1995. (QD381.9.E4 M66 1995eb)
6	“Mathematical optimization”, http://en.wikipedia.org/wiki/Mathematical_optimization
7	“Molecular dynamics”, http://en.wikipedia.org/wiki/Molecular_dynamics