PHY4172: COMPUTATIONAL PHYSICS

Effective Term
Semester A 2022/23

Part I Course Overview

Course Title
Computational Physics

Subject Code
PHY - Physics

Course Number
4172

Academic Unit
Physics (PHY)

College/School
College of Science (SI)

Course Duration
One Semester

Credit Units
3

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

Medium of Instruction
English

Medium of Assessment
English

Prerequisites
Nil

Precursors
AP3172/MSE3172 Electronic Properties of Solids (for students from Bachelor of Engineering in Materials Engineering);
BCH3017 Molecular Biology (for students from Bachelor of Science in Applied Biology / Biological Sciences)
BCH3016 Physical Chemistry (for students from Bachelor of Science in Chemistry)
BCH4022 Environmental Toxicology (for students from Bachelor of Science in Environmental Science and Management)
AP3130/MSE3130 Biomaterials (for students from Bachelor of Engineering in Biomedical Engineering)

Equivalent Courses
AP4172 Simulation and Modelling in Multidisciplinary Sciences

Exclusive Courses
Nil

Part II Course Details

Abstract

This course covers a range of topics and methods in multidisciplinary sciences that involve simulation and modelling. Its central aims are: (1) to describe basic theory and its numerical computation, (2) to introduce existing software that can be used to solve problems in multidisciplinary sciences, and (3) to guide students from the materials science, physics, chemistry, life science, and finance to do a discovery oriented multidisciplinary project such as new materials design, new physics exploration, energy conversion, DNA repair, drug design, or finance market prediction.

Course Intended Learning Outcomes (CILOs)

	CILOs	Weighting (if app.)	DEC-A1	DEC-A2	DEC-A3
1	Recognize the importance of simulation and modelling in multidisciplinary sciences.	10	x		
2	Demonstrate a few problems in multidisciplinary sciences 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, energy, environment, life science, and finance.	30			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, energy conversion, pollutant degradation, DNA repair, drug design, financial market prediction, etc.	30			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	1	Lectures	1, 2, 3, 4	14hrs/7wks (wk: 1-7)
2	2	Tutorials	1, 2, 3, 4	6hrs/6wks (wk: 2-7)
3	3	Projects	5	21hrs/6wks(last 6 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	30	Inc. project report and presentation

Continuous Assessment (%)

50

Examination (%)

50

Additional Information for ATs

For a student to pass the course, at least 30% of the maximum mark for the examination must be obtained

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. 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

Assessment Task
3. Examination

Criterion
He/she can thoroughly identify and explain how the principles are applied to science and technology for solving multidisciplinary sciences 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

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, energy, environment, life science, and finance.
- 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.
- Numerical optimization methods
  Conjugate gradient method. Simulated annealing. Genetic algorithms.
- Project
  A discovery oriented multidisciplinary project such as new materials design, new physics exploration, energy conversion, pollutant degradation, DNA repair, drug design, or financial market prediction.

Reading List

Compulsory Readings

	Title
1	“Monte Carlo method”, http://en.wikipedia.org/wiki/Monte_Carlo_method
2	“Molecular dynamics”, http://en.wikipedia.org/wiki/Molecular_dynamics
3	“Mathematical optimization”, http://en.wikipedia.org/wiki/Mathematical_optimization

Additional Readings

	Title
1	Daan Frenkel, Berend Smit, “Understanding Molecular Simulation: From Algorithms to Applications”, San Diego: Academic Press, 1996. (QD461 .F86 1996)
2	K Binder, D W Heermann, “Monte Carlo Simulation in Statistical Physics: An Introduction”, Berlin : Springer-Verlag, 1988. (C0092255)
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)