PHY8502: ADVANCED COMPUTATIONAL METHODS

Effective Term

Semester B 2024/25

Part I Course Overview

Course Title

Advanced Computational Methods

Subject Code

PHY - Physics

Course Number

8502

Academic Unit

Physics (PHY)

College/School

College of Science (SI)

Course Duration

One Semester

Credit Units

3

Level

R8 - Research Degree

Medium of Instruction

English

Medium of Assessment

English

Prerequisites

Nil

Precursors

Nil

Equivalent Courses

AP8172 Simulation and Modelling in Multidisciplinary Sciences

Exclusive Courses

AP6172 Simulation and Modelling in Multidisciplinary Sciences, PHY6502 Advanced Computational Methods

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, 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 modeling 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, life science, and finance.	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, DNA repair, drug design, financial market prediction, 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.

Learning and Teaching Activities (LTAs)

	LTAs	Brief Description	CILO No.	Hours/week (if applicable)
1		Lectures	1, 2, 3, 4	14hrs/7wks (wk: 1-7)
2		Tutorials	1, 2, 3, 4	6hrs/6wks (wk: 2-7)
3		Projects	5, 6	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	Mid-term Test	1, 2, 3, 4	30	performance assessment purpose (week 7)
3	Project	5, 6	50	Inc. project report and presentation

Continuous Assessment (%)

100

Examination (%)

0

Minimum Continuous Assessment Passing Requirement (%)

0

Minimum Examination Passing Requirement (%)

0

Assessment Rubrics (AR)

Assessment Task

Assignments (for students admitted before Semester A 2022/23 and in Semester A 2024/25 & thereafter)

Criterion

The student completes all assessment tasks/activities including answers to questions and simulations of representative systems relating to the topics taught and the work demonstrates excellent understanding of the scientific principles and the working mechanisms.

Excellent

(A+, A, A-) High(excellent accomplishment with creativity and correct understanding)

Good

(B+, B, B-) Significant(good accomplishment withmostly correct understanding)

Fair

(C+, C, C-) Moderate(fair accomplishment with some correct understanding)

Marginal

(D) Basic(essential accomplishment withbasic understanding)

Failure

(F) Notreaching marginal level

Assessment Task

Mid-term Test (for students admitted before Semester A 2022/23 and in Semester A 2024/25 & thereafter)

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(excellent accomplishment with creativity and correct understanding)

Good

(B+, B, B-) Significant(good accomplishment withmostly correct understanding)

Fair

(C+, C, C-) Moderate(fair accomplishment with some correct understanding)

Marginal

(D) Basic(essential accomplishment withbasic understanding)

Failure

(F) Notreaching marginal level

Assessment Task

Project (for students admitted before Semester A 2022/23 and in Semester A 2024/25 & thereafter)

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(excellent accomplishment with creativity and correct understanding)

Good

(B+, B, B-) Significant(good accomplishment withmostly correct understanding)

Fair

(C+, C, C-) Moderate(fair accomplishment with some correct understanding)

Marginal

(D) Basic(essential accomplishment withbasic understanding)

Failure

(F) Notreaching marginal level

Assessment Task

Assignments (for students admitted from Semester A 2022/23 to Summer Term 2024)

Criterion

The student completes all assessment tasks/activities including answers to questions and simulations of representative systems relating to the topics taught and the work demonstrates excellent understanding of the scientific principles and the working mechanisms.

Excellent

(A+, A, A-) High(excellent accomplishment with creativity and correct understanding)

Good

(B+, B) Significant(good accomplishment with mostlycorrect understanding)

Marginal

(B-, C+, C) Basic(essential accomplishment with basic understanding)

Failure

(F) Not reaching marginal level

Assessment Task

Mid-term Test (for students admitted from Semester A 2022/23 to Summer Term 2024)

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(excellent accomplishment with creativity and correct understanding)

Good

(B+, B) Significant(good accomplishment with mostlycorrect understanding)

Marginal

(B-, C+, C) Basic(essential accomplishment with basic understanding)

Failure

(F) Not reaching marginal level

Assessment Task

Project (for students admitted from Semester A 2022/23 to Summer Term 2024)

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(excellent accomplishment with creativity and correct understanding)

Good

(B+, B) Significant(good accomplishment with mostlycorrect understanding)

Marginal

(B-, C+, C) Basic(essential accomplishment with basic understanding)

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, 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.
- Machine leaning methods: Supervised learning. Unsupervised learning. Reinforcement learning.
- Project: A discovery oriented multidisciplinary project such as new materials design, new physics exploration, 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
4	“Finite element method”, https://en.wikipedia.org/wiki/Finite_element_method
5	“Finite difference Methods” https://en.wikipedia.org/wiki/Finite_difference_method

Additional Readings

	Title
1	K Binder, D W Heermann, “Monte Carlo Simulation in Statistical Physics: An Introduction”, Berlin : Springer-Verlag, 1988. (C0092255)
2	Daan Frenkel, Berend Smit, “Understanding Molecular Simulation: From Algorithms to Applications”, San Diego: Academic Press, 1996. (QD461 .F86 1996)
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	“The Finite Element Method: Basic Concepts and Applications with MATLAB, MAPLE, and COMSOL”, D. W. Pepper and J. C. Heinrich, CRC Press, 2017.
7	“Finite Difference Methods for Ordinary and Partial Differential Equations: Steady-State and Time-Dependent Problems”, R. LeVeque, SIAM, 2007.