City University of Hong Kong
Course Syllabus

offered by Department of Physics
with effect from Semester A 2022/23

Part I Course Overview

Course Title:	**Advanced Computational Methods**
Course Code:	**PHY6502**
Course Duration:	**One semester**
Credit Units:	**3**
Level:	**P6**
Medium of Instruction:	**English**
Medium of Assessment:	**English**
Prerequisites: *(Course Code and Title)*	**Nil**
Precursors: *(Course Code and Title)*	**Nil**
Equivalent Courses: *(Course Code and Title)*	**AP6172 Simulation and Modelling in Multidisciplinary Sciences**
Exclusive Courses: *(Course Code and Title)*	**AP8172 Simulation and Modelling in Multidisciplinary Sciences** **PHY8502 Advanced Computational Methods**

Part II Course Details

1. 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.

2. Course Intended Learning Outcomes (CILOs)

(CILOs state what the student is expected to be able to do at the end of the course according to a given standard of performance.)

No.	CILOs	Weighting (if applicable)	Discovery-enriched curriculum related learning outcomes (please tick where appropriate)		
			A1	*A2*	*A3*
1.	Recognize the importance of simulation and modeling in multidisciplinary sciences.	10%	√		
2.	Demonstrate a few problems in multidisciplinary sciences using simulation and modelling tools.	20%		√	
3.	Identify the key variables that determine the quality and reliability of simulation and modelling.	10%	√		
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%			√
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%			√
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%	√		
		100%			

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 self-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.

3. Teaching and Learning Activities (TLAs)

(TLAs designed to facilitate students' achievement of the CILOs.)

TLA	Brief Description	CILO No.						Hours/week (if applicable)
		1	**2**	**3**	**4**	**5**	**6**	
1	Lectures	√	√	√	√			14hrs/7wks (wk: 1-7)
2	Tutorials	√	√	√	√			6hrs/6wks (wk: 2-7)
3	Projects					√	√	21hrs/6wks (last 6 wks)

4. Assessment Tasks/Activities (ATs)

(ATs are designed to assess how well the students achieve the CILOs.)

Assessment Tasks/Activities	CILO No.						Weighting	Remarks
	1	2	3	4	5	6		
Continuous Assessment: 100%								
Assignments	√	√	√	√			20%	performance assessment purpose
Mid-term Test	√	√	√	√			30%	performance assessment purpose (week 7)
Project					√	√	50%	Inc. project report and presentation
Examination: 0%								
							100%	

5. Assessment Rubrics

(Grading of student achievements is based on student performance in assessment tasks/activities with the following rubrics.)

<u>Applicable to students admitted in Semester A 2022/23 and thereafter</u>

Assessment Task	Criterion	Excellent (A+, A, A-)	Good (B+, B)	Marginal (B-, C+, C)	Failure (F)
1. Assignments	The student completes all assessment tasks/activities and the work demonstrates excellent understanding of the scientific principles and the working mechanisms.	High	Significant	Basic	Not reaching marginal level
2. Mid-term Test	He/she can thoroughly identify and explain how the principles are applied to science and technology for solving multidisciplinary sciences problems.	High	Significant	Basic	Not reaching marginal level
3. Project	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.	High	Significant	Basic	Not reaching marginal level

Applicable to students admitted before Semester A 2022/23

Assessment Task	Criterion	Excellent (A+, A, A-)	Good (B+, B, B-)	Fair (C+, C, C-)	Marginal (D)	Failure (F)
1. Assignments	The student completes all assessment tasks/activities and the work demonstrates excellent understanding of the scientific principles and the working mechanisms.	High	Significant	Moderate	Basic	Not reaching marginal level
2. Mid-term Test	He/she can thoroughly identify and explain how the principles are applied to science and technology for solving multidisciplinary sciences problems.	High	Significant	Moderate	Basic	Not reaching marginal level
3. Project	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.	High	Significant	Moderate	Basic	Not reaching marginal level

Part III Other Information (more details can be provided separately in the teaching plan)

1. Keyword Syllabus

(An indication of the key topics of the course.)

● 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.

● Numerical methods for solving partial differential equations (PDEs)

Finite difference method. Finite element method.

● Project

A discovery oriented multidisciplinary project such as new materials design, new physics exploration, DNA repair, drug design, or financial market prediction.

2. Reading List

2.1 Compulsory Readings

(Compulsory readings can include books, book chapters, or journal/magazine articles. There are also collections of e-books, e-journals available from the CityU Library.)

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

2.2 Additional Readings

(Additional references for students to learn to expand their knowledge about the subject.)

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.