Hong Kong Baptist University
Faculty of Science – Department of Physics

Title (Units): **PHYS 3045** **SCIENTIFIC COMPUTING AND MODELING (3, 3, 1)**

Course Aims: This is an introductory course on scientific computing, modeling and computer simulations. By working through selected examples in physics and energy science, e.g., orbital motion of planet, heat transfer, OLED emission etc., students will learn basic computing algorithms and programming strategies, as well as an appreciation of important concepts in numerical analysis, such as accuracy, stability, and deficiency of various algorithms. The course includes a lab component which gives the student hands-on experience on computer simulation, for example, through higher level languages or subroutines.

Pre-requisite: Year 3 standing or consent of instructor

Course Reviewed by: Dr. Changsong Zhou, Dr. Kin-Yiu Wong and Dr. Jack T.F. Ng.

Course Intended Learning Outcomes (CILOs):

No.	Upon successful completion of this course, students should be able to:
1.	Describe basic data processing, numerical integration and the Monte Carlo sampling technique, and list the key criteria in choosing a numerical algorithm or library routine to perform integration of differential equations and matrix operations such as inversion and diagonalization.
2.	Perform basic data processing of regression, fitting and spectral analysis.
3.	Integrate ordinary differential equations, and assess the accuracy, stability, and quality of a given algorithm.
4.	Formulate eigenvalue and boundary value problems on a line as matrix problems.
5.	Write computer codes that implement the first or a higher order method to integrate the Newton's equation or other differential equations related to physics and energy science such as orbital motion of planet or light emission in OLED.
6.	Use higher level languages or subroutines such as MatLab and Mathematica to solve problems.

Teaching & Learning Activities (TLAs)

CILOs	**TLAs will include the following:**
1-4	Lectures are given to provide a systematic exposition of the subject in relation to the course objectives. Students are encouraged to ask questions during the class, and to make frequent summaries of the classroom discussion.
5-6	Lab sessions are organized to train the programming skills of students and to teach them useful software packages for data analysis, simulations and graphing. Students need to complete about five lab assignments and their performance will be evaluated.
1-6	The instructor is suggested to include a miniproject where the students work in groups to solve a problem using numerical techniques learned in class.

Assessment:

No.	Assessment Methods	Weighting	CILOs to be addressed	Remarks
1	Continuous Assessment	50%	1-6	The continuous assessment based on lab reports and miniproject is designed to measure how well the students have learned the basic concepts and developed skills to solve problems numerically.
2	Final Examination	50%	1-6	Final Examination questions are designed to see how far students have achieved their intended learning outcomes. Questions will primarily be analysis and skills based to assess the student's versatility in breaking up a physic problem into numerical form, and in writing the pseudo code to obtain the numerical solution.

Learning Outcomes and Weighting:

Content	LO No.	Teaching (in hours)
I. Introduction and basic data processing	1,2	9
II. Integration of function and Monte Carlo methods	1	6
III. Numerical integration of ODEs	1,3	8
IV. Matrix manipulation and eigenvalue problems.	1,4	8
V. Higher level languages and mini-project	5,6	5

Textbook: W.H. Press, S.A. Teukolsky, W.T. Vetterling and B.F. Flannery, Numerical Recipes: The Art of Scientific Computing, 3nd Ed., Cambridge, 2007.

References:

1. N.J. Giordano and H. Nakanisi, Computation Physics, 2nd Ed., Pearson Prentice Hall, 2006.
2. H. Gould, J. Tobochnik, and W. Christian, An Introduction to Computer Simulation Methods: Applications to Physical Systems (3rd Edition), Addision-Wesley, 1996.
3. D. Stauffer, F.W. Hehl, N. Ito, V. Winkelmann, J.G. Zabolitzky, Computer Simulation and Computer Algebra, 3rd Ed., Springer, 1993.
4. S.E. Koonin and D.C. Meredith, Computation Physics, Addision-Wesley, 1990.

Hong Kong Baptist University
Faculty of Science – Department of Physics

Course Content in Outline:

	Topic	Hours
I.	Introduction	3
	A. Computer simulation– a new discipline.	
	B. Working with numbers on a computer, accuracy vs. precision	
II.	Basic data processing	6
	A. Regression and fitting	
	B. Fourier transform and spectral analysis	
	C. Applications to experimental data	
III.	Integration of Function	6
	A. Numerical differentiation and integration of function	
	B. Random numbers and Monte Carlo sampling	
	C. Monte Carlo integration.	
IV.	Integrating dynamical equations	8
	A. Solving the Newton's or other differential equations: The Euler method.	
	B. Methods of higher accuracy, accuracy and stability.	
	C. Applications to problems such as population growth, orbital motion in solar system	
V.	Boundary value and eigenvalue problems	8
	A. Laplace methods	
	B. Matrix inversion	
	C. Applications to problems such as heat transfer, OLED emission, hydrogen atom	
VI.	Higher level languages and subroutines or mini-project, such as energy saving by layers of insulation of a building.	5