Centre for High Energy Physics
Faculty of Science
University of the Punjab, Lahore

Course Outline

Program	BSCP	Course Code	CPHY 483	Credit Hours	3 (2+1Lab)
Course Title	**Computational Physics Simulations II**				

Course Introduction

This course is about studying mainly quantum mechanical systems through simulations. Simulations are aimed at providing information about the physical systems very near to the reality. In this course the details of different deterministic as well as non-deterministic problems will be explored with or without using random numbers. This course will provide detailed mechanism of solving Schrodinger wave equation through different methods. It will also cover the details of using Monte Carlo method for solving different microscopic systems. The simulations will be performed by using computer programming environments of C++/C#/Python/Mathematica/MatLab, etc.

Learning Outcomes

Following objectives are expected at the end of this course:

1. Students will be able to convert differential forms of any physical problems into iterative forms.
2. The students will enhance their expertise of programming languages such as Python while performing simulations.
3. The students will be able to better understand the underlying physics details in the topics involved in this course.

Course Content

Week 1	Course Introduction involving its scope and applications, etc.
	Introductory Lab work in the programming environment of C++/C#/Python, etc.
Week 2	Schrödinger Equation (SE) and Its solutions
	Lab work for simulation of plane wave solution of SE
Week 3	1D (Shooting and Matching methods) for solving SE
	Lab work for simulation of Shooting and Matching solution of SE
Week 4	Variational approach for Solving SE
	Lab work for simulation ofVariational approach solution of SE
Week 5	Basis diagonalization method for SE
	Lab work for basis diagonalization method for SE
Week 6	Spectral methods for SE
	Lab work for spectral method solutions of SE
Week 7	Bound state solutions of SE
	Lab work for bound state solutions of SE

Week 8	Direct solutions of SE	
	Lab work for direct solutions of SE	
Week 9	Fourier Transform, Bound states in momentum space	
	Lab work for Random walk solutions of SE	
Week 10	Quantum mechanical scattering, Monte Carlo Integration, Diffusion Monte Carlo (DMC)	
	Lab work for diffusion Monte Carlo	
Week 11	Path Integral Monte Carlo (PIMC), Quantum Monte Carlo Methods: Variational Monte Carlo for atoms	
	Lab work for PIMC	
Week 12	The Born- Oppenheimer Approximation; The Hydrogen Atom; Metropolis sampling for the hydrogen atom and the harmonic oscillator	
	Lab work for sampling of atomic statistics such as for Hydrogen atom	
Week 13	The Ising Model and Statistical Mechanics; Mean-Field theory, Monte Carlo Method	
	Lab work for simulation of Mean Field Theory	
Week 14	The Isingmodel and second order phase transitions	
	Lab work for simulation of second order phase transitions	
Week 15	The Isingmodel and first order phase transitions	
	Lab work for simulation of first order phase transitions	
Week 16	Comparison of Mean Field Theory and Monte Carlo method for Ising Model	
	Lab work for simulation of Mean Field Theory Versus Monte Carlo Method of Ising Model	

Textbooks and Reading Material

1. Computational Quantum Mechanic, J. Izaac and Jingbo Wang, *Springer* (2019).
2. Quantum Mechanics Simulations, J. R. Hiller, I. D. Johnston, and D. F. Styer, *Wiley* (1995).
3. Computational Physics: Problem Solving with Computers (2^{nd}edition), Rubin H. Landau, *John Wiley & Sons* (2000).
4. Computational Physics (2^{st}edition), Nicholas J. Giordano, *Prentice Hall* (2005).
5. Computational Physics, Jos Thijssen, *Cambridge University Press* (2007).
6. Applied Computational Physics, J. F. Boudreau and E. S. Swanson, *Oxford University Press* (2017).

Teaching Learning Strategies

1. The instructor will detail out the process/concept of converting the information of quantum mechanical and statistical problems into forms which can be used for computer simulations.
2. The instructor will provide the details about the programming environment of C++/C#/Python etc. for implementation of Monte Carlo method.

3. Students will learn the concept of converting the differential equations, especially Schrodinger equation into iterative form and will practice by solving the exercise problems of main textbooks.
4. Students will practice the process of making algorithms and implementing them in the available arbitrary programming language, for using Monte Carlo method.
5. Students will learn how to analyze the simulation results in order to have better physics understanding.

Assignments: Types and Number with Calendar

At least two assignments and two quizzes. A course project may also be assigned.

Assessment

Sr. No.	Elements	Weightage	Details
1.	Midterm Assessment	35%	Written Assessment at the mid-point of the semester.
2.	Formative Assessment	25%	Continuous assessment includes: Classroom participation, assignments, presentations, viva voce, attitude and behavior, hands-on-activities, short tests, projects, practical, reflections, readings, quizzes etc.
3.	Final Assessment	40%	Written Examination at the end of the semester. It is mostly in the form of a test, but owing to the nature of the course the teacher may assess their students based on term paper, research proposal development, field work and report writing etc.