

DEPARTMENT OF PHYSICS				CLASS: I M.Sc. Physics				
Sem	Course Type	Course Code	Course Title	Credits	Contact Hours/week	CIA	Ext	Total
II	Elective 4	21P12PME4	Computational Physics	4	5	25	75	100

Nature of Course			
Knowledge and skill			Employability oriented
Skill oriented	✓		Entrepreneurship oriented

### Course Objectives:

The objective of the course is

- To learn and practice the fundamental programming concepts and methodologies subjected to develop C++ programs.
- To tackle the problems in the physical sciences using computer and C++ as a numerical tool
- To Numerically solve systems of nonlinear equations, Eigenvalues and eigenvectors of a matrix, integrals
- To identify appropriate numerical strategies to deal the problems in physics

### Course Content :

Unit	Description	Hours	K-level	CLO
I	<b>Data types, Operators, Expressions and Control Statements:</b> Identifiers and Keywords – Data types – C++ Simple data types – Literals – Variables – The Const Data type – C++ Operators – Type conversion – Declaration of variables – Simple C++ Programs – Features of I/O stream – keyboard and screen I/O - Manipulators Functions - Conditional Expressions – Loop statements – Nested Control Structures – Breaking Control Statements.	15	Up to K2	1
II	<b>Functions, arrays and pointers:</b> Defining a function – ‘Return’ statement – Types of functions – Actual and formal arguments – Local and global variables – Default arguments – Multifunction program – Recursive function – Header files – Standard functions – Array notation, declaration and initialization – Processing with array – Arrays and functions – Multidimensional arrays – Character array – Pointer operator – Address operator – Pointer expressions – Pointer arithmetic – Pointers and functions – Pointers and arrays - Pointers and strings – Arrays of pointers – Pointers to pointers.	15	Up to K4	2

III	<b>Structures, Classes and objects :</b> Declaration of structure – Initialization – Functions and structures – Arrays of structures- Arrays within a structure – Nested structure – Pointers and structures – Declaration of class – Member functions – Object of a class – Accessing a member of a class - Array of class objects – Pointers and classes – Nested class – Copy constructors – Default constructors – Destructors – Static data member – Static member functions – Friend functions – ‘ this’ pointer.	15	Up to K3	3
IV	<b>Approximation of a function and Numerical Calculus</b> Interpolation-Least-squares Approximation – Random number generators-Introduction to Lagrange polynomials –Numerical Differentiation-Numerical Integration- Trapezoidal rule – Simpson’s rules – Newton - Cotes formulas – Gaussian quadrature formula – Estimation of errors in evaluating the integrals Roots of Equation-Extremes of a function - Bond length of a molecule.	15	Up to K4	4
V	<b>Ordinary differential equation and applications</b> Initial-value problems- Taylor’s series method - The Euler and Picard methods - Predictor-corrector methods-The Runge - Kutta method – Chaotic dynamics of a driven pendulum–Boundary-value and eigenvalue problems-The Shooting Method-Linear equations and the Sturm - Liouville problem-The 1-D Schrödinger equation.	15	Up to K4	5

#### Books for study:

UNIT I, II and III: Programming with C++ - By D. Ravichandran –Tata McGraw – Hill Pub. Co. Ltd., New Delhi.

UNIT IV and V: An Introduction to Computation Physics (2<sup>nd</sup>Edn) – TAO PANG, Cambridge, 2006 (Chap.2,3(selected sections) 4,7).

#### Books for References:

1. Object oriented programming with C++ - E.Balagurusamy - Tata McGraw Hill Pub. Co. Ltd.
2. Let us C++ - YashwantP.Kanetkar – BPB Publications, New Delhi.
3. Numerical Methods – Conte and deBoer.

#### Web Resources

- 1.<https://www.programiz.com/cpp-programming>
- 2.<https://doc.lagout.org/Others/An%20Introduction%20to%20Computational%20Physics%2C%20Second%20Edition.pdf>
- 3.<https://www.uio.no/studier/emner/matnat/fys/FYS3150/h09/undervisningsmateriale/Lecture%20Notes/lectures2009.pdf>

### **Rationale for Nature of the course**

Contemporary research in physics and related sciences almost always involves the use of computers. They are used for data collection and analysis, numerical analysis, simulations, and symbolic manipulation. Computational physics has become a third way of doing physics and complements traditional modes of theoretical and experimental physics.

### **Activities having direct bearing on Skill development / Employability Entrepreneurship**

Developing Programming skill in students

Applying principles of mathematical modelling of physical systems

Students would write and execute C++ Program

### **Pedagogy**

Chalk and Talk, PPT, Quiz, Group discussion, Seminar, Interaction, Problem solving.

### **Course Designer:**

1. Dr.R.Vishnu Priya

### Lecture Schedule

Unit	Topics	Hours	Mode
<b>Unit I</b>	Identifiers and Keywords – Data types – C++ Simple data types – Literals – Variables – The Const Data type	3	Chalk and talk, Quiz and assignment
	C++ Operators – Type conversion – Declaration of variables	3	
	Simple C++ Programs – Features of I/O stream – keyboard and screen I/O	3	
	Manipulators Functions - Conditional Expressions – Loop statements	3	
	Nested Control Structures – Breaking Control Statements	3	
<b>Unit II</b>	Defining a function – ‘Return’ statement – Types of functions	3	PPT, Chalk and talk, and Group discussion
	Actual and formal arguments – Local and global variables – Default arguments – Multifunction program	3	
	Recursive function – Header files – Standard functions – Array notation, declaration and initialization	3	
	Multidimensional arrays – Character array – Pointer operator – Address operator – Pointer expressions – Pointer arithmetic	3	
	Pointers and functions – Pointers and arrays - Pointers and strings – Arrays of pointers – Pointers to pointers	3	
<b>Unit III</b>	Declaration of structure – Initialization – Functions and structures – Arrays of structures	3	PPT, Chalk and talk, Quiz and Group discussion
	Arrays within a structure – Nested structure – Pointers and structures – Declaration of class	3	
	Member functions – Object of a class – Accessing a member of a class - Array of class objects	3	
	Pointers and classes – Nested class – Copy constructors – Default constructors – Destructors	3	
	Static data member – Static member functions – Friend functions – ‘this’ pointer.	3	
<b>Unit IV</b>	Interpolation-Least-squares Approximation - Random number generators - Introduction to Lagrange polynomials	3	PPT, Chalk and talk, Assignment
	Numerical Differentiation-Numerical Integration-	3	
	Trapezoidal rule – Simpson’s rules	3	
	Newton - Cotes formulas – Gaussian quadrature formula	3	
	Estimation of errors in evaluating the integrals Roots of Equation-Extremes of a function - Bond length of a molecule.	3	
<b>Unit V</b>	Initial-value problems- Taylor’s series method - The Euler and Picard methods	3	Chalk and talk, Quiz and Interaction
	Predictor-corrector methods-The Runge - Kutta method	3	
	Chaotic dynamics of a driven pendulum–Boundary-value and eigenvalue problems	3	
	The Shooting Method-Linear equations and the Sturm - Liouville problem-The 1-D Schrödinger equation	3	

### Course learning Outcomes

On the successful completion of the course, students will be able to

CLOs	Course Learning Outcomes	Knowledge Level
CLO-1	Understand the concepts of object-oriented programming	Up toK2
CLO-2	Contrasts the difference between the various types of functions	Up toK4
CLO-3	Make use of Structures and function programming techniques to solve problems in the C++ programming language	Up toK3
CLO-4	Implement programming techniques to solve problems in the C++ programming language.	Up toK4
CLO-5	Apply the concepts and principles of the programming language to the real-world problems and solve the problems through project-based learning	Up toK4

### Mapping with CLOs with PSOs

#	PSO-1	PSO-2	PSO-3	PSO-4	PSO-5
CLO-1	3	3	2		1
CLO-2	3	3	2		1
CLO-3	3	3	2		1
CLO-4	3	3	2		1
CLO-5	3	3	2		1

Advance application -3, Intermediate level -2, Basic level-1

**Learning Outcome Based Education (LOBE) & Assessment**  
**Summative Examination – Blue Print**  
**Articulation Mapping-K Levels with Courses Learning Outcomes (CLOs)**

Units	CLOs	K- Level	SectionA		SectionB		Section C (Either/Or)	Section D (Open Choice)
			MCQs		Short answers			
			No. of Questions	K- Level	No. of Questions	K- Level		
1	CLO 1	Up to K2	2	K1 & K1	1	K1	2(K1 & K1)	1(K2)
2	CLO 2	Up to K4	2	K2 & K3	1	K2	2(K4 & K4)	1(K3)
3	CLO 3	Up to K3	2	K2 & K3	1	K1	2(K2 & K2)	1(K3)
4	CLO 4	Up to K4	2	K3 & K4	1	K2	2(K3 & K3)	1(K4)
5	CLO 5	Up to K4	2	K2 & K3	1	K3	2(K4 & K4)	1(K4)
No. of Questions to be asked			10			5	10	5
No. of Questions to be Answered			10			5	5	3
Marks for each question			1			2	5	10
Total Marks for each Section			10			10	25	30

K1- Remembering and recalling facts with specific answers

K2- Basic understanding of facts and stating main ideas with general answers

K3- Application oriented –Solving Problems

K4-Examining, analyzing, presentation and make inferences with evidences

**Distribution of Section-wise Marks with K Levels**

K Levels	Section A (No Choice)	Section B (No Choice)	Section C (Either/or)	Section D (Open Choice)	Total Marks	% of Marks without choice
K1	2	4	10	-	<b>16</b>	13.33
K2	2	4	10	10	<b>26</b>	21.67
K3	4	2	10	20	<b>36</b>	30.00
K4	2	-	20	20	<b>42</b>	35.00
Total Marks	10	10	50	50	<b>120</b>	100.00