

Course Code	Course Title	L	T	P	C
BPHY301E	Computational Physics	2	0	2	3
Pre-requisite	NIL	Syllabus version			
		1.0			
Course Objectives					
1. To introduce Numerical methods necessary for computational physics.					
2. Apply the techniques learned to Classical problems.					
3. Apply the techniques learned to Quantum problems.					
Course Outcomes					
At the end of the course, the student will be able to					
1. Explain basics of the numerical methods and techniques.					
2. Explain basics of differential equations and their applications.					
3. Explain basics of Neural networks and their applications.					
Module:1	Introduction to Numerical Methods - 1	4 hours			
Numerical methods - Lagrange's interpolation method - Forward difference and central difference methods - Numerov's algorithm					
Module:2	Introduction to Numerical Methods - 2	4 hours			
Newton - Cotes expression for integral - Trapezoidal rule - Simpson's rule - Gauss quadrature method					
Module:3	Differential Equations - 1	4 hours			
Taylor series method - Euler method - Runge Kutta method - Polynomial equations - Graphical methods - Bisectional method					
Module:4	Differential Equations - 2	4 hours			
Newton-Raphson method - False position method - Linear and non-linear curve fitting					
Module:5	Fourier Transform	4 hours			
Properties. Convolution and Correlation - Discrete Sampled Data: Sampling Theorem - Discrete Fourier Transform - Fast Fourier Transform (FFT) - Oscillators - Realistic Pendula - Fourier analysis of oscillations					
Module:6	Application to Quantum Mechanics	4 hours			
Solving differential equations - Schrodinger equation in Quantum Mechanics with Numerov's algorithm - Determinant of a matrix - Characteristic equation of a matrix - Eigen values and eigen vectors of a matrix - Power method					
Module:7	Physics Informed Neural Networks (PINNs)	4 hours			
Introduction to Neural Networks - Data-driven Solutions of Nonlinear Partial Differential Equations - Continuous Time Models (Schrodinger's Equation)					
Module:8	Contemporary Issues	2 hours			
Guest lecture from industry and R & D organisations					
		Total Lecture hours:		30 hours	
Text Book(s)					
1.	Tao Pang, An Introduction to Computational Physics, 2006, Cambridge University Press.				
2.	Darren Walker, Computational Physics, 2015, 1 st Edition, Medtec, New Delhi, India.				
3.					

	E. Balaguruswamy, Numerical Methods, 2017, 1 st Edition, McGraw Hill Education, New Delhi, India.		
Reference Books			
1.	A. Gezerlis, Numerical methods in physics with Python, 2020, Cambridge University Press.		
2.	O. J. Philipp, Computational Physics Simulation of Classical and Quantum Systems. 2013, Springer.		
3.	J. Izaac and J. Wang, Computational Quantum Mechanics, 2018, Berlin: Springer.		
4.	A. B. Stickler and E. Schachinger, Basic concepts in Computational Physics, 2016, Springer International Publishing Switzerland.		
5.	Rubin H Landau and Manuel Jose Paez Mejia, Computational Physics, John Wiley & Sons.		
6.	S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, Numerical Recipes: The Art of Scientific Computing W. H. Press.		
7.	https://github.com/maziarraissi/PINNs		
Mode of Evaluation: CAT, Written Assignment, Quiz and FAT			
Indicative List of Experiments			
1.	Finding solutions of first order differential equations using the Runge-Kutta (RK-1) method		
2.	Finding solutions of first order differential equations using the Runge-Kutta (RK-4) method		
3.	Solving Integration by Trapezoidal and Simpson's rule		
4.	Solving the roots of equations by Bisection Method		
5.	Solving the roots of equations by False position Method		
6.	Solving the roots of equations Newton Raphson method		
7.	Solving the Linear Interpolation, Lagrange and Newton Interpolation; Linear curve fitting		
8.	Solving the Linear Interpolation, Lagrange and Newton Interpolation; Non-linear curve fitting		
9.	Solving Schrodinger differential equation in Quantum Mechanics with Numerov's algorithm		
10.	Solutions of Nonlinear Partial Differential Equations using Neural Networks		
Total Laboratory hours			30 Hours
Mode of assessment: Continuous assessment / FAT / Oral examination and others			
Recommended by Board of Studies		20-06-2023	
Approved by Academic Council		No. 70	Date 24-06-2023