

1.	Title of the course	Computer Programming and Numerical Methods in Chemistry
2.	Course number	CY511M
3.	Structure of credits	2-0-3-4
4.	Offered to	PG
5.	New course/modification to	Modification To CY5210/10
6.	To be offered by	Department of Chemistry
7.	To take effect from	July 2022
8.	Prerequisite	Nil
9.	Course Objective(s): To provide a basic knowledge in computer language and an overall exposure about numerical methods that are widely used in computational chemistry. To equip students with the necessary numerical techniques to deal with some chemical and physical phenomena that can not be tackled analytically.	
10.	Course Content: Data statements, logical and arithmetic expressions, operators, I-O statements, loops, control statements, functions, subroutines, array, strings, characters, format, data analysis; Numerical methods: root finding using successive bisection and Newton Raphson method; Interpolation: Newton's forward and backward interpolation, Lagrange method; Numerical integration: trapezoidal and Simpson's one-third rule; Ordinary differential equation: initial value problem - Euler and Runge Kutta Method, Verlet algorithm, harmonic oscillators, chaotic pendulum, projectile motion; Boundary value problem : relaxation technique, shooting method; Monte Carlo Methods: random number, random walk and diffusion, Monte Carlo integration; Ising model: Metropolis algorithm, paircorrelation function; Langevin dynamics: underdamped and overdamped.	
11.	Textbook(s): 1. Balagurusamy E, <i>Numerical Methods</i> , Tata McGraw-Hill Education (2010). 2. Rajaraman V, <i>Computer Programming in Fortran 90 and 95</i> , PHI Learning (1997).	
12.	Reference(s): 1. Atkinson K E, <i>An Introduction to Numerical Analysis</i> , John Wiley & Sons (1989). 2. Press W H, Teukolsky S A, Vetterling W T and Flannery B P, <i>Numerical Recipes in FORTRAN 90</i> , Cambridge University Press (1996). 3. Xavier C, <i>Fortran 77 and Numerical Methods</i> , New Age International Publisher (1994).	