BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI K. K. Birla Goa Campus

INSTRUCTION DIVISION FIRST SEMESTER 2017-18 Course Handout (Part-II)

Date: 02/08/2017

In addition to part I (General handout for all courses appended to the timetable) this portion gives further details regarding the course.

Course Number : PHY F313

Course Title : Computational physics

Instructor-in-Charge : Toby Joseph

Text Book:

1. A first course in computational physics, Paul L. DeVries & Javier E. Hasburn, 2nd ed, Jones and Bartlett

Reference Books:

- 1. An Introduction to Computational Physics, Tao Pang, 2nd ed., Cambridge University Press
- 2. A Survey of Computational Physics, R. H. Landau, M. J. Paez & C. C. Bordeianu, Princeton University Press

In the study of physics, analytical solutions are not always easy to come by. Numerical techniques come to our rescue to solve many of the problems that are not analytically tractable. With the advent of easily accessible high end computational power, the field of Computational Physics has become main stream and has started playing a crucial role in the advancement of physics.

The take away from this course would be:

- Learn to explore physics using computational methods
- Introduction to numerical techniques
- Proficiency in writing computer codes to implement various numerical methods.
- Exposure to programming environment, Matlab

Every week there will be two lectures and two lab sessions.

Lec. Nos. (Labs)	Objective	Contents	Reference
1 (Lab:1)	Introduction	Course discussion; MATLAB basics	Class Notes
2 – 4 (Labs:2 - 4)	Roots of equations	Particle in a finite well; Kronig – Penny model; Bisection method; Newton-Raphson; Hybrid methods; Review of some of the other methods	DeVries
5 – 8 (Labs:5-8)	Numerical Linear Algebra	Masses on a string; Spectrum of heavy nuclei; Solving Linear equations- Gauss elimination; LU decomposition; Sparse matrices; Eigenvalues and eigenvectors – Power method	DeVries + Class Notes
9 – 11 (Labs: 9-11)	Interpolation, extrapolation and data fitting	Millikan's oil drop; Measurement of g using pendulum; Lagrange interpolation; Cubic spline; Richardson extrapolation; Least square fitting	DeVries + Class Notes
12 – 15 (Labs:12-15)	Numerical Integration	Simple Pendulum; Classical Scattering; Wave function evolution; <i>Elementary</i> methods; Simpson's rule; Romberg's method; Gaussian quadrature; Improper integrals	DeVries + Class Notes
16 – 20 (Labs:16-20)	Ordinary differential equation	Celestial Mechanics; van der Pol oscillator; 1-d Schrodinger equation; Euler methods; Runge-Kutta methods; Runge-Kutta-Fehlberg method; Approaches for coupled differential equations; 2 nd order differential equations; Finite difference schemes – Jacobi scheme, Gauss-Seidel scheme; Discretization error; successive over relaxation	DeVries + Class Notes
21 – 23 (Labs:21-23)	Mote Carlo – Metropolis method	Microcanonical ensemble; Canonical ensemble; Ising Model; <i>Monte Carlo methods; Metropolis algorithm</i>	Class Notes
24 – 27 (Labs:24-27)	Partial differential equations	Vibration string; Problems from electrostatics; Scattering problems; Finite difference in equations in 1-d and higher-dimensions with Dirichlet boundary conditions; stability; Finite difference equations with Neumann boundary conditions	DeVries + Class Notes

Evaluation Scheme:

No.	Component	Duration	Weight	Date	Nature of
					component
1	Mid-term test	90 min	25%	14/10/2017 (9:30)	Closed book
2	Quizzes	10 min each	10%	Continuous	Closed book
3	Lab Work	2 hrs./week	10%	Continuous	Open book
4	Lab exam	2 hrs.	15%	29/11/2017 (18:00)	Open text book
6	Comprehensive	3 hrs.	40%	13/12/2017 (FN)	Closed book

<u>Chamber Consultation Hour:</u> To be announced in lecture

<u>Notices</u>: Notices will put up on **Photon** course server: http://photon.bits-goa.ac.in <u>Make-up Policy</u>: Make up will be given only to really genuine cases, *i.e.* (i) <u>Sickness leading to **hospitalization**</u>, (ii) out-of-station with prior **intimation** and **permission**.

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