FIRST SEMESTER 2016-17

Course Handout Part II

Date: 2 Aug 2016

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

Course No. **: CHEM F324**
Course Title **: Numerical Methods in Chemistry**
Instructor-in-charge **: S. C. SIVASUBRAMANIAN**
Instructor(s) **: -**

1. Course Description: Selected problems in chemistry from diverse areas such as chemical kinetics and dynamics, quantum mechanics, electronic structure of molecules, spectroscopy, molecular mechanics and conformational analysis, thermodynamics, and structure and properties of condensed phases will be discussed. The problems chosen will illustrate the application of various mathematical and numerical methods such as those used in the solution of systems of algebraic equations, differential equations, and minimization of multidimensional functions, Fourier transform and Monte Carlo methods.

Scope and Objective of the Course: The course aims at covering topics in numerical methods of analysis with examples of direct applications in chemistry. The basics, limitations and algorithmic way of implementation of different numerical methods mentioned in the course description will be exposed in the theory session. Also in the same session one or more areas of chemistry where such method is applicable will be exposed. The practical session will give the students hands on experience to implement and test the methods in FORTRAN or C. At the end of the course the student will be able to utilize most of the numerical methods taught in many areas of science and analyze the results in a meaningful way.

2. Text and Reference Books:

Text Books:

T1. W. H .Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, "Numerical Recipes in Fortran", 2nd ed., Cambridge University Press, Cambridge UK(1992). *(Note: 1. There is a version in C language by the same publishers; interested students can get it on their own. 2. The 2005 Indian reprint is by Foundation Books Pvt. Ltd. New Delhi)*

Reference Books:

R1. S. S. Sastry, "Introductory Methods of Numerical Analysis", 4th ed., Prentice-Hall of India - New Delhi (2005)
R2. V. Rajaraman, "Computer Oriented Numerical Methods",3rd ed., Prentice-Hall of India - New Delhi (2013)
R3. Attila Szabo and N.S. Ostlund, "Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory", Dover Publications, New York (1996).
R4. Frank Jensen, "Introduction to Computational Chemistry", John-Wiley & Sons, New York (1999).
R5. A.C. Norris, "Computational Chemistry", John-Wiley& Sons, New York (1981).
R6. V. Rajaraman, "Computer Programming in FORTRAN 90 and 95", Prentice-Hall of India - New Delhi (1997)
R7. Levine Ira N., Physical Chemistry, 6th ed., Tata McGraw-Hill, New Delhi (2009).

3. Course Plan: (*One or two chemical applications are cited for each topic; however, many more applications are possible; an appropriate application will be discussed in the class*)

Lec. No.	Topics to be covered	Learning Objectives	Ref: Chap./Sec.#(Book)
1-3	Introduction to FORTRAN	FORTRAN constructs; Simple problems	Ch.1 (T1), R6
4-8	Solution of Linear Algebraic equations	Gauss-Jordan elimination and Gaussian Elimination; *Application: Quantitative estimation of components in a multi-component system from spectral data.*	Ch. 2(T1)
9-12	Interpolation and Extrapolation	Polynomial and cubic spline interpolations; multi dimensional interpolations; *Application: Plotting isenthalpic curves from Joule-Thomson expt. data and obtaining JT coefficient.*	Ch. 3(T1), *p. 57(R7)*
13-16	Integration of Functions	Classical and Romberg integrations; Gaussian quadrature; multidimensional integrations; *Applications: a) Integration of spectral absorption lines for quantitative estimation; b) estimation of enthalpy change, absolute entropy from a temperature dependent heat capacity function.*	Ch.4(T1), *p.151and p.158(R7)*
17-20	Root finding and Nonlinear Sets of equations	Roots of polynomials, Newton-Ralphson and other methods; *Application: estimation of pH of a weak acid given the dissociation constant.*	Ch.9(T1), *p.335(R7)*
21-24	Minimization and Maximization of functions.	Different methods of search for minimization and maximization of one dimensional and multidimensional functions; *Application: Simple potential energy surfaces*	Ch.10 (T1), *p.880 (R7)*
25-28	Eigen-systems	Concepts of diagonalization of a matrix, Eigen values, and different transformations used for specific type of matrices; *Application: finding the principle values from the data obtained in a magnetic susceptibility experiment, some examples from group theory, quantum chemistry etc.*	Ch. 11 (T1), *p.805 (R7)*
29-31	Fourier Transform	FFT, convolution and deconvolution, computing Fourier integrals; *Application: Time domain to frequency domain spectral conversions, x-ray crystallography examples etc.*	Ch. 12-13 (T1), *p770-771,788-791 (R7)*
32-34	Monte Carlo Methods	Uniform random deviates, transformation to normal deviates, simple and adaptive MC integrations; *Application: Distribution functions of gas velocities, Radial distribution function for liquids, Spectral simulations etc.*	Ch. 7 (T1), *p.451-452, p.947(R7)*
35-36	Integration of ordinary differential equations	Runge-Kutta and other methods; *Application: Chemical Kinetics, oscillating chemical reactions etc.*	Ch. 16(T1),
37-38	Partial differential equations	Initial and boundary value problems, multidimensional cases. *Application: vibrating string, wave equation etc.*	Ch. 19(T1)

4. **Evaluation Components:**

Components	Weightage (%)	Dates	Remarks
Mid-Sem. Test	25%	7/10 2:00 - 3:30 PM	OB/Com.Lab
Computer Lab/Tutorials Assignments/Quizzes/	25%	Continuous	Partly Closed Book
Project	10%		
Comprehensive Examination	30%	12/12 FN	OB/Comp. Lab

Regarding Continuous Evaluation: Assignments will be given periodically to supplement the material discussed in the class. Students will come with prior preparation to the Laboratory session and execute these assignments in computer.

Regarding Project:

See Evaluation Scheme above for weightage. These will include problem sets and certain literature based exercises, some of which may be of routine, and others of advanced nature. The problem sets and other exercises will be discussed in the class or chamber consultation hour. Students will also be asked to solve some problem(s) during the class hour for evaluation. Students will also have to deliver seminars on some topics.

5. **Chamber Consultation Hour:** Friday 9th Hr. (4-5pm); 3165 (CAHU).

Instructor-in-charge
CHEM F324