NUMERICAL METHODS AND SIMULATION TECHNIQUES FOR SCIENTISTS AND ENGINEERS

PROF. SAURABH BASU

Department of Physics

IIT Guwahati

INTENDED AUDIENCE : Sudents, Lecturers from Engineering colleges and Universities. Also Industry people may be interested who do simulation

PREREQUISITES : Basic level Mathematics course

INDUSTRY SUPPORT : Industry people in the R&D sectors of Fluid Mechanics, Material Science may value the course

COURSE OUTLINE :

The course contains very important aspects of modern day course curriculum, namely, numerical methods and simulation techniques that are going to be of utmost importance to both undergraduate and graduate level. Most of the real life problems are unsolvable using known analytic techniques, thus depending on numerical methods is imperative. The course introduces basic numerical methods and the key simulation techniques that are going to be useful to academia and industry alike. Even if the software packages, such as Mathematica, Matlab etc are available for most of the numeric computations, yet one should be aware of the techniques that are inbuilt into the softwares.

ABOUT INSTRUCTOR :

Prof. Saurabh Basu is a Professor at the Department of Physics, IIT Guwahati. His area of expertise is Theoretical Condensed Matter Physics, with special emphasis on the correlated boson and fermion systems, topological insulators. He has about 90 research publications in different refereed international journals.

COURSE PLAN :

Week 1: Introduction to Numerical analysis, Importance of error and their calculations, Examples

Week 2: Root Finding Method of non-linear equations, Bisection Method, Newton Raphson Method, Secant method, Regula- Falsi method, Practical examples

Week 3: Curve fitting method, linear and non-linear fitting, Linear interpolation, Lagrange interpolation method, Newton Interpolation formula, Practical examples

Week 4: Numerical differentiation, central difference methods, higher order derivatives, errors, practical examples

Week 5: Numerical integration, Simpson's 1/3 rd rule, Simpson's 3/8 th rule, local and global error analysis, practical examples

Week 6: Eigenvalue problems, Heun's method, Euler's method, Runge Kutta Method, Gerschgorin disc theorem , Jacobi method, Practical examples

Week 7: Simulation Techniques, Random numbers, Monte Carlo Method, Importance Sampling, Metropolis Algorithm, Heat- bath algorithm, practical Examples

Week 8: Molecular dynamics, interaction and forces in molecular systems, MD and Verlet algorithm, correlations, practical examples