



COMPUTATIONAL SCIENCE IN ENGINEERING

PROF. ASHOKE DE

Department of Aerospace Engineering

IIT Kanpur

PRE-REQUISITES : Basics of Mathematics and programming

INTENDED AUDIENCE : Freshman/Sophomore undergraduate students and postgraduate students of Aerospace/Mechanical/Chemical/Civil Engineering

INDUSTRIES APPLICABLE TO : Aerospace, Automobile, Chemical and Power Generation and Defense Industries

COURSE OUTLINE :

The Computational Science in Engineering is a rapidly evolving field that exploits the power of computation as an approach to major challenges on the frontiers of natural and social science and all engineering fields. The primary focus lies on developing problem-solving methodologies and robust tools for numerical simulation. The goal is to present the fundamentals of scientific computing, with short codes to implement the key concepts. This includes a framework for applied mathematics such as Linear Algebra, ODEs and PDEs. To understand phenomena and processes from science and engineering, these simulations require advanced skills in mathematical modelling, numerical analysis, efficient algorithms, computer architecture, software design and implementation, validation, and visualization of results.

ABOUT INSTRUCTOR :

Prof. Ashoke De is currently working as Associate Professor in the Department of Aerospace Engineering at Indian Institute of Technology Kanpur. He leads large scale initiatives in the modeling of turbulent reacting and non-reacting flows at IIT Kanpur. So far, he has authored more than 130 peer reviewed articles in journals and conferences. His primary research focus is the emerging field of computational mechanics with particular interest in combustion and turbulent flows.

COURSE PLAN :

Week 1: Linear Algebra: Introduction to Vectors, Vector spaces and subspaces, Solving Linear systems

Week 2: Linear Algebra: Orthogonality, Determinants, Eigenvalues & Eigen vectors, SVD

Week 3: Ordinary Differential Equations: ODE, homogeneous and non-homogeneous ODEs, second order linear ODE, higher order ODEs

Week 4: Partial Differential Equations: Classification, 1D & 2D equations, BC, 2nd order PDEs

Week 5: Basis of numerical analysis, errors, stability, Interpolation and extrapolation

Week 6: Root finding: Polynomials; Newton-Raphson Method, Secant Method

Week 7: System of linear algebraic equations and eigenvalue problems: Direct methods, Iterative methods, convergence analysis, Eigenvalues and Eigenvectors, bounds on eigenvalues, Methods for symmetric matrices and arbitrary matrices

Week 8: Solution of ODEs: Difference equation, Numerical methods, convergence, stability, Single step and multistep methods, Predictor-corrector methods, stability analysis of multistep methods, IVP (shooting methods), BVP (methods and solutions)