SECOND SEMESTER

NTPC201 MATHEMATICAL MODELING AND SIMULATION

Unit-I FUNDAMENTAL PRINCIPLES OF NUMERICAL METHODS: Scientific Modeling – Numerical operations – Numerical Algorithms – Numerical Programs – Numerical Software – Approximations in Mathematical Model building – Numerical integration - Differentiation – Variation finite element methods-Rayleigh's method –Ritz method.

MATHEMATICAL MODELING: Mathematical modeling- physical simulation- advantage and limitations-process control – Transport phenomena- concept of physical domain and computation domain assumption and limitations in numerical solutions- Finite element method and Finite difference method.

Unit-II DIFFERENTIAL EQUATIONS & APPLICATIONS: Euler method, Multi step-differential equations-boundary values-Elliptic equations-one dimensional parabolic equation-hyperbolic equation- partial differential equations-separation of variables-wave equation-Laplace equation-nonlinear partial differential equations-approximation methods of nonlinear differential equations.

Unit-III SIMULATION: Base concepts of simulation-data manipulation, data exchange of the structure, properties and processing of materials- Three dimensional model for capillary nanobridges and capillary forces, Molecular dynamics simulation.

Unit-IV MONTE CARLO METHODS: Basics of the Monte Carlo method-Algorithms for Monte Carlo simulation- Applications to systems of classical particles-modified Monte Carlo techniques-percolation system-variation Monte Carlo method-diffusion Monte Carlo method – Quantum Monte Carlo method.

References:

1. S.C Chapra and R.P Canale, "Numerical methods for Engineers",Tata McGraw Hill, New Delhi, 2002.
2. Enwin Kreyzig,"Advance Engineering Mathematics ", John Wiley & Sons, 2004.
3. R.J Schilling and S.L. Harris, "Applied Numerical Methods for Engineers using MATLAB and C", Thomson publishers, New Delhi, 2004.
4. D. Frenkel and B Smith, "Understanding molecular simulation from algorithm to applications", Kluwar Academic Press, 1999.
5. K. Ohno, K. Esfarjani and Y. Kawazoe, "Introduction to Computational Materials Science from ab Carlo Methods", Springer-verlag, 1999.