

SYLLABUS :-

Prerequisite: CY41003, CY40102 Use of random numbers to evaluate area under a curve. Application of numerical methods to solve differential equations. Quantum chemical calculations for simple molecular systems. Code development to evaluate potential energy and force acting on complex molecules in a system. Development of a classical MD code for simple monatomic systems. Development of a classical Metropolis MC code for simple monatomic systems. Use of various commercially available molecular modeling and simulation software. Books: Computer Simulation of Liquids, by M. P. Allen and D. J. Tildesley; Clarendon Press (Oxford). Understanding Molecular Simulations: From Algorithms to Applications, by D. Frenkel and B. Smit (Academic Press); Molecular modeling by A.R. Leach.