Second Semester Area C

CSE 389D, Introduction to Mathematical Modeling in Science and Engineering II

1. Introduction to Statistical Mechanics
   1.1. Basic Concepts: Ensembles, Distribution Functions, and Averages
   1.2. Ergodic Theory: Phase Functions and Time Averages
   1.3. Microcanonical, Canonical, and Grandcanonical Ensembles
   1.4. Statistical Mechanics Basis of Classical Thermodynamics
   1.5. Entropy and the Partition Function
   1.6. Maxwell-Gibbs Relations
   1.7. Introduction to Molecular Dynamics
   1.8. Boltzman’s Equations: Non-Equilibrium Thermodynamics

2. Mathematical Modeling in Biochemistry
   2.1. Overview of Cell Biology
   2.2. Components of the cells: Proteins, DNA, RNA and membranes
   2.3. Proteins and RNA I: expression and regulation
   2.4. Protein and RNA II: Folding
   2.5. Cell machinery at work: activation and allosteric transitions
   2.6. Cell signaling and transport: Ion channels
   2.7. Protein aggregation and macromolecular assembly: Molecular diseases, viruses