

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. Boltzmann'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