

Introduction to Modelling and Simulation

Topics

1. Mechanical behavior of materials (10 hours).....Exercise-1 (60 points)
 - Structure of materials
 - Elastic and plastic properties of materials (stress-strain behavior)
 - Elastic constants of materials
 - Theoretical tensile and shear strength of materials
 - Point and line defects
 - About fracture mechanics
2. Classical mechanics of continua (7 hours).....Exercise-2 (40 points)
3. Classical mechanics of particles (8 hours).....Exercise-3 (60 points)
 - Newton's mechanics
 - Lagrange's mechanics
 - Hamiltonian mechanics
4. Statistical mechanics (12 hours).....Exercises 4 (40 points)
 - Classical and statistical thermodynamics
 - Statistical ensembles

Midterm (500 points)

5. Introduction to computational methods of material modelling (9 hours)
 - Classical molecular dynamics simulation
 - Molecular interactions and interatomic potentials
 - Linkage between atomistic and continuum description
 - Virial theorem (link to stress)

Project (300 points)

Total Grade =1000 points, Total sessions = 32, Total hours =48

Reference:

E.B. Tadmor and R.E. Miller, Modeling Materials, Cambridge University Press.