

Course Code: JF305
Course Title: Advanced Computational Science
Instructors: Santosh Ansumali
Credits: 3.0

1. **Introduction to High Performance Computing (6 Hours)**
 - I. Introduction to distributed computing
 - II. Amdahl's law and Gustafson's law
 - III. MPI parallelization and SIMD vectorization
 - IV. Memory Bandwidth optimizations and Roofline Model
2. **Ordinary Differential Equations (6 Hours)**
 - I. One-step methods
 - II. Forward and Backward Error Analysis
 - III. Runga Kutta and Multi-step methods
 - IV. Symplectic Integrators
 - V. Stiff Equations
3. **Particle Based Methods – (9 Hours)**
 - I. Molecular Dynamics, Hard Sphere Dynamics,
 - II. Discrete simulation Monte Carlo
 - III. Multi-Particle Collision Dynamics,
 - IV. Brownian Dynamics Method
4. **Finite Difference Method (6 hours)**
 - I. Introduction to Finite difference
 - II. Von Neumannn Analysis
 - III. Discrete Differential Operators
 - IV. Modified Equation and Artificial viscosity Methods
 - V. Lax-Wandroff Method
 - VI. Crank-Nicholson Method
 - VII. Mac-Cormack Method for Advection equation
 - VIII. Fractional Step Methods
5. **Introduction to Kinetic Theory of Gases (8 Hours)**
 - I. Distribution function, Mean Free path, Maxwell-Boltzmann Distribution,
 - II. Transport Properties,
 - III. Models of Boltzmann Equation and moment Chain
 - IV. Methods of Reduced Description and Hydrodynamic Limit, Chapman-Enskog Method, Grad's Moment Method, Maximum Entropy's Method
6. **Introduction to Lattice Boltzmann Models (9 Hours)**
 - I. Discrete Velocity Models for Hydrodynamics,
 - II. Basic 2D and 3D implementations, Boundary Conditions,
 - III. Entropic Lattice Boltzmann
 - IV. Multiphase Flow
 - V. LBM as PDE solver
7. **Introduction to Computational Fluid Dynamics (4 hours)**
 - I. Pseudo-compressibility Method
 - II. Pressure Projection Method
 - III. Pseudo-Spectral Method