

ADVANCED NUMERICAL METHODS

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CONTENTS

Basic concepts of Newtonian dynamics and Statistical Mechanics: energy conservation, time reversibility and phase-space incompressibility, Liouville Theorem, Ergodicity.

Derivation of the microcanonical, canonical and grandcanonical statistical ensemble from principle of maximum entropy.

Integration schemes for molecular dynamics: Verlet, Trotter splitting, Velocity Verlet.

Dependence of the results on the time step.

Sampling the canonical ensemble with Monte Carlo: Metropolis-Hastings rule, balance and detailed balance, hybrid Monte Carlo.

Sampling the canonical ensemble with molecular dynamics: velocity rescaling, Berendsen thermostat, Andersen thermostat, Langevin dynamics.

Stochastic equations: Ito rule, Fokker-Planck equation.