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## **Computational Statistical Physics: A Mathematical Overview**

This talk is meant to be a mathematical introduction to computational statistical physics and molecular dynamics simulations. After a brief presentation of the most important notions of statistical physics (in particular thermodynamic ensembles, which are probability measures on the phase-space), I will present some standard numerical techniques to compute macroscopic or average properties of systems described at the microscopic level. I will focus on - the microcanonical ensemble (NVE), sampled by a long-time integration of the Hamiltonian dynamics with symplectic algorithms; - the canonical ensemble (NVT), sampled by irreducible stochastic dynamics (Markov chains or stochastic differential equations) leaving the Boltzmann-Gibbs measure invariant. I will also briefly mention the computation of free energy differences.