Dynamical Non-Equilibrium Molecular Dynamics

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In the talk we will discuss the Dynamical approach to Non-Equilibrium Molecular Dynamics (D-NEMD), which extends stationary NEMD to time-dependent situations, be they responses or relaxations.
Based on the original Onsager regression hypothesis, implemented in the nineteen-seventies in computer simulation, the approach permits to separate the problem of dynamical evolution from the problem of sampling the initial condition.
D-NEMD provides the theoretical framework to compute time-dependent macroscopic dynamical behaviors by averaging on a large sample of non-equilibrium trajectories starting from an ensemble of initial conditions generated from a suitable (equilibrium or stationary non-equilibrium) distribution at time zero.
We discuss how to generate a large class of initial distributions. Indeed, the same approach applies to the calculation of the rate constants of activated processes and to the generation of hydrodynamic patterns (convective motion, relaxation of interfaces). The generality of the method will be illustrated by presenting applications to few key hydrodynamic processes (the "classical" flow under shear, the formation of convective cells and the relaxation of an interface between two immiscible liquids).