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Thermal fluctuations in a kinetic model for multicomponent fluids

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Thermal fluctuations and non-ideal multicomponent effects are important ingredients for a proper mesoscale description of a wide variety of flows in soft matter and biological physics [1, 2, 3]. Theoretically, thermally fluctuating mesoscopic flows are most conveniently dealt within the framework of fluctuating hydrodynamics [4]. An important ingredient in this formulation is the fluctuation-dissipation theorem (FDT) relating the noises covariances to the Onsager coefficients of the fluid.
Even without the presence of thermal fluctuations, modeling and simulation of multicomponent and multiphase fluid flows is extremely difficult, especially because of the problems in simulating complex diffusion processes, phase separation, and interface dynamics. This has triggered the development of a whole range of innovative numerical methods to solve the Navier-Stokes equations, of which the lattice Boltzmann equations (LBE) [5, 6] stands out due to the capability of handling boundary conditions associated with highly irregular geometries, its nearly ideal amenability to parallel computing, and the possibility to describe non-ideal fluids with phase transitions/phase separation.
The original contribution of the work will result in formulating a kinetic model able to reproduce the desired equilibrium correlation functions for the density and velocity fields invoking FDT directly at the kinetic level. These results will serve as a basis for the development of LBE, embedding both the effects of fluctuations and non-ideality with a limited set of kinetic velocities.

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Summary

A model based on the continuum Boltzmann equation for describing multicomponent fluids is extended to incorporate the effects of thermal fluctuations. The resulting equation is then linearized around the equilibrium and noise correlations for all the modes are determined by invoking the fluctuation-dissipation theorem directly at the kinetic level. By suitable discretizations of time, space and velocity, the results are then transferred on the lattice and numerical simulations are performed. From numerical results, it can be appreciate the importance of using our noise correlations, instead of using uncorrelated noise, to get a proper thermalization of the system in a homogeneous case, while capillary fluctuations of a fluid-fluid interface in a non-homogeneous case are well reproduced.

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