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(G*) Colloidal suspensions near the fluid phase interface of coupled Lattice-Boltzmann and molecular-dynamics simulations

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Lattice-Boltzmann (LB) simulations have been used extensively over the past several decades in the study of hydrodynamics. With computational power increasing, LB methods have been coupled with various molecular dynamics (MD) methods to better simulate complex fluids, phase transitions, and their behaviour at interfaces. Using a modified LB package from the Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), we couple colloidal particles and the LB fluid mesh under critical conditions to investigate particle dynamics at and near the liquid-gas interface due to variable wetting potentials. This work is preliminary to studying interfacial behaviour of complex fluid suspensions in LAMMPS, such as that of a liquid crystal (LC) colloid suspension, where distinct defect patterns are known to emerge at the LC-gas interface at equilibrium. We expect these defects to disturb the uniformity of the colloidal suspension.

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