TOWARDS A NEW ALGORITHM FOR MULTIPHASE LATTICE BOLTZMANN SIMULATIONS

Jasna Zelko¹ and Burkhard Dünweg^{2,3}

 ¹ Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany, <u>zelko@mpip-mainz.mpg.de</u>, http://www.mpip-mainz.mpg.de/polymer_theory
² Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany, <u>duenweg@mpip-mainz.mpg.de</u>, http://www.mpip-mainz.mpg.de/~duenweg
³ Department of Chemical Engineering, Monash University, Clayton, Victoria 3800, Australia, <u>burkhard.duenweg@monash.edu</u>, http://www.monash.edu

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A new lattice Boltzmann (LB) method for simulating multiphase flows is developed theoretically. The LB method is adjusted such that its continuum limit is the Navier-Stokes equation, with a driving force derived from the Cahn-Hilliard free energy. In contrast to previous work, however, the bulk and interface terms are decoupled, the former being incorporated into the model through the local equilibrium populations, and the latter through a forcing term. We focus on gas-liquid phase equilibria with the possibility to implement an arbitrary equation of state. The most novel aspect of our approach is a systematic Chapman-Enskog (CE) expansion up to the third order. Due to the third-order gradient in the interface forcing term, this is needed to obtain an LB model that is fully consistent with both hydrodynamics and thermodynamics. In order to satisfy all conditions, we need 59 velocities in three dimensions, and 21 velocities for simulating two-dimensional systems.

The commonly noticed inconsistency of the existing models is thus traced back to their insufficient number of degrees of freedom. Therefore, the gain of the new model is in its clear derivation, full thermo-hydrodynamic consistency, and expected complete elimination of spurious currents in the continuum limit, which is achieved by the construction of various counter-terms in both the definition of the momentum density and the collision operator. Numerical tests are deferred to future work.