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Multiphysic Two-Phase Flow Lattice Boltzmann: Droplets with Realistic Representation of the Interface

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Abstract. Free energy lattice Boltzmann methods are well suited for the simulation of two phase flow problems. The model for the interface is based on well understood physical grounds. In most cases a numerical interface is used instead of the physical one because of lattice resolution limitations. In this paper we present a framework where we can both follow the droplet behavior in a coarse scale and solve the interface in a fine scale simultaneously. We apply the method for the simulation of a droplet using an interface to diameter size ratio of 1 to 280. In a second simulation, a small droplet coalesces with a 42 times larger droplet producing on it only a small capillary wave that propagates and dissipates.

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Key words: Two-phase flow, diffuse interface model, multi-scale, real interface.

1 Introduction

The main problem present in meso-scale multi-phase flow simulation is resolving the interfacial phenomena. These are disregarded when working at macroscopic scales and even for millimeter size droplet interactions [15] where only interfacial tension forces and phase tracking are relevant when solving mass and momentum balances. High resolution techniques are needed for performing mesoscale experiment studies on droplets,

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bubbles or colloids. These results are needed as closure relationships for describing the interactions of such entities.

The actual problem is that the computational models are able to model droplets or bubbles and can be trusted when no pinch-off or interface rupture is expected to occur. On the other hand, thermodynamical models of the interface can give a better description of the interface at the nanoscale but can not model an entire droplet at the same time because of the difference in scales.

In this work, transient mesoscale two phase problems are proposed modeled in a new way where the homogeneity of traditional CFD solvers is broken up in a method that implements multiscale lattices that go beyond a local mesh refinement concept [1]. The work distinguishes between interfacial physics and bulk phase hydrodynamics. The interfacial physics are modeled using the Cahn-Hilliard equation. This physical model takes into account not only the tracking between phases, but also the shape of the interface and the mass diffusion process through it. Therefore it is also suitable for phase change simulations [3, 11]. The hydrodynamic-only model is much simpler.

The lattice Boltzmann method is adopted for solving the both present models. Relevant papers can be found in the lattice Boltzmann literature addressing the more general concepts of mesh refinement in both single [4] and multiphase [18, 21]. These can be used as a complement to the concept introduced in this work. The scope of this work is to show how a multimodel approach can be used for simulation of 2D droplets to have large droplets with more realistic interfaces. For the gas and liquid bulk hydrodynamics, traditional single phase lattice Boltzmann methods are used. In a region affected by the liquid-gas interphase a two phase flow lattice Boltzmann method is used based on the free energy approach: Cahn-Hilliard equation with a pressure and momentum lattice Boltzmann distribution. In short, each model has its own space-time scales, equations and solution method.

The models are described in Section 2; how to solve them and the multiscale implementation in Section 3; the simulation results in Section 4; and finally concluding remarks are given in Section 5.

2 Model considerations

The main idea is to separate the physics by a domain decomposition technique, distinguishing in the highest hierarchy two regions: simple single phase fluid flow in the bulk and two phase fluid flow with concentration gradients present in the interfaces. Two scales are defined: the interfacial physics scale and a bulk hydrodynamic scale, where the corresponding lattice topographies are fine and coarse respectively. The problem is better explained at the coarse level, where only a single phase is present. There are coarse voxels containing only liquid phase, only gas phase, or a part of the interface defined as a non-negligible variation of the concentration (density). A coarse interface voxel is overlapped with an entire lattice block composed of fine voxels. A scale change is made