MULTIPHASE CAPABILITY DEVELOPMENT FOR A LATTICE BOLTZMANN SOLVER

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MSc Thesis Specification: The main objective of this MSc Thesis is to develop the existing in-house fully parallelized 2D/3D lattice Boltzmann code for multiphase flows. The Lattice Boltzmann Method (LBM) [8] has become a widely used CFD tool for analysis of complex flows. It is a mesoscopic method, developed as an extension of the Lattice Gas Cellular Automata (LGCA) [3]. It consists in a single linear partial differential equation in contrast with the system of coupled and non-linear PDE which form the Navier-Stokes equations, hence, its implementation is far easier. Its locality nature makes it a fully parallelizable method, which is one of its main advantages. Due to its simplicity, it provides an excellent framework to describe complex flows such as the multiphase flows [1].

Among the multiphase LB models proposed in the literature, three of them will be developed and implemented in the context of this MSc thesis.

The first one is the color-gradient model, also known as two-colors model or Rothman-Keller (RK) model [9], who firstly proposed. Gunstensen et al. [5] introduced it for simulating immiscible binary fluids based on 2D hexagonal lattice. Later on, Grunau et al. [4] provided the technique to allow variations of density and viscosity. This model considers two immiscible fluids, red and blue, which are associated to their own density distribution functions (DDF). To take into account the interaction between the fluids, an additional operator is introduced in the collision step. This additional term are related to the surface tension and the so called gradient color function. The phase separation is achieved by a recoloring step which involves the optimization of a function. The original recoloring step proposed by Gunstensen et al. is very computational expensive and difficult to program. For these reasons it was substituted by the recoloring strategy proposed by D'Ortana et al. [2], which consists in a simple operator. Later on Latva-Kokko and Rothman [6] put the basis to extend its application to the speed models D2Q9 and D3Q19. An excellent review of this approach is provided by Leclaire et al. [7]. This cheaper and simpler approach allows the capability of interface thickness adjustment.

The second model; and the most employed one, was developed by Shan and Chen (SC) [10]. It uses an interaction force between particles to mimic microscopic interactions and automatically separate the concentrated and diluted phases. This automatic segregation, and the achieved surface tension isotropy are the reason behind its great popularity. The main drawback of this method is the fact that it does not satisfy the local conservation of the total momentum.

Finally, the third model is the Free-Energy method of Swift et al. [11]. It describes an approach which leads in equilibrium to a steady state that can be associated with a free energy. The collision rules employed by this method ensure that the system evolves to the minimum energy state. The energy functional includes both the pure fluid part and the interface part. Like the SC model, the phase separation is automatic. This model is the most complex one of the studied in this thesis, but it relies on stronger physical foundations.

The efficient implementation of these models will be tackled by the software engineer student Jose Oliveira. In order to close the development of the multiphase capability for the LB code, a validation process will be accomplished. The main validation cases from LB multiphase flows literature are, the circular steady bubble, the steady bubble deformation, the coalescence of bubbles, the Rayleigh-Taylor instability and Taylor-Dispersion experiment.

The Gant Chart of this MSc Thesis is shown below.

References

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