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Discrete simulation of fluid dynamics

Study of hydrodynamic instabilities with a multiphase lattice Boltzmann model

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ABSTRACT

Rayleigh–Taylor and Kelvin–Helmholtz hydrodynamic instabilities are frequent in many natural and industrial processes, but their numerical simulation is not an easy challenge. This work simulates both instabilities by using a lattice Boltzmann model on multiphase fluids at a liquid-vapour interface, instead of multicomponent systems like the oil–water one. The model, proposed by He, Chen and Zhang (1999) [1] was modified to increase the precision by computing the pressure gradients with a higher order, as proposed by McCracken and Abraham (2005) [2]. The resulting model correctly simulates both instabilities by using almost the same parameter set. It also reproduces the relation $\gamma \propto \sqrt{A}$ between the growing rate γ of the Rayleigh–Taylor instability and the relative density difference between the fluids (known as the Atwood number A), but including also deviations observed in experiments at low density differences. The results show that the implemented model is a useful tool for the study of hydrodynamic instabilities, drawing a sharp interface and exhibiting numerical stability for moderately high Reynolds numbers.

1. Introduction

Hydrodynamic instabilities are very common processes in daily life. The clouds of periodic curls in a sunny day, how the water jet from the tap breaks into droplets and the beautiful mushroom-like patterns that can be seen when the coffee mixes with water are some examples of hydrodynamic instabilities. Hydrodynamic instabilities use to appear when two fluids in contact generate a metastable interface. Due to the involved forces, an initial perturbation grows to form complex structures with certain grade of periodicity. As a matter of fact, perturbations with a specific wavelength grow faster than others and, in consequence, their evolution will generate periodic patterns with that wavelength. This is the secret behind the shape of the jet contrails that break into similar puffs, the periodicity of droplets at the ceiling of the shower or the geometric structure of supernovas. In addition, hydrodynamic instabilities are relevant in many industrial processes, not only as undesirable phenomena, as in the field of inertial confinement fusion where instabilities reduce the fusion rate, but also as something that can be useful to create homogeneous drops and grains. Even more, the set of differential equations governing the behaviour of hydrodynamic instabilities are common to other fields of non-linear dynamics (as plasma physics and general relativity); therefore, they use to be handled as paradigms to investigate other non-linear—but hardly reproducible—systems. The equations used to describe the hydrodynamic instabilities are non-linear partial differential equations, and their analytical solution is only plausible for the simpler cases. For all others it is necessary to use computational methods.

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Multiphase lattice-Boltzmann models (MLBM), unlike other numerical methods, do not discretize the differential equations of fluid mechanics, but they simulate the transport and collision of the probability distributions for the molecules of the fluid. By adding interaction forces between the molecules, the fluid segregates into differentiated phases and the surface tension appears naturally. Thus, MLBM are specially appropriated to simulate hydrodynamic instabilities. The first MLBM was proposed in 1993 by Shan and Chen [3], who included interactions among particles. Through the adequate choice of interaction potentials, phase segregation occurs automatically. Next, He Shan and Doolen [4] obtained a more realistic equation of state by including two terms in the interaction potential: a strong short-range interaction, due to the volume exclusion among molecules, and a weak long-range component, from a Van der Waals mean-field approximation of the attractive forces. This proposal solves some thermodynamic inconsistencies of the Shan and Chen model and allows us to use the Maxwell's equal-area rule (see [5]). Later on, He, Chen and Zhang [1] included an index function (an extra set of distribution functions) to identify the two phases by a number, and used it to simulate the Rayleigh–Taylor instability (RTI). This index function improves the stability and keeps a sharp interface through the time evolution. More recently, Xu et al. [6] introduced a multiphase lattice-Boltzmann model with multiple relaxation times that simulates both the Kelvin–Helmholtz (KHI) and the Richmyer–Meshkov (RMI) instabilities, but it has a huge amount of parameters to be adjusted (actually, a different set for each instability), instead of including interparticle forcing terms, and the equation of state for the fluid has not being established yet.

Our aim is to simulate both the RTI and KHI via the lattice-Boltzmann model for a single-component multiphase system, i.e. a liquid-vapour configuration. For this purpose, we use the model introduced by He, Chen and Zhang, but using the hybrid scheme proposed by McCracken and Abraham [2] to calculate the pressure gradient, which improves accuracy and stability. In the next section, we describe the model. Section 3 contains our results for the RTI and KHI, where we focus on the effect of the parameters of the equation of state and the Atwood Number on the development of the instabilities and give a set of optimal parameters for the instability onset. Finally, our conclusions are summarized in Section 4, which also suggests future research works in this interesting area.

2. Model description

Standard lattice-Boltzmann models can be described by the continuous Boltzmann equation,

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla f = \frac{1}{\tau}(f^{(\mathrm{eq})} - f) \tag{1}$$

representing the propagation (left-hand side) and interaction or collision (right-hand side) of some distribution functions f, which can be taken as the probability of finding a particle with position $\boldsymbol{x}$ and velocity $\boldsymbol{\xi}$. Eq. (1) uses the BGK (Bhatnagar, Gross, Krook) approximation [7] in order to write the collision term in a simplified form. Here $f^{(\mathrm{eq})}$ is called the equilibrium distribution function (corresponding to a Maxwell–Boltzmann distribution) and τ is the relaxation time. By assuming a low-velocity regime and approximating the Maxwellian up to second order, the equilibrium distribution function takes the form

$$f^{(\mathrm{eq})} = \frac{\rho}{(2\pi RT)^{D/2}} \exp\left(-\frac{\boldsymbol{\xi}^2}{2RT}\right)\left[1 + \frac{(\boldsymbol{\xi}\cdot\boldsymbol{u})}{RT} + \frac{(\boldsymbol{\xi}\cdot\boldsymbol{u})^2}{2(RT)^2} - \frac{|\boldsymbol{u}|^2}{2RT}\right] \tag{2}$$

with D the dimension, R the ideal-gas constant and T the temperature. The quantities ρ and $\boldsymbol{u}$ are the density and macroscopic velocity at a given point, respectively. If time and space are discrete in steps δt and $\boldsymbol{x} + \boldsymbol{\xi}\delta_t$ respectively, Eq. (1) takes the form

$$f(\boldsymbol{x} + \boldsymbol{\xi}\delta_t, \boldsymbol{\xi}, t + \delta_t) - f(\boldsymbol{x}, \boldsymbol{\xi}, t) = -\frac{1}{\tau}\left[f(\boldsymbol{x}, \boldsymbol{\xi}, t) - f^{(\mathrm{eq})}(\boldsymbol{x}, \boldsymbol{\xi}, t)\right] \tag{3}$$

In this work, we set $\delta t = 1$, and the stability of the system is controlled by restricting the Reynolds number and the magnitude of the velocities in order to maintain the low-velocity assumption made above. Finally, the velocity space is chosen discrete in such a way that the macroscopic quantities

$$\rho = \sum_{i=1}^{n} f_i \qquad \rho\boldsymbol{u} = \sum_{i=1}^{n} f_i\xi_i \qquad 2\rho\varepsilon + \rho|\boldsymbol{u}|^2 = \sum_{i=1}^{n} f_i\xi_i^2 \tag{4}$$

where $\varepsilon = 3RT/2$ is the internal energy, which is maintained constant, with T the temperature and R the ideal gas constant, coincide with the density, the momentum and the energy computed from Gaussian quadrature up to second order in cell size, with one distribution function per discrete velocity, $f(\boldsymbol{x}, \boldsymbol{\xi_i}, t) = f_i$. An example of such a velocity set is D2Q9 (Fig. 1), which can be written as

$$\boldsymbol{\xi}_i = \begin{cases} \mathbf{0} & i = 0 \\ c\cdot\left(\cos\left[(i-1)\frac{\pi}{2}\right], \sin\left[(i-1)\frac{\pi}{2}\right]\right) & i = 1,2,3,4 \\ \sqrt{2}c\cdot\left(\cos\left[(i-5)\frac{\pi}{2} + \frac{\pi}{4}\right], \sin\left[(i-5)\frac{\pi}{2} + \frac{\pi}{4}\right]\right) & i = 5,6,7,8 \end{cases} \tag{5}$$