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Improved Lattice Boltzmann Without Parasitic Currents for Rayleigh-Taylor Instability

Daniele Chiappini[1,*], Gino Bella[1], Sauro Succi[2], Federico Toschi[2,3] and Stefano Ubertini[4]

[1] *University of Rome Tor Vergata, Via del Politecnico 1, I-00133, Rome, Italy.*
[2] *IAC-CNR, Viale del Policlinico 137, I-00161, Rome, Italy.*
[3] *Department of Physics and Department of Mathematics and Computer Science, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands.*
[4] *University of Naples Parthenope, Isola C4 - Centro Direzionale, I-80143, Naples, Italy.*

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Abstract. Over the last decade the Lattice Boltzmann Method (LBM) has gained significant interest as a numerical solver for multiphase flows. However most of the LB variants proposed to date are still faced with discreteness artifacts in the form of spurious currents around fluid-fluid interfaces. In the recent past, Lee et al. have proposed a new LB scheme, based on a higher order differencing of the non-ideal forces, which appears to virtually free of spurious currents for a number of representative situations. In this paper, we analyze the Lee method and show that, although strictly speaking, it lacks exact mass conservation, in actual simulations, the mass-breaking terms exhibit a self-stabilizing dynamics which leads to their disappearance in the long-term evolution. This property is specifically demonstrated for the case of a moving droplet at low-Weber number, and contrasted with the behaviour of the Shan-Chen model. Furthermore, the Lee scheme is for the first time applied to the problem of gravity-driven Rayleigh-Taylor instability. Direct comparison with literature data for different values of the Reynolds number, shows again satisfactory agreement. A grid-sensitivity study shows that, while large grids are required to converge the fine-scale details, the large-scale features of the flow settle-down at relatively low resolution. We conclude that the Lee method provides a viable technique for the simulation of Rayleigh-Taylor instabilities on a significant parameter range of Reynolds and Weber numbers.

AMS subject classifications: 76T02, 68U02

Key words: Lattice-Boltzmann, multiphase, parasitic currents, Rayleigh-Taylor Instability.

*Corresponding author. *Email addresses:* `chiappini@ing.uniroma2.it` (D. Chiappini), `bella@uniroma2.it` (G. Bella), `succi@iac.cnr.it` (S. Succi), `toschi@iac.cnr.it` (F. Toschi), `stefano.ubertini@uniparthenope.it` (S. Ubertini)

1 Introduction

Multiphase flows are ubiquitous in industrial processes (i.e. chemical, pharmaceutical, electronic, and power-generation industries) and natural phenomena alike [1]. Consequently, numerical methods for the investigation of their complex behaviour is in constant demand. However, the task of simulating the behavior of multi-phase flows is very challenging, due to the inherent complexity of the involved phenomena (emergence of moving interfaces with complex topology, droplet collision and break-up), and represents one of the leading edges of computational physics [2, 8]. As a matter of fact, a general computational approach encompassing the full spectrum of complexity exposed by multiphase flows is still not available.

The numerical methods based on the traditional continuum approach (i.e. Navier-Stokes with closure relationships) are usually based on rather complex correlations and often require transient solution algorithms with very small time steps. In the last two decades, a new class of mesoscopic methods, based on minimal lattice formulation of Boltzmann kinetic equation, have gained significant interest as an efficient alternative to continuum methods based on the discretization of the NS equations for non ideal fluids [16].

Since its early days, the Lattice Boltzmann shed promises of becoming a tool for the modeling of multiphase flows. The earliest Lattice Boltzmann simulations of multicomponent flows have been performed by Gunstensen et al. [14, 15] and Grunau et al. [16], based on the pioneering Rothman-Keller lattice gas multi-phase model [13]. Ever since, many models have been proposed in order to simulate multiphase flows with the LBM, most of them aiming at incorporating the physics of phase-segregation and interface dynamics, typically hard to model with traditional methods, through simple mesoscopic interaction laws. In particular, the pseudo-potential LBM, due to Shan and Chen [18], has gained increasing popularity on account of its conceptual simplicity and computational efficiency. In the Shan-Chen (SC) method, potential energy interactions are represented through a density-dependent, mean-field, pseudo-potential and phase separation is achieved by imposing a short-range attraction between the light and dense phases. This method allows to track and maintain diffuse interfaces with no need of any special treatment of the interface. However, it is known to present unphysical features (i.e spurious velocities), namely the presence of non-zero velocities even for fluids at rest, with a steady density profile. These spurious currents are disturbing for practical applications, and they may cast doubts on the quantitative accuracy of the simulations methods [28]. The spurious currents have been recently addressed by many authors [3, 4, 17]. He et al. [17] proposed a multi-phase LBM scheme with improved numerical stability. It still incorporates molecular interactions, but unphysical features are alleviated by introducing a pressure distribution function instead of the single-particle density distribution function. A particularly remarkable option has been suggested by Lee et al. [3–6], who proposed a higher order finite difference treatment of the kinetic forces arising from non-ideal interactions (potential energy). In this model, spurious currents are allegedly tamed