Journal of Computational Physics 285 (2015) 251–264

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Numerical stability of explicit off-lattice Boltzmann schemes: A comparative study

Parthib R. Rao *, Laura A. Schaefer

Department of Mechanical Engineering and Material Science, University of Pittsburgh, 636 Benedum Hall, 3700 O'Hara St., Pittsburgh, PA 15261, USA

ARTICLE INFO

Article history:
Received 17 July 2014
Received in revised form 17 December 2014
Accepted 10 January 2015
Available online 16 January 2015

Keywords:
Off-lattice Boltzmann method
Finite-difference
Numerical stability

ABSTRACT

The off-lattice Boltzmann (OLB) method consists of numerical schemes which are used to solve the discrete Boltzmann equation. Unlike the commonly used lattice Boltzmann method, the spatial and time steps are uncoupled in the OLB method. In the currently proposed schemes, which can be broadly classified into Runge–Kutta-based and characteristics-based, the size of the time-step is limited due to numerical stability constraints. In this work, we systematically compare the numerical stability of the proposed schemes in terms of the maximum stable time-step. In line with the overall LB method, we investigate the available schemes where the advection approximation is explicit, and the collision approximation is either explicit or implicit. The comparison is done by implementing these schemes on benchmark incompressible flow problems such as Taylor vortex flow, Poiseuille flow, and lid-driven cavity flow. It is found that the characteristics-based OLB schemes are numerically more stable than the Runge–Kutta-based schemes. Additionally, we have observed that, with respect to time-step size, the scheme proposed by Bardow et al. (2006) [1] is the most numerically stable and computationally efficient scheme compared to similar schemes, for the flow problems tested here.

1. Introduction

The lattice Boltzmann (LB) method is an alternative and powerful numerical technique used for modeling a variety of complex hydrodynamic flows [2,3]. Unlike conventional numerical methods which discretize the macroscale governing equations directly, the LB method solves a fully-discrete kinetic equation for distribution functions (DFs) $f_i(\boldsymbol{x}, t)$, designed to reproduce the Navier–Stokes equation in the hydrodynamic limit. The LB method has advantages such as ease of parallelization, simplicity of programming, and a capability for incorporating model interactions for simulating complex flows.

A defining feature of the LB method is the coupling between the velocity and space–time discretizations. That is, for a particular discrete-velocity set, $\boldsymbol{\xi}_i$, the coupling automatically fixes the temporal and spatial steps through the relation $\Delta\boldsymbol{x} = \boldsymbol{\xi}_i \Delta t$. This procedure has some advantages such as numerical-diffusion free (exact) advection and computational efficiency (copy-operation). The coupling is, in fact, a carryover from the earliest LB models, which were based on Lattice Gas Automata (LGA). However, the LGA link was broken when it was shown more than a decade ago that the LB method can be derived directly from the discrete Boltzmann equation as a special finite-difference scheme [4–6]. Consequently, the

* Corresponding author. Tel.: +1 412 624 9720.
E-mail addresses: prr28@pitt.edu (P.R. Rao), las149@pitt.edu (L.A. Schaefer).

http://dx.doi.org/10.1016/j.jcp.2015.01.017

velocity-space can be discretized according to the flow-physics to be modeled. The discretization of space and time is a numerical requirement and, importantly, is not tied to the discretization of the velocity-space.

As a consequence, a subset of the LB method, called the off-lattice Boltzmann (OLB) method, was developed where space and time are *independently* discretized, i.e. $\Delta \boldsymbol{x} \neq \boldsymbol{\xi}_i \Delta t$. In the OLB method, we do not have the simplicity of a Lagrangian-type of evolution (streaming), rather the evolution of f_i takes place in an Eulerian sense. The earliest OLB schemes were geared mainly towards extending the geometric flexibility of the LB method, which was previously limited, due to the requirement of a uniform Cartesian mesh. Several OLB schemes with different spatial discretization methods such as finite-volume (FV), finite-element (FE), and finite-difference (FD), along with their variants, have been developed. For example, OLB schemes were used for non-uniform mesh [7], curvilinear co-ordinates [8,9], unstructured mesh [10–12], finite element mesh [13,1] among others. These advancements have made the LB method feasible for many practical engineering problems.

In addition to improving the geometric flexibility of the LB method, OLB schemes can also be used to solve the discrete Boltzmann equation (DBE) with higher-order lattices. Higher-order lattices are sets of discrete velocities, which are more suited to model more complex flows such as thermal flows, micro-scale (high Knudsen number) flows, etc. In many of these velocity sets (also termed as *non-space-filling or off-lattice*), the discrete velocities cannot be expressed as an integer multiple of the smallest non-trivial speed. The D2Q16 velocity-set listed in [6] and [14] and the D2V17n velocity-set in [15] are typical examples. Since the regular stream-collide type of evolution scheme cannot be employed with these lattices, OLB schemes provide a viable evolution scheme for the DBE.

While several sophisticated spatial-discretization methods have been developed, many of the studies use time-marching schemes such as explicit Euler or Runge–Kutta (RK) for temporal discretization. Typically, these schemes require very small values of Δt relative to the relaxation parameter τ, to maintain numerical stability [16,17]. Small Δt requirement is particularly restrictive in the case of flows with high Reynolds number (*Re*) flows where τ is very small. Moreover, in the LB method, the Mach number *Ma* in the simulations has to be kept small (generally less than 0.1) to limit the compressibility errors. Small values of *Ma* lead to a slower convergence rate, especially for steady-state flow problems [18,19]. Thus, the combined effects of small *Ma* and Δt increase the overall computational cost of the RK-based OLB schemes.

Many alternative time-marching schemes have been proposed that maintain the numerical stability of the OLB method at higher values of Δt, relative to the relaxation parameter τ, i.e. at higher $\Delta t/\tau$ values. These schemes vary greatly in their numerical stability due to the different approximations of the collision and advection part of the DBE. Hence, there is a need to systematically compare their *relative* performance in terms of the numerical stability of these schemes. This work addresses this need.

More specifically, we assess the stability of various OLB schemes, as quantified in terms of their maximum allowable $\Delta t/\tau$ ratio. This is done via benchmark testing on incompressible flow problems such as Taylor-vortex flow, Poiseuille flow and lid-driven cavity flow. The on-lattice D2Q9 velocity set, which is used here for evaluation purposes, is described in Section 2.1. The various time-marching (OLB) schemes used in the comparative analysis are described in brief in Section 2.2.

2. Numerical formulation

2.1. Discrete Boltzmann equation

The basis for all OLB schemes is the Boltzmann equation with the Bhatnagar–Gross–Krook collision approximation [20], which is given as:

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

where $f \equiv f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ is the single-particle distribution function, $\nabla f \equiv \frac{\partial}{\partial x_\alpha}$ is the spatial gradient of f, $\boldsymbol{\xi}$ is the microscale velocity, τ is the relaxation time of the collision process, and $f^{eq} = f^{eq}(\boldsymbol{x}, \boldsymbol{\xi}, t)$ is the local Maxwell–Boltzmann (equilibrium) distribution function. Eq. (1) is continuous in velocity and configuration $(\boldsymbol{x}, t)$ space. To discretize the velocity space $\boldsymbol{\xi}$, the equation is non-dimensionalized using a chosen speed of sound, and the resulting f^{eq} is expanded in a Taylor-series of fluid velocity $\boldsymbol{u}$ up to second-order. The discrete velocities are then obtained from the requirement that the lower-order hydrodynamic moments with respect to the truncated f^{eq} satisfy the conservation of mass, momentum, and energy [5,6]. Following this procedure, we obtain the widely-used discrete velocity set of the D2Q9 lattice, for which the discrete Boltzmann–BGK equation can be written as:

$$\frac{\partial f_i}{\partial t} + \boldsymbol{\xi}_i \cdot \nabla f_i = -\frac{1}{\tau}\left(f_i - f_i^{eq}\right), \tag{2}$$

where $f_i \equiv f_i(\boldsymbol{x}, \boldsymbol{\xi}_i, t)$, $f_i^{eq} \equiv f_i^{eq}(\boldsymbol{x}, \boldsymbol{\xi}_i, t)$ and $i = 0, 1, 2, \cdots, 8$. Here, while the Greek subscripts $\alpha \equiv \{x, y\}$ in 2D imply summation, the Latin subscripts (over velocity) *do not* imply summation. Eq. (2) is termed as the *discrete Boltzmann equation*