Journal of Computational Physics 228 (2009) 236–256

Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

Non-negativity and stability analyses of lattice Boltzmann method for advection–diffusion equation

Borja Servan-Camas [1], Frank T.-C. Tsai *

Department of Civil and Environmental Engineering, Louisiana State University, 3418G Patrick F. Taylor Hall, Baton Rouge, LA 70803-6405, United States

A R T I C L E I N F O

Article history:
Received 30 April 2007
Received in revised form 2 July 2008
Accepted 8 September 2008
Available online 13 September 2008

Keywords:
Lattice Boltzmann equation
Stability
BGK
Mass transport

A B S T R A C T

Stability is one of the main concerns in the lattice Boltzmann method (LBM). The objectives of this study are to investigate the linear stability of the lattice Boltzmann equation with the Bhatnagar–Gross–Krook collision operator (LBGK) for the advection–diffusion equation (ADE), and to understand the relationship between the stability of the LBGK and non-negativity of the equilibrium distribution functions (EDFs). This study conducted linear stability analysis on the LBGK, whose stability depends on the lattice Peclet number, the Courant number, the single relaxation time, and the flow direction. The von Neumann analysis was applied to delineate the stability domains by systematically varying these parameters. Moreover, the dimensionless EDFs were analyzed to identify the non-negative domains of the dimensionless EDFs. As a result, this study obtained linear stability and non-negativity domains for three different lattices with linear and second-order EDFs. It was found that the second-order EDFs have larger stability and non-negativity domains than the linear EDFs and outperform linear EDFs in terms of stability and numerical dispersion. Furthermore, the non-negativity of the EDFs is a sufficient condition for linear stability and becomes a necessary condition when the relaxation time is very close to 0.5. The stability and non-negativity domains provide useful information to guide the selection of dimensionless parameters to obtain stable LBM solutions. We use mass transport problems to demonstrate the consistency between the theoretical findings and LBM solutions.

1. Introduction

The lattice Boltzmann method (LBM) is a mesoscopic numerical method that simulates macroscopic fluid dynamics based on mesoscopic kinetic equations [1]. Developed as an improvement of the lattice gas automata (LGA) [2], the LBM has received great attention not only in hydrodynamic problems, but also in mass transport problems, e.g. the reaction–diffusion equation [3], the contaminant transport equation [4], and coupled density-dependent flow and heat/mass transfer problem [5,6]. Most studies using the LBM have focused on the lattice Boltzmann equation with the Bhatnagar–Gross–Krook collision operator [7] (LBGK), and this will be the focus of our study.

The numerical stability of the LBM still remains a challenge because it involves linear and non-linear stability. While the linear stability analysis might be sufficient to analyze stability when hydrodynamic gradients are weak, it is not sufficient in the general case where hydrodynamic gradients can lead to non-linear instabilities.

One of the earliest works that investigated the stability problem in the LBM was provided by Sterling and Chen [8], where the LBGK was linearized for the fluctuating quantities of particle distribution functions with respect to the equilibrium

* Corresponding author. Tel.: +1 225 578 4246; fax: +1 225 578 4945.
E-mail addresses: bserva1@lsu.edu (B. Servan-Camas), ftsai@lsu.edu (F.T.-C. Tsai).
[1] Tel.: +1 225 620 3296; fax: +1 225 578 4945.

0021-9991/$ - see front matter © 2008 Elsevier Inc. All rights reserved.
doi:10.1016/j.jcp.2008.09.005

distribution functions (EDFs). The von Neumann analysis was carried out to identify the most unstable directions and wave numbers, and their relationship with the mean flow field, relaxation time, and mass distribution parameters. Worthing et al. [9] extended the work of Sterling and Chen [8] to non-uniform flows. In particular, the case of a shear background flow was studied and some stability boundaries were found.

In order to improve the stability of the LBM, several approaches have been introduced. The entropic LBM (ELBM) considers that the instability arises from violating the second law of thermodynamics. Therefore, inclusion of the H theorem in the LBM was suggested to ensure positive production of entropy [10,11]. The equilibrium state in the ELBM is not explicitly needed since the collision integral can be formulated based on knowledge of the H function [12]. To ensure the implementation of the H theorem, one must first find the kinetic state after collision that does not increase entropy during the collision process, and this kinetic state fixes a limit for the new state after the collision. The ELBM provides unconditional stability [13], but was computationally expensive because the isentropic state must be obtained by solving a non-linear equation at each lattice and at every time step [14]. In Chikatamarla et al. [15], an analytical solution to the collision step was found, improving the efficiency of the ELBM.

Comparisons between the LBGK and ELBM show that the ELBM is more stable and allows increasing the Reynolds number [16]. Despite the increase of stability, the ELBM still suffers from spurious oscillations in regions with strong hydrodynamic gradients, such as shock waves [17]. However, a great reduction of the spurious oscillations in the ELBM can be achieved by selecting proper lattice velocities to retain complete Galilean invariance [18].

Improving stability can also be achieved by enforcing the non-negativity of particle distributions. Li et al. [19] introduced a FIX-UP method, which consist of increasing the relaxation time in the LBGK to the minimum value that ensured non-negativity of all particle distribution functions after the collision. Tosi et al. [20] compared the stability behavior of the ELBM and FIX-UP methods with the traditional LBGK, and both methods showed improved stability. While the computational cost is double for the ELBM with respect to the FIX-UP method in one single time step, the ELBM allows increasing the Reynolds number by about an order of magnitude, which makes the ELBM more suitable for high Reynolds number flows.

Brownlee et al. [21] introduced the idea of Enrenfests' steps, in which artificial viscosity is added by returning the particle distributions to their equilibrium states in those points where the variation of entropy between the kinetic state after the collision and the equilibrium state is superior to some threshold. This idea evolved to the concept of the entropy limiters [22], where the particles are smoothly relaxed to their equilibrium based on deviations of entropy from the equilibrium considering also the entropy deviation at the neighbor nodes.

The multi-relaxation times (MRT) method has also shown improvement on the stability of the LBM [23,24]. The main difference of the MRT over the LBGK is that all the particle distributions are not relaxed to the equilibrium state at the same rate. A particular case of MRT is the two relaxation times (TRT), which has been applied to solve mass transport equations and is capable of reducing numerical instabilities [25].

In this work, we focus on the stability of the LBM when solving the advection–diffusion equation (ADE). To our knowledge, the stability problem of using the LBGK to solve the ADE has not been fully discussed, and the aforementioned methods have mainly focused on hydrodynamics equations. To date, no clear stability boundaries have been provided for the LBGK when solving the ADE.

In this study, we carry out linear stability analysis of the LBGK and investigate the relationship between the stability of LBGK and the non-negativity of EDFs since some studies have reported that negative values of the EDFs could quickly lead to numerical instability [26,27]. Linear stability analysis is suitable and can provide insightful information when the hydrodynamic gradients are weak and the flow varies slowly in time (e.g. flows in porous media). Suga [28] carried out linear stability analysis on the LBGK for the ADE, and delineated stability boundaries for several two-dimensional lattices. However, only linear EDFs were considered and the ratio between the lattice speed and the speed of sound was constrained to a specific value, which creates a dependency among the lattice Peclet number, the Courant number, and the relaxation time. In this study, we eliminate this constraint and investigate the linear stability analysis and non-negativity of EDFs in three different lattices. We found that it is crucial for the linear stability and non-negativity analyses to identify the dimensionless parameters locally governing the LBGK.

The rest of this paper is organized as follows: Section 2 formulates the dimensionless EDFs in terms of a scaled Peclet number, Courant number, relaxation time, and flow direction. Section 3 derives non-negative domains for three different lattices and two types of EDFs. Section 4 introduces the linear stability analysis of the LBGK. Section 5 implements the linear stability analysis on the LBGK to delineate stability domains and compares them to the non-negative domains. Section 6 implements numerical examples to validate the stability and non-negativity domains found in Section 5. Section 7 concludes this study.

2. Dimensionless analysis in LBM

2.1. LBM with Bhatnagar–Gross–Krook (BGK) collision operator

The LBM was first developed to solve the equations of hydrodynamics based on the kinetic theory of gases described by the Boltzmann equation. The discrete Boltzmann equation for describing dynamics of local particle distribution functions in a discrete velocity field is