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On a superconvergent lattice Boltzmann boundary scheme[☆]

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ABSTRACT

In a seminal paper [20], Ginzburg and Adler (1994) analyzed the bounce-back boundary conditions for the lattice Boltzmann scheme and showed that it could be made exact to second order for the Poiseuille flow if some expressions depending upon the parameters of the method were satisfied, thus defining so-called "magic parameters". Using the Taylor expansion method that one of us developed, we analyze a series of simple situations (1D and 2D) for diffusion and for linear fluid problems using bounce-back and "anti bounce-back" numerical boundary conditions. The result is that "magic parameters" depend upon the detailed choice of the moments and of their equilibrium values. They may also depend upon the way the flow is driven.

1. Introduction

The theoretical analysis of the lattice Boltzmann scheme [1–7] is an active subject of research. Recall that the method was first analyzed by d'Humières [5] with a Chapman–Enskog expansion coming from statistical physics; we also refer to Asinari and Ohwada [8] for a method of analysis based on the Grad moment system. A fruitful idea followed by Junk et al. [9–11] is to use the so-called equivalent equation method derived independently by Lerat–Peyret [12] and Warming and Hyett [13] (see also [14]). An infinitesimal parameter is introduced and the finite differences operators are expanded into a family of equivalent partial differential equations. The main goal of this study is to use the Taylor expansion method [10,11] in order to increase the accuracy of boundary conditions for simple problems with analytical solutions. We first consider a one-dimensional (1D) diffusion problem and study the influence of the definition of the moments and of their equilibrium value. We then consider a two-dimensional (2D) Poiseuille flow using several ways to enforce a pressure gradient.

We consider regular lattices parametrized by a space step Δx. We introduce a time step Δt and adopt "acoustic" scaling: the ratio $\lambda \equiv \frac{\Delta x}{\Delta t}$ is a **fixed** reference velocity for each study. As a consequence, the parameters Δx and Δt are equivalent infinitesimals. Note that as this work is devoted to boundaries, we shall use a particular way to test the accuracy of a numerical scheme as will be discussed later.

2. Diffusion problem in one space dimension

We consider the classical Lattice Boltzmann model D1Q3 with three discrete velocities and one conservation law to model diffusion problems. We choose the velocities v_i $(0 \le i \le 2)$ such that $v_0 = 0$, $v_1 = \lambda$, $v_2 = -\lambda$. At each mesh point, there

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are three functions $\{f_j\}$ that can be interpreted as populations of fictitious particles. These populations evolve according to the lattice Boltzmann scheme which we write as in [10]:

$$f_j(x, t+\Delta t) = f_j^*(x - v_j \Delta t, t), \quad 0 \le j \le 2, \tag{1}$$

where the superscript $*$ denotes post-collision quantities and x a vertex of the lattice. Therefore during each time increment Δt there are two fundamental steps: advection and collision. The **advection** step describes the motion of a particle which has undergone collision at node $x - v_j \Delta t$ and goes to the jth neighboring node. Following d'Humières [5], the **collision** step is defined in the space of moments. For D1Q3 three moments $\{m_\ell\}$ are obtained by a linear transformation of vectors f_j:

$$m_0 = f_0 + f_1 + f_2 \equiv \rho(\text{density}), \qquad m_1 = \lambda(f_1 - f_2), \qquad m_2 = \frac{\lambda^2}{2}(f_1 + f_2). \tag{2}$$

In consequence, we introduce a matrix of moments M to represent moments like (2); it takes the form

$$M = \begin{pmatrix} 1 & 1 & 1 \\ 0 & \lambda & -\lambda \\ 0 & \dfrac{\lambda^2}{2} & \dfrac{\lambda^2}{2} \end{pmatrix} \tag{3}$$

and the relations (2) can be simply written as $m = Mf$. To simulate diffusion problems, we conserve only the density moment ρ in the collision step and obtain one macroscopic scalar equation. The other quantities (nonconserved moments) are assumed to relax towards equilibrium values (m_1^{eq}, m_2^{eq}) following:

$$m_\ell^* = (1 - s_\ell)\, m_\ell + s_\ell\, m_\ell^{eq}, \quad 1 \le \ell \le 2, \tag{4}$$

where s_ℓ ($0 < s_\ell < 2$, for $\ell = 1, 2$) are relaxation rates, not necessarily equal to a single value as in the BGK case [4]. The equilibrium values m_ℓ^{eq} of the nonconserved moments in Eq. (4) determine the macroscopic behavior of the scheme. Indeed with the following choice of equilibrium values (neglecting nonlinear contributions):

$$m_1^{eq} = 0, \qquad m_2^{eq} = \zeta \frac{\lambda^2}{2} \rho \tag{5}$$

and using the Taylor expansion method we find (see e.g. [15]) that the equivalent partial differential equation of the numerical scheme up to order three in Δx is a diffusion equation:

$$\frac{\partial \rho}{\partial t} - \kappa \frac{\partial^2 \rho}{\partial x^2} = \mathrm{O}(\sigma_1 \Delta x^3). \tag{6}$$

The value of the diffusivity κ is given according to

$$\kappa = \Delta t \lambda^2 \sigma_1 \zeta \tag{7}$$

where $\sigma_\ell \equiv \frac{1}{s_\ell} - \frac{1}{2}$, $\ell = 1, 2$.

Remark that the thermal diffusivity κ is imposed by the Physics. Moreover the scale velocity λ is fixed and the coefficient ζ is also imposed. When we refine the mesh, the coefficient σ_1 must be chosen in order to enforce relation (7). In other terms, the product $\sigma_1\, \Delta t$ must be maintained constant. Then the right hand side of relation (6) exhibits a **second order truncation error** of the lattice Boltzmann scheme for a **given** thermal diffusivity κ. Associated with stability properties (see Junk and Yong [16]), convergence properties of lattice Boltzmann scheme can be established, as in [17].

3. Localization of a 1D boundary

Let us introduce a constant c and consider the following 1D Poisson problem:

$$-\mathbf{K}\frac{\mathrm{d}^2 \rho}{\mathrm{d}x^2} = c \quad \text{in }]0, 1[, \qquad \rho(0) = \rho(1) = 0. \tag{8}$$

We take an "anti bounce-back" numerical boundary condition at $x = 0$:

$$f_1(x_b, t+\Delta t) = -f_2(x_e, t+\Delta t) = -f_2^*(x_b, t), \tag{9}$$

with x_b the fluid node and x_e the external node as presented in Fig. 1, and a similar condition for $x = 1$. A uniform body source (δp) is added to the Boltzmann scheme to model the right hand side c of Eq. (8). So we can write the lattice Boltzmann scheme as follows: (i) $m = Mf$, (ii) $\widetilde{m}_0 = m_0 + \frac{1}{2}\delta p$, (iii) evaluate the other moments, (iv) relaxation (4) of the other moments, (v) $\widetilde{m}_0 = m_0 + \frac{1}{2}\delta p$, (vi) $f = M^{-1} m$, (vii) advection step (1) and boundary conditions. The exact solution of problem (8) is elementary: $u(x) = \frac{c\,x\,(1-x)}{2\,\mathrm{K}}$. We analyze the behavior of the discrete model to show whether it can be tuned so that the location of the "numerical boundary" can be fixed at mid-point as expected from "anti bounce-back". Thus we shall use as criterion for accuracy the difference between the imposed boundary and the "numerically determined" boundary.