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To cite this article: A. Renda *et al* 1998 *EPL* **41** 279

EUROPHYSICS LETTERS 1 February 1998

Europhys. Lett., **41** (3), pp. 279-283 (1998)

Thermohydrodynamic lattice BGK schemes with non-perturbative equilibria

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(received 18 September 1997; accepted in final form 1 December 1997)

PACS. 47.11+j – Computational methods in fluid dynamics.
PACS. 05.20Dd – Kinetic theory.

Abstract. – A new class of lattice BGK models is proposed which is based on a non-perturbative discrete Maxwellian ansatz for the local equilibria. This new class extends the range of stability of previous models.

In the recent years, the Lattice Boltzmann (LB) and the Lattice BGK (LBGK) models have raised a considerable interest for the simulation of complex hydrodynamic phenomena, ranging from single and multiphase flows in periodic and bounded geometries [1], [2]. The main drivers behind LBGK methods are: i) physical soundness, ii) handy treatment of complex boundary conditions, and iii) outstanding amenability to parallel computing. In spite of its undeniable success, there are two main aspects of the LBGK method which call for further developments: a) extension to nonuniform, generalized coordinates, and b) nonlinear stability in the thermohydrodynamic regime. In this letter we present a contribution to the latter item.

The LBGK method is based on the following set of equations:

$$f_i(\mathbf{x}+\mathbf{c}_i, t+1) - f_i(\mathbf{x}, t) = -\omega[f_i(\mathbf{x}, t) - f_i^{\mathrm{eq}}(\mathbf{x}, t)], \tag{1}$$

where f_i is the probability of finding a fluid particle at the site $\mathbf{x}$ and time t with the speed $\mathbf{c}_i$. The set of discrete speeds $[\mathbf{c}_i,\ i = 1, \ldots, b]$ must be chosen in such a way that the tensor $\sum_i \mathbf{c}_i\mathbf{c}_i\mathbf{c}_i\mathbf{c}_i$ be isotropic. Otherwise, eq. (1) would not reproduce the Navier-Stokes equations in the continuum limit.

The right-hand side of eq. (1) represents a discrete version of the well-known BGK collision operator [3], [4], where ω is a free parameter (the inverse relaxation time). This parameter controls the relaxation of the discrete distribution function f_i to its local thermodynamic equilibrium f_i^{eq}. At the same time, ω controls the fluid viscosity ν via the relation $\nu = 2T(\omega^{-1} - 2^{-1})$, where T is the temperature.

This local equilibrium plays a pivotal role in the theory of the LBGK methods. First, it must secure the correct mass, momentum and energy conservations

$$\begin{cases} \sum_i f_i^{\mathrm{eq}} = \rho, \\ \sum_i f_i^{\mathrm{eq}} \mathbf{c}_i = \rho \mathbf{u}, \\ \sum_i f_i^{\mathrm{eq}} c_i^2 = \rho(u^2 + DT), \end{cases} \tag{2}$$

where ρ, $\mathbf{u}$, and T are the fluid mass, speed and temperature, respectively, and D is the spatial dimension. The number of conservation laws will be denoted as $N = D + 2$. Second, the local equilibrium must ensure the correct form of the pressure tensor, $\sum_i f_i^{\mathrm{eq}} \mathbf{c}_i \mathbf{c}_i = p\mathsf{I} + \mathbf{u}\mathbf{u}$, where $p = \rho T$ is the scalar pressure, and I is the unit tensor.

At first glance, the most natural choice for f_i^{eq} would fall on the discrete version of a local Maxwellian:

$$f_i^{\mathrm{eq}} = (2\pi T)^{-D/2} \exp[-(2T)^{-1}(\mathbf{c}_i - \mathbf{u})^2]. \tag{3}$$

The problem with this expression is that, owing to the finite number of discrete speeds, eq. (3) does not fulfill the conservation laws, eq. (2). The conventional way out of this problem is to replace the function f_i^{eq} (3) by an expansion in powers of the local Mach number, $M = u/c_{\mathrm{s}}$, where c_{s} is the sound speed. For isothermal, incompressible flows, the second-order expansion is enough to recover the Navier-Stokes equations. However, for thermal and/or compressible flows, terms up to $O(M^4)$ are required. This implies an extension of the discrete speeds stencil $\{\mathbf{c}_i\}$ and a corresponding proliferation of Lagrange multipliers in the expression of f_i^{eq}, eq. (3).

The main advantage of truncated Maxwellian equilibria is that they can be precomputed at the outset, once and for all, as a function of the local hydrodynamic fields, ρ, $\mathbf{u}$, and T. This makes the LBGK scheme very efficient from the computational point of view.

The downside is that, at variance with the full-Maxwellians, truncated equilibria are positive definite only within some subset $\Omega^{\mathrm{eq}} \subset \mathcal{H}$, where $\mathcal{H}$ is the hydrodynamic space spanned by ρ, $\mathbf{u}$, and T. This problem is relatively harmless for "cold" incompressible computations, but becomes much more disturbing —according to most authors— whenever compressibility and especially temperature dynamics have to be accounted for [5].

In this letter we suggest a new class of equilibria which may considerably soften this problem. The idea is as follows: for a system with a *finite* number of velocities, the constraints, eq. (2), can be precomputed in such a way that N equilibrium populations (primary equilibria) will be expressed in terms of the hydrodynamic fields, and in terms of the $b - N$ remaining equilibrium populations (secondary equilibria). Further, the full, unexpanded, discrete Maxwellian form (3) is suggested as an ansatz to deliver the closure of the secondary equilibria in terms of the hydrodynamic fields.

We will illustrate this idea with the one-dimensional five-speed model (1D5V) [6]. The 1D5V model contains five discrete velocities: $c_0 = 0$, $c_{1+} = 1$, $c_{1-} = -1$, $c_{2+} = 2$, and $c_{2-} = -2$. These velocities correspond to three energy levels: $\epsilon_0 = 0$ (c_0), $\epsilon_1 = 1/2$ (c_{1+} and c_{1-}), and $\epsilon_2 = 2$ (c_{2+} and c_{2-}). The number of equilibrium populations is five, the number of conservation laws, eq. (2), is three.

For the primary equilibria, we take the low-energy populations f_0^{eq}, f_{1+}^{eq}, and f_{1-}^{eq}. The closure ansatz is done in two steps. First, we write the high-energy equilibria, $f_{2\pm}^{\mathrm{eq}}$ as a fraction of the low-energy populations $f_{1\pm}^{\mathrm{eq}}$:

$$f_{2\pm}^{\mathrm{eq}} = \lambda_{\pm} f_{1\pm}^{\mathrm{eq}}, \tag{4}$$

where $\lambda_{\pm} \geq 0$. Substituting eq. (4) into the system of constraints, eq. (2), we come to a 3×3 linear system for the primary equilibria:

$$\begin{aligned} f_0^{\mathrm{eq}} + (1+\lambda_+) f_{1+}^{\mathrm{eq}} + (1+\lambda_-) f_{1-}^{\mathrm{eq}} &= \rho, \\ (1+2\lambda_+) f_{1+}^{\mathrm{eq}} - (1+2\lambda_-) f_{1-}^{\mathrm{eq}} &= \rho u, \\ (1+4\lambda_+) f_{1+}^{\mathrm{eq}} + (1+4\lambda_-) f_{1-}^{\mathrm{eq}} &= \rho(u^2+T). \end{aligned}$$

The solution to this system reads

$$\begin{cases} f_{1+}^{\mathrm{eq}} = \rho \dfrac{(1+4\lambda_-)u + (1+2\lambda_-)(u^2+T)}{(1+2\lambda_+)(1+4\lambda_-) + (1+2\lambda_-)(1+4\lambda_+)}, \\[2ex] f_{1-}^{\mathrm{eq}} = \rho \dfrac{(1+2\lambda_+)(u^2+T) - (1+4\lambda_+)u}{(1+2\lambda_+)(1+4\lambda_-) + (1+2\lambda_-)(1+4\lambda_+)}, \\[2ex] f_0^{\mathrm{eq}} = \rho - (1+\lambda_+) f_{1+}^{\mathrm{eq}} - (1+\lambda_-) f_{1-}^{\mathrm{eq}}. \end{cases} \tag{5}$$

Second, the factors $\lambda_{\pm}$ are subject to the Maxwellian closure (3). Specifically, we substitute the expression (3) for the functions $f_{2\pm}^{\mathrm{eq}}$ and $f_{1\pm}^{\mathrm{eq}}$ in eq. (4), and derive

$$\lambda_{\pm} = \exp\left[-\frac{(c_{2\pm}-u)^2 - (c_{1\pm}-u)^2}{2T} \right]. \tag{6}$$

Thus, eqs. (4), (5), and (6) specify all the five equilibrium populations unambiguously in terms of the hydrodynamic fields. We further refer to the LBGK model with the Maxwellian closure (6) as to the MBGK model.

The positivity domain of the equilibrium populations defined by eqs. (5) and (6) was found to be considerably wider than that of the conventional LBGK model [6]. To compare the stability of the MBGK with the LBGK, we have performed simulations of the Riemann problem, the 1D propagation of an initial pressure-density discontinuity. All simulations have been performed with $\omega = 1.0$ on a 2000-point grid, in the domain where both the LBGK and the MBGK models have positive equilibrium. Here we represent the typical results for the two sets of initial conditions:

Case 1:

$$u_{\mathrm{L}} = 0.0, \quad P_{\mathrm{L}} = 1.0, \quad \rho_{\mathrm{L}} = 1.6,$$

$$u_{\mathrm{R}} = 0.0, \quad P_{\mathrm{R}} = 0.25, \quad \rho_{\mathrm{R}} = 0.7;$$

Case 2:

$$u_{\mathrm{L}} = 0.0, \quad P_{\mathrm{L}} = 1.0, \quad \rho_{\mathrm{L}} = 1.6,$$

$$u_{\mathrm{R}} = 0.0, \quad P_{\mathrm{R}} = 0.13, \quad \rho_{\mathrm{R}} = 0.4.$$

Here L and R refer to the quantities on the left and on the right of the initial density and pressure (P) discontinuity in the Riemann problem.

The pressure profiles for the case 1 are shown in fig. 1. The analytical solution is reported for the sake of comparison. As we see, both methods demonstrate a nice agreement with the analytical solution.

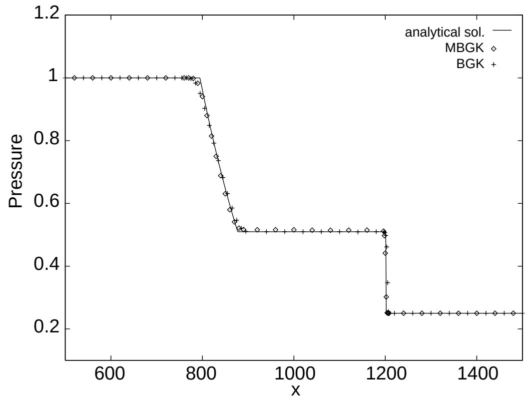

Fig. 1

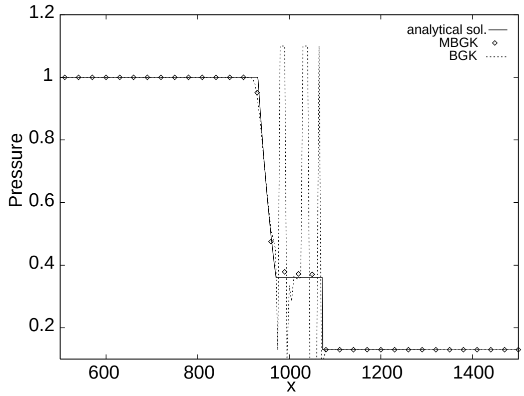

Fig. 2

Fig. 1. – Pressure profiles for the Riemann problem after 150 time steps: Case 1.
Fig. 2. – Pressure profiles for the Riemann problem after 40 time steps: Case 2.

However, for the case 2, the MBGK performs much better than the LBGK (see fig. 2). Here one sees clearly that the LBGK simulation goes unstable in the central region, while the MBGK keeps on sticking to the analytical solution quite smoothly everywhere except in the front of the expansion fan (pressure drop from 1 to about 0.4). This is a typical example of the superiority in the nonequilibrium regime of the MBGK method. To date, we have no evidence of situations where LBGK is stable and MBGK is not. We close this letter with a number of comments.

There are several motivations behind our approach. The first point concerns the choice of primary and secondary equilibria. The choice made above implements the following idea: the low-energy "core" of the equilibrium population at each lattice site is mostly responsible for an adequate account of the conservation laws. We require that the high-energy "tail" of the population be a smooth function of the core, such that if the core is positive so is the tail.

The second point concerns the origin of the Maxwellian closure. The true discrete local Maxwell equilibrium distribution maximizes the entropy $S = -\sum_i f_i \ln f_i$, subject to the constraints (2). The solution to this problem, in terms of the Lagrange multipliers, reads: $f_i^{\mathrm{M}} = A\exp[-b(c_i - \mathbf{v})^2]$. The functions A, b, and $\mathbf{v}$ do not have a simple expression in terms of the hydrodynamic fields, as in eq. (3) (in particular, $b \neq (2T)^{-1}$, and $\mathbf{v} \neq \mathbf{u}$). However, in the framework of the 1D5V model, we can write an exact relation:

$$f_{2\pm}^{\mathrm{M}}/f_{1\pm}^{\mathrm{M}} = \exp[-b(c_{2\pm} - v)^2 + b(c_{1\pm} - v)^2].$$

Since the conservation laws are satisfyed in the exact solution (5), they will be not violated by assigning the values $b = (2T)^{-1}$ and $v = u$ in the latter expression to give the closure (6).

The procedure outlined above can be extended to higher dimensions. The distinction between the primary and the secondary equilibria populations depends on the geometry of a lattice, and should be considered separately in each case. Results for the 2D16V model [6] are currently in preparation.

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We are grateful to an anonymous referee for his useful comments. SS acknowledges stimulating discussions with S. Chen, S. Orszag, A. Wagner, and J. Yeomans. IVK acknowledges the support of the Italian Research Council (CNR), and of the RFBR (Grant No. 95-02-03836-a).

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