

Taylor expansion method for linear lattice Boltzmann schemes with an external drift. Application to boundary conditions

François Dubois, Pierre Lallemand, Mohamed Mahdi Tekitek

► To cite this version:

François Dubois, Pierre Lallemand, Mohamed Mahdi Tekitek. Taylor expansion method for linear lattice Boltzmann schemes with an external drift. Application to boundary conditions. EUROPEAN WORKSHOP on High Order Nonlinear Numerical Methods for Evolutionary PDEs., Mar 2013, Bordeaux, France. pp.350. hal-00864541v1

HAL Id: hal-00864541 https://hal.science/hal-00864541v1

Submitted on 23 Sep 2013 (v1), last revised 3 Dec 2014 (v2)

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Taylor expansion method for linear lattice Boltzmann schemes with an external drift. Application to boundary conditions

François Dubois^{1,2}, Pierre Lallemand³ and Mohamed-Mahdi Tekitek^{4,*}

¹ CNAM Paris, Department of Mathematics and LMSSC, France.

² Department of Mathematics, University Paris Sud, Orsay, France.

³ Centre National de la Recherche Scientifique, Paris, France.

⁴ Université El Manar, Faculté des Sciences de Tunis, Tunis, Tunisie.

francois.dubois@math.u-psud.fr, pierre.lallemand1@free.fr, mohamedmahdi.tekitek@fst.rnu.tn * corresponding author.

31 May 2013 *

Abstract

This contribution is divided into two parts. In the first part, we show that it is possible to get the macroscopic fluid equations of a lattice Boltzmann scheme with an external force using the Taylor expansion method. In a second part, we validate this general expansion by a detailed application to boundary conditions. We precise the result for quartic condition for Poiseuille flow with an external drift with the D2Q13 scheme.

Key words : LBM, Poiseuille flow, thermal, force term, bounce-back, anti-bounce-back.

PACS numbers : 02.60Cb (numerical simulation, solution of equations), 43.20.+g (General linear acoustics), 47.10.+g (Navier-Stokes equations).

^{*} This contribution has been presented by Mohamed-Mahdi Tekitek at the conference "HONOM", INRIA, Bordeaux, 18-22 March 2013. Edition 12 August 2013.

1) Lattice Boltzmann method

• The Lattice Boltzmann scheme is a mesoscopic method. It deals with a small number of functions $\{f_i\}$ that can be interpreted as populations of fictitious particles. It has been developed more than 20 years ago by Qian *et al.* [11], Succi *et al.* [12] among others. This method can simulate various fluid dynamics problems. In the following, the notation "DdQq" denotes a lattice Boltzmann scheme with d space dimensions and q dicrete velocities. Space is descretized by a regular lattice \mathcal{L} parametrized by a spatial scale Δx . The time step is denoted by Δt . A numerical celerity λ is naturally defined by $\lambda \equiv \frac{\Delta x}{\Delta t}$. The q discrete velocities can be written as $v_j = \lambda e_j$ for $0 \leq j \leq q-1$. A classical example is given by the D2Q9 scheme illustrated on the Figure 1.



Figure 1. Stencil for the D2Q9 lattice Boltzmann scheme.

• The lattice Boltzmann scheme is formulated in both spaces of particles and moments m_k , proposed by d'Humières [8]. We introduce an invertible matrix $M = (M_{kj})$ for $0 \le k, j \le q-1$. Then the moments m_k for $0 \le k \le q-1$ are defined by linearity: $m_k \equiv \sum_j M_{kj} f_j$. The moment vector is composed of two kinds of quantities: the first one of conserved moments $V \in \mathbb{R}^N$ which are not affected by the collision step when there is no forcing term. If N = 1 we have exactly one scalar Partial Differential Equation. If N > 1 we study an underlying of N PDEs. The second one of non conserved moments Y relax during the collision step. So the moment vector $m \in \mathbb{R}^q$ can be written as

(1)
$$m = \begin{pmatrix} V \\ Y \end{pmatrix}.$$

An elementary time evolution of a lattice Boltzmann scheme with a force is composed by four steps (see Guo *at al.* [6]) : computation of the dynamical variables, collision (through simple relaxation), forcing of the conserved moments and advection.

• The computation of the dynamical variables W from the first component V of the moments (1), is given by:

(2)
$$W = V + \theta \Delta t F,$$

where θ is a fixed scalar in]0,1[and $F \in \mathbb{R}^N$ is a given drift term. Remark that the post-processing in this contribution is obtained from the knowledge of these dynamical variables.

TAYLOR EXPANSION METHOD WITH AN EXTERNAL DRIFT

• The collision and relaxation step is a redistribution of the populations $\{f_i\}$ at each node x. The N first moments W are not affected by the relaxation. The other "nonconserved" moments relax with a time constant τ_k towards the equilibrium values m_k^{eq} . where θ is a fixed scalar in]0, 1[and F is a given drift term. This equilibrium value is only fonction of the conserved variables W. In this contribution, we suppose that the equilibrium values Y^{eq} of the non-conserved moments are linear function of dynamical variables. We have

$$Y^{eq} = E W,$$

where E is a fixed matrix with q - N lines and N columns. Thus the relaxation is simply described by an ordinary differential equation: $\frac{d}{dt}(m_k - m_k^{eq}) + \frac{1}{\tau_k}(m_k - m_k^{eq}) = 0$ for $k \ge N$. Using an explicit first order Euler scheme, we obtain the algorithm:

(4)
$$m_k^* = (1 - s_k) m_k + s_k m_k^{eq},$$

where the superscript * indicates "post-collision" state and where the relaxation rates $s_k \equiv \frac{\Delta t}{\tau_k}$ have to satisfy $0 < s_k < 2$ in order to maintain stability of the scheme. With the notation (1) the relaxation step is performed in the moment space as follows:

(5)
$$Y^* = (\mathrm{Id} - S)Y + SY^{eq},$$

where S is the diagonal matrix of the relaxation times s_k for $k \ge N$. We remark that this collision step is local in space.

• Due to the force term, the conserved moments during the collision step, evolve according to

(6)
$$V^* = V + \Delta t F.$$

If ()^t denotes the transpose of the matrix (), the moments $m^* \equiv (V^*, Y^*)^{t}$ after collision are determined by the relations (5) and (6). After the forcing and collision steps, the particle distribution f_j^* is recovered by the inversion of a linear system of small size: $f_j^* = \sum_k M_{jk}^{-1} m_k^*$.

• The advection step corresponds to a method of characteristics with CFL= 1 for the advection with velocity v_j . The particles moves from a lattice node x to either itself (for $v_0 = 0$) or one of the q - 1 neighbors $x_j = x + v_j \Delta t$ for velocities $v_j \neq 0$ as presented in the Figure ??. We assume here that for each node x and each velocity v_j , the vertex $x - v_j \Delta t$ is also a node of the lattice. So a time step of a lattice Boltzmann scheme can be written as:

(7)
$$f_i(x, t + \Delta t) = f_i^*(x - v_i \Delta t, t), \quad 0 \le i \le q - 1, \ x \in \mathcal{L},$$

where f_i^* denotes the post-collision population of particles evaluated at the end of the previous step.

F. DUBOIS, P. LALLEMAND AND MM. TEKITEK.

2) Taylor expansion for equivalent equation

• In this contribution, we extend the "Berliner version" [1] of the Taylor expansion method in order to derive macroscopic equivalent equations when an external forcing term is present. We suppose here that the dynamical variables W satisfy a partial differential equation:

(8)
$$\partial_t W = \alpha_1 W + \Delta t \ \alpha_2 W + \Delta t^2 \ \alpha_3 W + \dots + \gamma_0 F + \Delta t \ \gamma_1 F + \dots$$

and the non conserved moments Y follow a dynamical variables of the type

(9)
$$Y = E W + \Delta t \beta_1 W + \Delta t^2 \beta_2 W + \dots + \Delta t \rho_0 F + \Delta t^2 \rho_1 F + \dots$$

Note here that the equation (8) will give the macroscopic (equivalent) equation of the physical problem. The equation (9) gives the expansion of the non conserved moments in function of the conserved quantities.

• The operators α_j and β_j are space partial differential operators of order j. Due to (5), we first write the collision step as follows: $Y^* = (\mathrm{Id} - S) Y + S Y^{eq} = (\mathrm{Id} - S) Y + S E W$ due to (3). Then, according to the relation (2), we have $Y^* = (\mathrm{Id} - S) Y + S E (V + \Delta t \theta F)$ = $S E V + (\mathrm{Id} - S)Y + \Delta t \theta S E F$.

Then the moments m^* after forcing and relaxation can be presented as follows:

(10)
$$m^* = \begin{pmatrix} V^* \\ Y^* \end{pmatrix} = \begin{pmatrix} I & 0 \\ SE & I-S \end{pmatrix} \begin{pmatrix} V \\ Y \end{pmatrix} + \Delta t \begin{pmatrix} I \\ \theta SE \end{pmatrix} F.$$

Secondly, we rewrite the scheme (7) in moment space:

$$\begin{pmatrix} V \\ Y \end{pmatrix}_{k} (x, t + \Delta t) = m_{k}(x, t + \Delta t) = \sum_{j,l} M_{k,j} M_{j,l}^{-1} m_{l}^{*}(x - v_{j}\Delta t, t)$$
$$= \sum_{j,l,\alpha} M_{k,j} M_{j,l}^{-1} (-v_{j})^{\alpha} \frac{\Delta t^{|\alpha|}}{\alpha!} \partial_{\alpha} m_{l}^{*}(x, t)$$

and we inject the value (10) of m^* in the previous expression. We arrange the previous formal series as increasing powers of Δt . We obtain the following equation:

(11)
$$\begin{pmatrix} V \\ Y \end{pmatrix} (t + \Delta t) = \sum_{n \ge 0} \Delta t^n \begin{pmatrix} A_n & B_n \\ C_n & D_n \end{pmatrix} \begin{pmatrix} V \\ Y \end{pmatrix} (t) + \sum_{n \ge 0} \Delta t^{n+1} \begin{pmatrix} G_n \\ H_n \end{pmatrix} F.$$

The order zero of the development (11) relative to Δt is deduced from (10) by identification:

(12)
$$\begin{pmatrix} A_0 & B_0 \\ C_0 & D_0 \end{pmatrix} = \begin{pmatrix} I & 0 \\ SE & I-S \end{pmatrix}, \quad \begin{pmatrix} G_0 \\ H_0 \end{pmatrix} = \begin{pmatrix} I \\ \theta SE \end{pmatrix}.$$

• Proposition 1. Taylor expansion at order 1.

The equivalent equations and the non conserved moments for linear lattice Boltzmann scheme with external force up to first order are given by the relations

(13)
$$\partial_t W = \alpha_1 W + \gamma_0 F + O(\Delta t), \quad Y = E W + \Delta t \left(\beta_1 W + \rho_0 F\right) + O(\Delta t^2)$$

with

(14)
$$\begin{cases} \alpha_1 = A_1 + B_1 E, & \beta_1 = S^{-1} (C_1 + D_1 E - E \alpha_1), \\ \gamma_0 = G_0 = I, & \rho_0 = S^{-1} (H_0 - E \gamma_0 - \theta S E). \end{cases}$$

Proof of Proposition 1.

We have from (11) and (12) $V(t + \Delta t) = V + \Delta t \ \partial_t V + O(\Delta t^2) = V + \Delta t (A_1 V + B_1 Y)$ + $\Delta t \ G_0 F + O(\Delta t^2)$ and $Y(t + \Delta t) = Y + \Delta t \ \partial_t Y + O(\Delta t^2) = (Id - S) Y + S E V + \Delta t (C_1 V + D_1 Y) + \Delta t \ H_0 F + O(\Delta t^2)$. Using the relation (2) we have $V = W - \theta \Delta t F$ and the development at equilibrium (order zero) $Y = E W + O(\Delta t)$, we obtain on one hand $\partial_t W = (A_1 + B_1 E) W + G_0 F + O(\Delta t)$ and on the other hand

$$Y = EW + \Delta t \, S^{-1} \left[C_1 + D_1 E - E \left(A_1 + B_1 E \right) W \right] + \left(H_0 - E \gamma_0 - \theta \, S \, E \right) F + \mathcal{O}(\Delta t^2) \,.$$

By identification of the previous relations with the Ansatz (8)(9), we obtain the relations (13) at first order with the coefficients α_1 , β_1 , γ_0 and ρ_0 explicited in (14).

• Proposition 2. Taylor expansion at order 2.

The equivalent equations for linear lattice Boltzmann scheme with external force, as described in first section, up to second order, are:

(15)
$$\begin{cases} \partial_t W = \alpha_1 W + \gamma_0 F + \Delta t \left(\alpha_2 W + \gamma_1 F \right) + \mathcal{O}(\Delta t^2) \\ Y = E W + \Delta t \left(\beta_1 W + \rho_0 F \right) + \Delta t^2 \left(\beta_2 W + \rho_1 F \right) + \mathcal{O}(\Delta t^3) \end{cases}$$

with coefficients α_1 , β_1 , γ_0 and ρ_0 proposed in (14) and

(16)
$$\begin{cases} \alpha_2 = B_1 \beta_1 + A_2 + B_2 E - \frac{1}{2} \alpha_1^2 \\ \gamma_1 = B_1 \rho_0 + G_1 - \theta A_1 - \frac{1}{2} [\alpha_1 \gamma_0 + (\gamma_0 - 2\theta) \partial_t] \\ \beta_2 = S^{-1} [D_1 \beta_1 - E \alpha_2 - \beta_1 \alpha_1 - E \frac{\alpha_1^2}{2} + C_2 + D_2 E] \\ \rho_1 = S^{-1} [D_1 \rho_0 + H_1 - E \gamma_1 - \beta_1 \gamma_0 - \frac{1}{2} E \alpha_1 \gamma_0 - \frac{1}{2} E \gamma_0 \partial_t - \rho_0 \partial_t - \theta C_1]. \end{cases}$$

Proof of Proposition 2.

We first differentiate relative to time the first relation of (13): $\partial_t^2 W = \partial_t (\alpha_1 W + F) + O(\Delta t) = \alpha_1 (\alpha_1 W + F) + \partial_t F + O(\Delta t) = \alpha_1^2 W + (\alpha_1 + \partial_t) F + O(\Delta t).$ We can therefore develop the dynamical variables W at time $t + \Delta t$ up to second order. Due to the definition (2), we have:

$$W(t + \Delta t) = V(t + \Delta t) + \theta \Delta t F(t + \Delta t)$$

= $V(t) + \Delta t \left(A_1 V(t) + B_1 Y(t)\right) + \Delta t^2 \left(A_2 V(t) + B_2 Y(t)\right) + \theta \Delta t F(t + \Delta t) + O(\Delta t^3)$
= $W(t) - \theta \Delta t F(t + \Delta t) + \theta \Delta t F(t + \Delta t) + \Delta t \left(A_1 (W - \theta \Delta t F) + B_1 (E W + \Delta t \beta_1 W + \Delta t \rho_0 F)\right) + \Delta t^2 \left(A_2 W + B_2 E W\right) + O(\Delta t^3).$

Then taking into account the Taylor formula at second order accuracy and the expression of $\partial_t^2 W$:

$$W + \Delta t \,\partial_t W + \frac{\Delta t^2}{2} \left(\alpha_1^2 W + (\alpha_1 + \partial_t) F + \mathcal{O}(\Delta t^3) = W - \theta \,\Delta t^2 \,\partial_t F + \Delta t \left(A_1 W + B_1 E W \right) + \Delta t^2 \left(-\Delta t F + B_1 \beta_1 W + B_1 \rho_0 F + A_2 W + B_2 E W \right) + \mathcal{O}(\Delta t^3).$$

After dividing by Δt :

$$\partial_t W = (A_1 + B_1 E) W + F + \Delta t \left[(A_2 + B_2 E + B_1 \beta_1 - \frac{1}{2} \alpha_1^2) \right] W + \Delta t \left[(G_1 + B_1 \rho_0 - \theta A_1 - \frac{1}{2} \alpha_1 + (\theta - \frac{1}{2}) \partial_t) F \right] + O(\Delta t^2)$$

and the expressions of α_2 and γ_1 in (16) are established.

• For establish the second set of relations of (15), we first look to the derivation relative to time of the non-conserved moments Y. We have

$$\begin{split} \partial_t Y &= \partial_t \left[E \, W + \Delta t \left(\beta_1 \, W + \rho_0 \, F \right) \right] + \mathcal{O}(\Delta t^2) \\ &= E \left[\alpha_1 \, W + F + \Delta t \left(\alpha_2 \, W + \gamma_1 \, F \right) + \mathcal{O}(\Delta t^2) \right] \\ &+ \Delta t \, \beta_1 \left(\alpha_1 \, W + F \right) + \Delta t \, \rho_0 \, \partial_t \, F + \mathcal{O}(\Delta t^2) \\ &= E \left(\alpha_1 \, W + F \right) + \Delta t \left[(E \, \alpha_2 + \beta_1 \, \alpha_1) \, W + (E \, \gamma_1 + \beta_1 + \rho_1 \, \partial_t) \, F \right] + \mathcal{O}(\Delta t^2) \, . \end{split}$$

We differentiate relative to time at second order:
$$\partial_t^2 Y &= \partial_t \left[E \left(\alpha_1 \, W + F \right) \right] + \mathcal{O}(\Delta t) = E \, \alpha_1 \left(\alpha_1 \, W + F \right) + E \, \partial_t \, F + \mathcal{O}(\Delta t) = E \, \alpha_1^2 \, W + (E \, \alpha_1 + E \, \partial_t) \, F + \mathcal{O}(\Delta t) \, . \end{split}$$

$$(E \, \alpha_1 + E \, \partial_t) \, F + \mathcal{O}(\Delta t) \, . \end{split}$$

$$SY(t) &= S \, E \, V - \left(Y (t + \Delta t) - Y (t) \right) + \Delta t \, (C_1 \, V + D_1 \, Y + \theta \, S \, E \, F) \right. \\ &+ \Delta t^2 \left(C_2 \, V + D_2 \, Y + H_1 \, F \right) + \mathcal{O}(\Delta t^3) \\ = S \, E \left(W - \theta \, \Delta t \, F \right) - \Delta t \left[E \left(\alpha_1 \, W + F \right) + \Delta t \left[(E \, \alpha_2 + \beta_1 \, \alpha_1) \, W + (E \, \gamma_1 + \beta_1 + \rho_1 \, \partial_t) \, F \right] \right. \\ &- \left. \frac{\Delta t^2}{2} \left[E \, \alpha_1^2 \, W + (E \, \alpha_1 + E \, \partial_t) \, F \right] + \Delta t \left[C_1 \left(W - \theta \, \Delta t \, F \right) + D_1 \left(E \, W + \Delta t \, \beta_1 \, W \right) \right] \right. \\ &+ \Delta t \, \rho_0 \, F \right) + \theta \, S \, E \, F \right] + \Delta t^2 \left(C_2 \, W + D_2 \, E \, W + H_1 \, F \right) + \mathcal{O}(\Delta t^3) \end{split}$$

$$= S \left[E W + \Delta t \beta_1 W + \Delta t \rho_0 F \right] + \Delta t^2 \left[\left(C_2 + D_2 E + D_1 \beta_1 - \frac{1}{2} E \alpha_1^2 - (E \alpha_2 + \beta_1 \alpha_1) \right) W + \left(H_1 + D_1 \rho_0 - \theta C_1 - \frac{1}{2} (E \alpha_1 + E \partial_t) - (E \gamma_1 + \beta_1 + \rho_0 \partial_t) \right) F \right] + O(\Delta t^3)$$

and the expressions of β_2 and ρ_1 proposed at the second line of the relations (16) are established because γ_0 is the identity matrix.

3) Application to boundary condition

• Boundary conditions are performed to impose a given velocity (or a given pressure) on somea given part of the physical boundary. These conditions have to be translated in terms of the numerical scheme. In general there is a difference between the assumed wall position and the "measured" one. For some particular lattice Boltzmann parameters, this difference is null up to order two on Δx . This defines so-called "quartic" parameters (see [3]). For the general framework of this kind of methodology, we refer to Ginzburg and Adler [4], Ginzburg *et al.* [5] and Ginzburg and d'Humières [9]. In this section, we study the impact of the knowledge given in the relations (15)(16) on the analysis of the boundary conditions for the lattice Boltzmann schemes. We focus on the D1Q3 scheme for a scalar problem and the D2Q9 and D2Q13 schemes for the linearized fluid.



Figure 2. Stencil of the lattice Boltzmann scheme D1Q3.

• D1Q3 for a thermics model problem.

We introduce the following matrix moment M for the D1Q3 lattice Boltzmann scheme:

D1Q3:
$$M = \begin{pmatrix} 1 & 1 & 1 \\ 0 & \lambda & -\lambda \\ -2\lambda^2 & \lambda^2 & \lambda^2 \end{pmatrix}$$
.

We consider only one conservation law (N = 1) and we set $\rho = W = f_0 + f_1 + f_2$. The equilibrium values Y^{eq} of the two non-conserved moments are given according to $Y^{eq} = E \rho$ with $E = (0, \lambda^2 \zeta)^{\text{t}}$. • Proposition 3. Diffusion model with the D1Q3 lattice Boltzmann scheme. With the previous lattice Boltzmann D1Q3 scheme, we have the equivalent equation $\frac{\partial \rho}{\partial t} - \kappa \frac{\partial^2 \rho}{\partial x^2} - F = O(\Delta t^2)$ at second order for a stationary force F, with the thermal diffusivity $\kappa = \frac{2+\zeta}{3} \Delta t \lambda^2 \sigma_1$ and $\sigma_1 \equiv \frac{1}{s_1} - \frac{1}{2}$.

Proof of Proposition 3.

There is only one sclar conservation and $W \equiv \rho$. According to the proposition 2, we have the equivalent equation up to order two: $\partial_t W = \alpha_1 W + F + \Delta t \left(\alpha_2 W + \gamma_1 F\right) + O(\Delta t^2)$. The associated coefficients can be computed easily: $\alpha_1 = 0$, $\alpha_2 = \lambda^2 \sigma_1 \frac{\zeta+2}{3}$, $\gamma_0 = 1$ and $\gamma_1 = \left(\theta - \frac{1}{2}\right) \partial_t$. We have in consequence $\gamma_1 F = 0$ if $\partial_t F = 0$ and the equivalent equation is established.

• Boundary Conditions for thermics

We consider the elementary one-dimensional Poisson problem with homogeneous Dirichlet boundary conditions:

(17)
$$-\Delta u(x) = c \text{ for } 0 < x < 1, \quad u(0) = u(1) = 0.$$

The solution of the problem (17) is quadratic and is presented in Figure 3. A uniform body force F is considered to take into account the source term c in the right hand side of the Poisson equation. We denote by x_b the first node at the left in the domain]0, 1[and by x_e a fictitious outside node. The node x_b is supposed to be located at a distance Δq of the solid wall position x_i (see Figure 3). We implement a so-called "anti-bounce-back" boundary condition (see Bouzidi *et al.* [2, 9]) to take into account the Dirichlet boundary conditions:

(18)
$$f_1(x_b, t + \Delta t) = -f_2^*(x_b, t) + \Phi$$

where Φ is a given boundary term that has to be precised.



Figure 3. Left: quadratic solution of a one-dimensional Poisson problem. Right: "anti-bounce-back" numerical boundary condition for the D1Q3 lattice Boltzmann scheme. The boundary node x_b is located at the distance Δq of the theoretical boundary. The incoming particles $f_1(x_b)$ are determined with the knowledge of the outgoing density of particles $f_2(x_b)$.

• Proposition 4. Quartic treatment of a D1Q3 boundary condition.

For the above D1Q3 lattice Boltzmann scheme, we define $\xi \equiv -3 + 8\sigma_1\sigma_2 - 8\sigma_1(1 - 2\theta)$. The numerical solution of the Poisson problem (17) vanishes at third order formal accuracy for the position $\Delta q = \frac{\Delta x}{2}$ if the condition $\xi = 0$ is satisfied.

F. DUBOIS, P. LALLEMAND AND MM. TEKITEK.



Figure 4. Solid wall position $\Delta q \, vs$. the parameter $\xi \equiv -3 + 8\sigma_1\sigma_2 - 8\sigma_1(1 - 2\theta)$ for the D1Q3 scheme for thermal model. We have considered variations of the parameter θ of the relation (2) for the forcing term ($\theta = 0.2$ with bullets, $\theta = 0.5$ with circles and $\theta = 0.7$ with boxes) and of the parameter σ_2 relative to the last moment.



Figure 5. Analogous to the figure 4. On the left: regular variation of the parameter θ for $\theta \in [0.1, 0.9]$. Right: zoom of the left figure for $\theta \in [0.31, 0.32]$.

Proof of Proposition 4.

Using the equation (9) on the nonconserved moment, we have $Y = EW + \Delta t \ \beta_1 W + \Delta t^2 \ \beta_2 W + \Delta t \ \rho_0 \ F + \Delta t^2 \ \rho_1 \ F$. Then we perform a collision step to get $Y^* = (I - S) \ Y + S \ E \ Y + \Delta t \ \theta \ S \ E \ F$. With the help of the inverse moments matrix M^{-1} , we deduce: $f_1^* = \frac{1}{2\lambda^2} [2m_2^* + \lambda \ m_1^*]$ and $f_2^* = \frac{1}{2\lambda^2} [2m_2^* - \lambda \ m_1^*]$. We impose the anti-bounce-back condition on the boundary: $f_1(x_b, t + \Delta t) = -f_2(x_e, t + \Delta t) + \Phi$. Due to the fundamental time iteration of a lattice Boltzmann scheme (7), we can write this relation under the form $f_1^*(x_e, t) = -f_2^*(x_b, t) + \Phi$. Using a Taylor development of the moments, we obtain: $f_1^*(x_e) + f_2^*(x_b) = \frac{(2+\zeta)}{3}\rho(x_i) + \Delta t^2\lambda^2\frac{(2+\zeta)}{72} \left[-3 + 8\sigma_1\sigma_2 - 8\sigma_1(1 - 2\theta) \right] \frac{\partial^2\rho}{\partial x^2}(x_i) + O(\Delta t^3)$. We can precise that $\Phi = \frac{1}{3}(2+\zeta)\rho(x_i)$ in the right hand side of (18). Then the conclusion holds if we give a null value for the second order term in the previous relation. We remark that for $\theta = \frac{1}{2}$ we found the same result that the one we proposed previously [3].

• D2Q9 for a linear acoustic type fluid

This scheme is described and analyzed in [10]. The matrix M is now 9×9 . For a fluid model, we have N = 3 and the conserved moments are the density $m_0 \equiv \rho$ and the two components of the momentum: $m_1 \equiv J_x$ and $m_2 \equiv J_y$. The nonconserved moments m_k for $k \geq 3$ are detailed in [10]. Their equilibrium values are classical: $m_3^{eq} = -2\rho$, $m_4^{eq} = \rho$, $m_5^{eq} = -\frac{J_x}{\lambda}$, $m_6^{eq} = -\frac{J_y}{\lambda}$ and $m_7^{eq} = m_8^{eq} = 0$. The relaxation rates are labelled from s_3 to s_8 with the two constraints $s_5 = s_6$ and $s_7 = s_8$ to recover an isotropic model compatible with the physics. The particle directions are represented on the figure 1. With a forcing term of the type $F = (0, F_x, 0)$, the partial equivalent equations at the order 2 are given by

$$\begin{cases} \frac{\partial \rho}{\partial t} + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} = O(\Delta t^2), \\ \frac{\partial J_x}{\partial t} + \frac{\lambda}{3} \frac{\partial \rho}{\partial x} - \frac{\lambda^2}{3} \Delta t \left[\sigma_3 \frac{\partial}{\partial x} \left(\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} \right) + \sigma_7 \Delta J_x \right] - F_x = O(\Delta t^2), \\ \frac{\partial J_y}{\partial t} + \frac{\lambda}{3} \frac{\partial \rho}{\partial y} - \frac{\lambda^2}{3} \Delta t \left[\sigma_3 \frac{\partial}{\partial y} \left(\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} \right) + \sigma_7 \Delta J_y \right] = O(\Delta t^2). \end{cases}$$

• Two-dimensional Poiseuille flow with the D2Q9 lattice Boltzmann scheme

We study this classical problem in $\Omega = [1, N_x] \times [1, N_y]$ with the help of an imposed volumic uniform body force F_x to model the pressure gradient. We enforce periodic condition at the inlet (i = 1) and at the outlet $(i = N_x)$. A "bounce-back" boundary condition is imposed on the walls to take into account the null velocity $J_x = 0$ on the upper and lower boundary.

• Proposition 5. Precise position of the Poiseuille boundary with D2Q9.

With the above choices for the lattice Boltzmann scheme, the solid wall is at $\Delta q = \frac{\Delta x}{2}$ up to third order when the parameter $\xi \equiv -3 + 8\sigma_8\sigma_5 - 8\sigma_8(1-2\theta)$ is equal to zero.

• The proof of Proposition 5 is elementary with traditional algebraic methods but quite long to develop. We have implemented it without difficulty with a formal computer softwave. In order to convince the reader, we test the resulting condition $\xi = 0$ with appropriate numerical experiments presented in Figure 6. These experiments extend the ones presented in [3].



Figure 6. Poiseuille flow with the D2Q9 lattice Boltzmann scheme. Left: solid wall position $\Delta q \, vs$. the parameter $\xi \equiv -3 + 8\sigma_8\sigma_5 - 8\sigma_8(1-2\theta)$. Variations of the parameter θ of the relation (2) for the forcing term ($\theta = 0.2$ with bullets, $\theta = 0.5$ with circles and $\theta = 0.7$ with boxes) and of the parameter σ_5 relative of the moment m_5 . Right: zoom of the left figure, with a variation $\Delta q \, vs$. the parameter $\theta \in [0.77, 0.78]$.



Figure 7. Stencil of the D2Q13 lattice Bolzmann scheme.

• D2Q13 for a linearized fluid

To construct the scheme D2Q13, we add four more velocities to the previous schme D2Q9 (see the figure 7). The details can be found *e.g.* in Higuera *et al.* [7]. Nine moments are analogous to those proposed previously. The equilibrium values are parameterized according to $m_3^{eq} = a_1 \rho$, $m_4^{eq} = m_5^{eq} = 0$, $m_6^{eq} = \frac{c_1}{\lambda} J_x$, $m_7^{eq} = \frac{c_1}{\lambda} J_y$, $m_8^{eq} = -\frac{65+63 c_1}{24\lambda} J_x$, $m_9^{eq} = -\frac{65+63 c_1}{24\lambda} J_y$, $m_{10}^{eq} = a_2 \rho$, $m_{11}^{eq} = a_3 \rho$ and $m_{12}^{eq} = 0$. In order to simulate isotropic models, the relaxation rates s_3 to s_{12} satisfy the following relations : $s_4 = s_5$, $s_6 = s_7$ and $s_8 = s_9$ as proposed *e.g.* in [1]. With the previous choices, with a forcing term $F = (0, F_x, 0)$ analogous to the one proposed previously for the D2Q9 scheme, the partial

equivalent equations take the form

$$\begin{cases} \frac{\partial \rho}{\partial t} + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} = O(\Delta t^2), \\ \frac{\partial J_x}{\partial t} + c_s^2 \frac{\partial \rho}{\partial x} - \zeta \frac{\partial}{\partial x} \left[\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} \right] - \nu \Delta J_x - F_x = O(\Delta t^2), \\ \frac{\partial J_y}{\partial t} + c_s^2 \frac{\partial \rho}{\partial y} - \zeta \frac{\partial}{\partial y} \left[\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} \right] - \nu \Delta J_y = O(\Delta t^2). \end{cases}$$

The sound speed c_s , the shear viscosity ν and the bulk viscosity ζ satisfy respectively $c_s^2 = \frac{28+a_1}{26} \lambda^2$, $\nu = \Delta t \, \sigma_5 \, \frac{\lambda^2}{2}$ and $\zeta = -\Delta t \, \sigma_3 \, \frac{2+a_1}{26} \, \lambda^2$.

• Two-dimensional Poiseuille flow with the D2Q13 lattice Boltzmann scheme

The general choices are analogous to the ones we did with the D2Q9 lattice Boltzmann scheme.

• Proposition 6. Precise position of the Poiseuille boundary with D2Q13. When the parameter $\xi \equiv -7 + 40\sigma_5 \sigma_7 - 8\sigma_5 (1 - 2\theta)$ is null and with the above choices for the lattice Boltzmann scheme, the solid wall is located at $\Delta q = \frac{\Delta x}{2}$ at third order accuracy if and only if $\xi = 0$.

• This proposition has been solved with the help of formal calculus. We did various experiments analogous to the one presented for the D2Q9 scheme. They are summarized in the captions of Figures 8 and 9.



Figure 8. Poiseuille flow for the D2Q13 scheme. Solid wall position $\Delta q \, vs$. the parameter $\xi \equiv -7 + 40\sigma_5 \sigma_7 - 8\sigma_5 (1 - 2\theta)$. Variations of the parameter θ of the relation (2) for the forcing term ($\theta = 0.2$ with bullets, $\theta = 0.5$ with circles and $\theta = 0.7$ with boxes) and of the parameter σ_5 .



Figure 9. Precise Poiseuille flow with the D2Q13 lattice Boltzmann scheme. Solid wall position Δq vs. the parameter θ for the forcing term in (2). Left: $\theta \in [0.1, 0.9]$, right: zoom of the left figure with $\theta \in [0.37, 0.38]$.

4) Conclusion

In this contribution, we have extended the "Berliner version" [1] of the formal Taylor expansion method for linear lattice Boltzmann scheme to the case of a possible external force. We have established that the quartic parameters to enforce the precision of the lattice Boltzmann scheme depend not only on the relaxation rate but also on the choice of the parameter θ for the time integration (2) of the source term. We have derived quartic parameters for the D2Q13 model for a Poiseuille flow. Our numerical results validate the formal Taylor development. Nevertheless, a rigorous numerical analysis is still an open question. In future work, we wish to extend the quest of quartic parameters for more general physical problems, study time dependent boundary conditions and give more general boundary conditions for any position of the wall relative to the lattice.

References

- A. Augier, F. Dubois, B. Graille. "On rotational invariance of lattice Boltzmann schemes", 9th ICMMES Conference, Taipei, july 2012. To appear in *Computers and Mathematics with Applications*.
- [2] M. Bouzidi, M. Firdaous, P. Lallemand. "Momentum transfer of a Boltzmann-lattice fluid with boundaries", *Physics of Fluids*, vol. 13, p. 3452-3459, 2001.
- [3] F. Dubois, P. Lallemand, MM. Tekitek. "On a superconvergent lattice Boltzmann boundary scheme", *Computers and Mathematics with Applications*, vol. 59, p. 2141-2149, 2010.
- [4] I. Ginzburg, P.M. Adler. "Boundary flow condition analysis for the three-dimensional lattice Boltzmann model", *Journal de Physique II*, vol. 4, p. 191-214, 1994.
- [5] I. Ginzburg, F. Verhaeghe, D. d'Humières. "Two-relaxation-time lattice boltzmann scheme: about parametrization, velocity, pressure and mixed boundary conditions", *Communications in Computational Physics*, vol. 3, p. 519-581, 2008.

TAYLOR EXPANSION METHOD WITH AN EXTERNAL DRIFT

- [6] Z. Guo, C. Zheng, B. Shi, "Discrete lattice effects on the forcing term in the lattice Boltzmann method", *Physical Review E*, vol. 65, p. 1-6, 2002.
- [7] F. J. Higuera, S. Succi, R. Benzi. "Lattice Gas Dynamics with Enhanced Collisions", *EuroPhysics Letters*, vol. 9, p. 345-349, 1989.
- [8] D. d'Humières. "Generalized Lattice-Boltzmann Equations", in Rarefied Gas Dynamics: Theory and Simulations, vol. 159 of AIAA Progress in Aeronautics and Astronautics, p. 450-458, 1992.
- [9] D. d'Humières, I. Ginzburg. "Multi-reflection boundary conditions for lattice Boltzmann models", *Physical Review E*, vol. 68, 2003.
- [10] P. Lallemand, L.-S. Luo. "Theory of the lattice Boltzmann method: Dispersion, dissipation, isotropy, Galilean invariance, and stability", *Physical Review E*, vol. 61, p. 6546-6562, 2000.
- [11] Y.H. Qian, D. d'Humières, P. Lallemand. "Lattice BGK Models for Navier-Stokes Equation", *EuroPhysics Letters*, vol. 17, p. 479-484, 1992.
- [12] S. Succi, R. Benzi, F. Higuera. "Lattice Gas Methods for Homogeneus and Inhomegeneus Hydrodynamics", Discrete kinetic theory, lattice gas dynamics and foundations of hydrodynamics, R. Monaco Editor, World Scientific Publishing, Singapore, p. 329-342, 1989.