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# Construction and Analysis of Lattice Boltzmann Methods Applied to a 1D Convection-Diffusion Equation

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## Abstract

We construct and we analyze two LBM schemes applied to a 1D convection-diffusion equation. We obtain these LBM schemes by showing that the 1D convection-diffusion equation is the fluid limit of a discrete velocity kinetic system. Then, we show that these LBM schemes are equivalent to a finite difference type scheme for different boundary conditions. This allows us, firstly, to prove the convergence in  $L^\infty$  of these LBM schemes and to obtain discrete maximum principles in the case of the 1D heat equation for any  $\Delta t$  of the order of  $\Delta x^2$ . Secondly, this allows us to obtain most of these results for the Du Fort-Frankel scheme for a particular choice of the first iterate. By proposing a probabilistic interpretation of these LBM schemes, we also obtain Monte-Carlo algorithms which approach the 1D heat equation. At last, we present numerical applications justifying these results.

### *Key words:*

Lattice Boltzmann method, Chapman-Enskog expansion, Hilbert expansion, convection-diffusion equation, heat equation, Du Fort-Frankel scheme, stability and convergence in  $L^\infty$ , discrete maximum principle, Monte-Carlo algorithm.

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## 1. Introduction

Lattice Boltzmann Methods (LBM) come from an attempt to simulate the incompressible Navier-Stokes system with cellular automata [1, 2] before being seen as deterministic schemes based on the resolution of discrete velocity kinetic systems [3]. LBM schemes are now often used to solve many type of PDEs. Among them, we find the heat equation [4] with or without phase change [5], the heat equation with radiative source term [6], the hyperbolic heat equation (also named telegraph equation) with or without radiative source term [7], the Richard equation for porous media [8], the incompressible Navier-Stokes system [9] eventually applied in porous media with heat and mass transfer [10] or in a diphasic situation [11, 12] or with a free-surface [13], the Bingham model for viscoplastic flows [14]. Among the reasons which justify the use of LBM schemes, we can cite its algorithmic simplicity, its time explicit nature, its scalability when the algorithm is parallelized. We can also cite the fact that all LBM schemes are formulated in a common way. More precisely, when  $W(t, x)$  is the solution of a PDEs system where  $t \geq 0$  is the time and  $x \in \Omega \subset \mathbb{R}^d$

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is the spacial variable ( $d \in \{1, 2, 3\}$ ), the approximation  $W_i^{n+1}$  of  $W(t^{n+1}, x_i)$  is obtained through a formula of the type

$$W_i^{n+1} = \sum_{q=1}^{q_{\max}} \varphi(v_q) f_{q,i}^{n+1}$$

where  $\varphi(\cdot)$  is a given function which depends on the PDEs, where  $v_q \in \mathbb{R}^d$  belongs to a discrete and finite set  $\{v_q\}_{1 \leq q \leq q_{\max}}$  and where  $f_{q,i}^{n+1}$  is deduced from a scheme of the type

$$f_{q,i}^{n+1} = L_{q,i}(W_i^n) \cdot \mathbf{f}_i^n$$

where  $L_{q,i}(W_i^n)$  is a matrix which acts on  $\mathbf{f}_i^n = (f_{q',j_i}^n)_{q',j_i}$ , where  $q' \in \{1, \dots, q_{\max}\}$  and where  $j_i$  belongs to a stencil centered on  $i$  ( $j_i \in \{i-1, i, i+1\}$  in 1D), and which does not depend on  $W_i^n$  when the PDEs are linear.

Although the LBM schemes have proven their efficiency both in academical and industrial situations (see for example the numerical applications in [13]), the numerical analysis of these schemes is not well developed. Moreover, this numerical approach suffers sometimes of a lack of precision in the way to introduce it. Nevertheless, there exists recent publications which give accurate informations on the LBM approach from a mathematical point of view. Among them, we find in [15, 16] a justification of LBM schemes applied to the 1D linear advection equation and to a 1D Navier-Stokes type model (which is a p-system with diffusive term). In [17, 18], a Chapman-Enskog expansion is applied to the LBM scheme to justify it in the case of the 1D convection-diffusion equation and in the case of the 1D wave equation with diffusive term. In [19], a Chapman-Enskog expansion is also applied to a LBM scheme applied to the incompressible Navier-Stokes system; moreover, a Chapman-Enskog expansion is also applied to a discrete velocity kinetic system. In [20, 21], a convergence result in  $L^2$  is proposed for LBM schemes in the case of the incompressible Navier-Stokes system under some assumptions and a stability result in  $L^2$  is obtained by linearizing the LBM schemes.

In this paper, we construct and we justify two LBM schemes in the case of the 1D convection-diffusion equation

$$\partial_t \rho + \partial_x(u\rho) = \nu \partial_{xx}^2 \rho \quad (1)$$

where  $\nu > 0$  and with periodic, Neumann or Dirichlet boundary conditions,  $u(x)$  being a given function. When  $u(x) = 0$ , one of these LBM schemes is classical and can be found in [4]; the second one seems to be less classical. These LBM schemes are obtained by discretizing a discrete velocity kinetic system whose the fluid limit is (1), this fluid limit being formally obtained with a Chapman-Enskog expansion but also with a Hilbert expansion. Then, we prove that in the case of the heat equation with periodic, Neumann or Dirichlet boundary conditions, these LBM schemes converge in  $L^\infty$  for any  $\Delta t$  of the order of  $\Delta x^2$  where  $\Delta t$  is the time step and where  $\Delta x$  is the mesh size. This result is obtained by noting that these LBM schemes are equivalent to a finite difference type scheme and by using the Lax Theorem. In the case of the heat equation, this finite difference type scheme is a particular Du Fort-Frankel scheme [22]. As it is easy to obtain discrete maximum principles with the LBM approach for any  $\Delta t = \mathcal{O}(\Delta x^2)$  (in the periodic and Neumann cases), due to this equivalence, we also obtain that this particular Du Fort-Frankel scheme converges in  $L^\infty$  and verifies discrete maximum principles (in the periodic and Neumann cases) for any  $\Delta t = \mathcal{O}(\Delta x^2)$ . These results are also new for the Du Fort-Frankel scheme which has been known for a long time to converge in  $L^2$  for any  $\Delta t = \mathcal{O}(\Delta x^2)$ . Thus, the LBM schemes have also been used in this study as a tool to give new results for a classical finite difference type scheme. Let us note that the case of Dirichlet boundary conditions is particular. Indeed, we have to modify the Dirichlet boundary conditions to obtain a discrete

maximum principle for any  $\Delta t = O(\Delta x^2)$ . Nevertheless, we lose the equivalence with the Du Fort-Frankel scheme which avoids to obtain the convergence of the LBM schemes by using the Lax Theorem. At last, we also propose Monte-Carlo algorithms for the heat equation which come from a probabilistic interpretation of the LBM schemes. Some basic properties of these Monte-Carlo algorithms are proposed. We hope that this probabilistic approach will be also a tool to analyze the LBM schemes. The end of the paper is devoted to numerical simulations which validate the proposed results.

The outline of this paper is the following. In §2, we introduce the discrete velocity kinetic system and its fluid limit (which is formally obtained in Annex A). In §3, we construct the LBM schemes. In §4, we obtain the equivalence of these LBM schemes with a finite difference type scheme. In §5, we obtain the stability and the convergence in  $L^\infty$  for any  $\Delta t = O(\Delta x^2)$  when  $u(x) = 0$ . In §6, we prove that discrete maximum principles are verified for any  $\Delta t = O(\Delta x^2)$  when  $u(x) = 0$ . In §7, we present some limitations of the LBM schemes. In §8, a probabilistic interpretation of the LBM schemes is proposed when  $u(x) = 0$ . In §9, we present some numerical results. At last, we conclude the paper in §10.

## 2. Fluid limit of a discrete velocity kinetic system

Let us define the function

$$M_q^\varepsilon(t, x) := \frac{\rho(t, x)}{2} \left[ 1 + \frac{u(x)}{v_q^\varepsilon} \right] \quad (2)$$

where  $\rho(t, x) \in \mathbb{R}_*^+$  and  $u(x) \in \mathbb{R}$ . The parameters  $t \in \mathbb{R}^+$  and  $x \in \Omega := [x_{\min}, x_{\max}]$  ( $\Omega \subset \mathbb{R}$ ) are the time and space variables. The set  $\{v_q^\varepsilon\}_{q \in \{1,2\}}$  is a discrete and finite set of velocities defined by

$$v_q^\varepsilon := (-1)^q c^\varepsilon \quad \text{with} \quad q \in \{1, 2\} \quad (3)$$

where  $c^\varepsilon \in \mathbb{R}^+$  depends on a parameter  $\varepsilon \in \mathbb{R}^+$  and will be defined later. In the LBM framework,  $\{v_q^\varepsilon\}_{q \in \{1,2\}}$  is named D1Q2. The function  $M_q^\varepsilon$  verifies

$$\sum_{q \in \{1,2\}} \begin{pmatrix} 1 \\ v_q^\varepsilon \end{pmatrix} M_q^\varepsilon = \begin{pmatrix} \rho \\ \rho u \end{pmatrix}. \quad (4)$$

To solve the convection-diffusion equation (1), we will propose two schemes which are built from a study of a system of equations of the type

$$\begin{cases} \partial_t f_1^\varepsilon + v_1^\varepsilon \partial_x f_1^\varepsilon = \frac{1}{\varepsilon} (M_1^\varepsilon - f_1^\varepsilon), \\ \partial_t f_2^\varepsilon + v_2^\varepsilon \partial_x f_2^\varepsilon = \frac{1}{\varepsilon} (M_2^\varepsilon - f_2^\varepsilon). \end{cases} \quad (5)$$

These schemes will belong to the family of LBM schemes. System (5) may be considered as a kinetic equation whose the kinetic velocities belong to the discrete and finite set  $\{v_q^\varepsilon\}_{q \in \{1,2\}}$  and whose the collision operator is a BGK-type collision operator where the classical maxwellian is replaced by  $M_q^\varepsilon$ . Thus,  $M_q^\varepsilon$  will be named "maxwellian" in the sequel,  $\rho(x)$  and  $u(x)$  being the macroscopic density and velocity associated to  $M_q^\varepsilon$ . We also define the normalized maxwellian

$$m_q^\varepsilon := \frac{1}{2} \left( 1 + \frac{u}{v_q^\varepsilon} \right) = \frac{1}{2} \left( 1 + (-1)^q \frac{u}{c^\varepsilon} \right). \quad (6)$$

By construction, we have  $M_q^\varepsilon = \rho m_q^\varepsilon$  and  $m_q^\varepsilon$  verifies

$$\sum_{q \in \{1,2\}} \begin{pmatrix} 1 \\ v_q^\varepsilon \end{pmatrix} m_q^\varepsilon = \begin{pmatrix} 1 \\ u \end{pmatrix}. \quad (7)$$

Let us underline that most of the variables above depend on the collision time  $\varepsilon$ . Thus, to clearly underline this dependency, we introduce the parameter  $\varepsilon$  in the notation of these variables. We will simplify the notations after this section by omitting the parameter  $\varepsilon$ .

The LBM schemes proposed to solve (1) will be deduced in §3 from a fluid limit of the discrete velocity kinetic system (5). This fluid limit is obtained for a particular choice of the kinetic velocity  $c^\varepsilon$ :

**Proposition 2.1.** *Let us suppose that  $\Omega$  is periodic and let  $f_q^\varepsilon(t, x)$  be solution of the discrete velocity kinetic system*

$$\forall q \in \{1, 2\} : \quad \begin{cases} \partial_t f_q^\varepsilon + v_q^\varepsilon \partial_x f_q^\varepsilon = \frac{1}{\varepsilon} (M_q^\varepsilon - f_q^\varepsilon), \\ f_q^\varepsilon(t=0, x) = f_q^{\varepsilon,0}(x) \end{cases} \quad (8)$$

where  $M_q^\varepsilon$  is given by

$$M_q^\varepsilon(t, x) := \frac{\rho^\varepsilon(t, x)}{2} \left[ 1 + \frac{u(x)}{v_q^\varepsilon} \right]$$

with  $\rho^\varepsilon := f_1^\varepsilon + f_2^\varepsilon$  and where  $v_q^\varepsilon := (-1)^q c^\varepsilon$ . Then, when  $\varepsilon \ll 1$ , when  $f_q^\varepsilon(t=0, x)$  is close to the Maxwellian equilibrium  $M_q^\varepsilon$  in such a way

$$f_q^\varepsilon(t=0, x) = M_q^\varepsilon(t=0, x) + \mathcal{O}(\sqrt{\varepsilon}) \quad (9)$$

and when

$$c^\varepsilon = \sqrt{\frac{v}{\varepsilon}}, \quad (10)$$

$\rho^\varepsilon$  is solution of

$$\begin{cases} \partial_t \rho^\varepsilon + \partial_x (u \rho^\varepsilon) = v \partial_{xx}^2 \rho^\varepsilon + \mathcal{O}(\varepsilon), \\ \rho^\varepsilon(t=0, x) = f_1^{\varepsilon,0}(x) + f_2^{\varepsilon,0}(x). \end{cases} \quad (11)$$

Moreover, we have

$$f_q^\varepsilon(t, x) = M_q^\varepsilon - (-1)^q \frac{\sqrt{\varepsilon v}}{2} \partial_x \rho^\varepsilon + (-1)^q \varepsilon^{3/2} \left[ \frac{u}{2\sqrt{v}} \cdot (\partial_x (u \rho^\varepsilon) - v \partial_{xx}^2 \rho^\varepsilon) - \frac{\sqrt{v}}{2} \partial_{xx}^2 (u \rho^\varepsilon) + \frac{v^{3/2}}{2} \partial_{xxx}^3 \rho^\varepsilon \right] + \mathcal{O}(\varepsilon^2)$$

that is to say

$$\begin{aligned} f_q^\varepsilon(t, x) &= \frac{\rho^\varepsilon}{2} \left[ 1 + (-1)^q \sqrt{\varepsilon} \left( \frac{u}{\sqrt{v}} - \sqrt{v} \frac{\partial_x \rho^\varepsilon}{\rho^\varepsilon} \right) \right. \\ &\quad \left. + (-1)^q \varepsilon^{3/2} \left( \frac{u}{\sqrt{v}} \cdot \frac{\partial_x (u \rho^\varepsilon) - v \partial_{xx}^2 \rho^\varepsilon}{\rho^\varepsilon} - \sqrt{v} \frac{\partial_{xx}^2 (u \rho^\varepsilon)}{\rho^\varepsilon} + v^{3/2} \frac{\partial_{xxx}^3 \rho^\varepsilon}{\rho^\varepsilon} \right) \right] + \mathcal{O}(\varepsilon^2). \end{aligned} \quad (12)$$

Let us note that we suppose that  $\Omega$  is periodic since kinetic boundary conditions are difficult to analyze when they are not periodic. Nevertheless, we will study in §4 how to take into account in the LBM schemes proposed in §3 Neumann and Dirichlet boundary conditions applied to (1).

The proof is written in Annex A: it is based on a Chapman-Enskog expansion (Annex A.1) or on a Hilbert expansion (Annex A.2). Proposition 2.1 means that the convection-diffusion equation (1) is the fluid limit of the discrete velocity kinetic system (8). Let us note that  $\varepsilon \ll 1$  means that  $\varepsilon \ll t_{fluid}$  where  $t_{fluid} = O(1)$  is the time scale of the fluid limit (1),  $\varepsilon$  being the kinetic time scale ((1) and (8) are supposed to be dimensionless).

Of course, we deduce from Proposition 2.1 the following corollary:

**Corollary 2.1.** *Let us suppose that  $\Omega$  is periodic and let  $f_q^\varepsilon(t, x)$  be solution of the discrete velocity kinetic system*

$$\begin{cases} \partial_t f_1^\varepsilon - \sqrt{\frac{v}{\varepsilon}} \partial_x f_1^\varepsilon = \frac{1}{2\varepsilon} (f_2^\varepsilon - f_1^\varepsilon), \\ \partial_t f_2^\varepsilon + \sqrt{\frac{v}{\varepsilon}} \partial_x f_2^\varepsilon = \frac{1}{2\varepsilon} (f_1^\varepsilon - f_2^\varepsilon), \\ f_1^\varepsilon(t=0, x) = f_1^{\varepsilon,0}(x), \\ f_2^\varepsilon(t=0, x) = f_2^{\varepsilon,0}(x). \end{cases} \quad (13)$$

Then, when  $\varepsilon \ll 1$  and when  $f_q^\varepsilon(t=0, x)$  is close to the maxwellian equilibrium  $M_q^\varepsilon(t=0, x) := \frac{f_1^{\varepsilon,0}(x) + f_2^{\varepsilon,0}(x)}{2}$  in such a way

$$f_q^\varepsilon(t=0, x) = M_q^\varepsilon(t=0, x) + O(\sqrt{\varepsilon}), \quad (14)$$

$\rho^\varepsilon := f_1^\varepsilon + f_2^\varepsilon$  is solution of

$$\begin{cases} \partial_t \rho^\varepsilon = v \partial_{xx}^2 \rho^\varepsilon + O(\varepsilon), \\ \rho^\varepsilon(t=0, x) = f_1^{\varepsilon,0}(x) + f_2^{\varepsilon,0}(x). \end{cases} \quad (15)$$

Moreover, we have

$$f_q^\varepsilon(t, x) = \frac{\rho^\varepsilon}{2} \left[ 1 + (-1)^q \sqrt{\varepsilon v} \left( \varepsilon v \frac{\partial_{xxx}^3 \rho^\varepsilon}{\rho^\varepsilon} - \frac{\partial_x \rho^\varepsilon}{\rho^\varepsilon} \right) \right] + O(\varepsilon^2). \quad (16)$$

Let us note that it is proven in [23, 24] that the fluid limit of

$$\begin{cases} \partial_t \rho + c \partial_x w = 0, \\ \partial_t w + \partial_x p(\rho) = -\frac{w}{\varepsilon} \end{cases} \quad (17)$$

is given by

$$\partial_t \rho = \varepsilon \partial_{xx}^2 p(\rho),$$

$p(\rho)$  being a given function which does not depend on  $\varepsilon$ . On the other side, we can note that when  $p(\rho) = c\rho$  where  $c$  is a constant, by defining  $f_1$  and  $f_2$  in such a way  $\rho = f_1 + f_2$  and  $w = f_2 - f_1$ , (17) is equivalent to

$$\begin{cases} \partial_t f_1 - c \partial_x f_1 = \frac{1}{2\varepsilon}(f_2 - f_1), \\ \partial_t f_2 + c \partial_x f_2 = \frac{1}{2\varepsilon}(f_1 - f_2) \end{cases} \quad (18)$$

whose the fluid limit is given by

$$\partial_t \rho = \varepsilon c^2 \partial_{xx}^2 \rho + \mathcal{O}(\varepsilon^2). \quad (19)$$

The discrete velocity kinetic system (18) is similar to (13). Nevertheless, the kinetic velocity  $c$  in (18) is a constant and, thus, does not depend on  $\varepsilon$  which is not the case of the kinetic velocity  $c^\varepsilon := \sqrt{\frac{\nu}{\varepsilon}}$  in (13). As a consequence, the fluid limits (15) and (19) are different.

The fact that the discrete velocity kinetic system (8) is such that the kinetic velocity  $c^\varepsilon$  depends on the collision time  $\varepsilon$  is not classical, and obliges us to perform carefully the expansions given the fluid limit (11) and the approximation (12) of  $f_q^\varepsilon$  (see Annex A). More precisely, this is a constraint imposed *a posteriori* by the LBM schemes that we want to obtain and justify through an *ad hoc* discretization of a discrete velocity kinetic system. Indeed, a LBM scheme is always characterized by the fact that  $c^\varepsilon = \Delta x / \Delta t$  where  $\Delta x$  and  $\Delta t$  are respectively the mesh size and the time step. Moreover, the proposed LBM schemes will be such that  $\Delta t = \mathcal{O}(\Delta x^2)$  (which is natural for a convection-diffusion equation) and such that  $\varepsilon = \mathcal{O}(\Delta t)$  (which is not natural: the fact that the collision time depends on a discretization parameter makes often difficult the analysis of the LBM schemes). As a consequence, we have to choose  $c^\varepsilon = \mathcal{O}(1/\sqrt{\varepsilon})$  and not  $c^\varepsilon = c$  to have a chance to obtain and justify LBM schemes for the convection-diffusion equation (1).

### 3. Construction of two LBM schemes

We define a 1D mesh  $\{x_i\}_{i \in \{1, \dots, N\}}$  whose the mesh size  $\Delta x$  is constant and we define an uniform time step  $\Delta t = t^{n+1} - t^n$  such that

$$\Delta t := C_d \frac{\Delta x^2}{\nu} \quad \text{with} \quad C_d = \mathcal{O}(1).$$

This definition is justified by the fact that we want to discretize a convection-diffusion equation whose the kinematic viscosity is equal to  $\nu$ . Proposition 2.1 encourages us to discretize

$$\forall q \in \{1, 2\} : \begin{cases} \partial_t f_q + (-1)^q \sqrt{\frac{\nu}{\varepsilon}} \partial_x f_q = \frac{1}{\varepsilon}(M_q - f_q), \\ f_q^\varepsilon(t=0, x) = f_q^0(x) \end{cases} \quad (20)$$

(to simplify the notations, we now omit  $\varepsilon$  in  $f_q^\varepsilon$  and  $M_q^\varepsilon$ ) instead of

$$\begin{cases} \partial_t \rho + \partial_x(u\rho) = \nu \partial_{xx}^2 \rho, \\ \rho(t=0, x) = \rho^0(x). \end{cases} \quad (21)$$

The difficulty is to find a numerical scheme applied to (20) which is enough accurate to capture the fluid limit (21) when  $\Delta t$  is of the order of  $\Delta x^2$  and when  $\Delta t \ll 1$  and  $\varepsilon \ll 1$ . This also underlines that  $\varepsilon$  depends on  $\Delta t$  which makes difficult the analysis of the LBM schemes.

### 3.1. Integration of the kinetic system

We have the following result whose the proof is based on an idea that we can find in [25, 15]:

**Proposition 3.1.** *Let  $f_q^\varepsilon(t, x)$  be solution of the kinetic system*

$$\forall q \in \{1, 2\} : \quad \partial_t f_q + (-1)^q c \partial_x f_q = \frac{1}{\varepsilon} (M_q - f_q) := \mathbf{Q}_q(f)(t, x)$$

and let

$$g_q(t, x) := f_q(t, x) - \frac{\Delta t}{2} \mathbf{Q}_q(f)(t, x). \quad (22)$$

Then, we have

$$g_1 + g_2 = f_1 + f_2$$

and

$$g_q[t + \Delta t, x + (-1)^q c \Delta t] = g_q(t, x)(1 - \eta) + M_q(t, x)\eta + \mathcal{O}\left(\frac{\Delta t^3}{\sqrt{\varepsilon}}\right) \quad \text{when} \quad \Delta t^3 \ll \sqrt{\varepsilon} \quad (23)$$

where

$$\eta = \frac{1}{\frac{\varepsilon}{\Delta t} + \frac{1}{2}}.$$

Since  $g_1 + g_2 = f_1 + f_2 := \rho$ , we will propose LBM schemes by using the approximation (23): this point underlines also that the LBM scheme will be based on the variable  $g_q$  instead of  $f_q$ . Nevertheless, it will be possible to deduce the LBM scheme based on  $f_q$  by applying the inverse transform of (22) to the LBM scheme based on  $g_q$ .

The proof of Proposition 3.1 is based on the following lemma:

**Lemma 3.1.** *Let us define the BGK kernel*

$$Q(f) = \frac{1}{\varepsilon} (\mathcal{M}_f - f) \quad (\varepsilon \in \mathbb{R})$$

where the distribution  $f$  is defined on a discrete or continuous velocity domain,  $\mathcal{M}_f$  being the maxwellian distribution associated to  $f$ , and let us define the distribution

$$g := f - \tilde{\varepsilon} Q(f) \quad (\tilde{\varepsilon} \in \mathbb{R}).$$

Then, when  $\tilde{\varepsilon} \neq -\varepsilon$ :

$$Q(f) = \frac{\varepsilon}{\varepsilon + \tilde{\varepsilon}} Q(g).$$

Let us underline that the lemma 3.1 is not restricted to a discrete velocity domain.

**Proof of Proposition 3.1:** The solution of the continuous EDP

$$\partial_t f_q + (-1)^q c \partial_x f_q = \frac{1}{\varepsilon} (M_q - f_q) =: \mathbf{Q}_q(f)(t, x)$$

is given by

$$f_q[t + \Delta t, x + (-1)^q c \Delta t] = f_q(t, x) + \int_0^{\Delta t} \mathbf{Q}_q(f)[t + s, x + (-1)^q c s] ds. \quad (24)$$



Since  $f_q^\varepsilon = M_q^\varepsilon + \mathcal{O}(\sqrt{\varepsilon})$  when  $\varepsilon \ll 1$  (see (12)), we can write that

$$Q_q^\varepsilon = \mathcal{O}\left(\frac{1}{\sqrt{\varepsilon}}\right) \quad \text{when} \quad \varepsilon \ll 1. \quad (25)$$

This implies that

$$\int_0^{\Delta t} Q_q(f)[t+s, x+(-1)^q c s] ds = \mathcal{O}\left(\frac{\Delta t}{\sqrt{\varepsilon}}\right) \quad \text{when} \quad \varepsilon \ll 1. \quad (26)$$

Thus, the easiest numerical integration formula applied to (24) would give

$$f_q[t+\Delta t, x+(-1)^q c \Delta t] = f_q(t, x) + \Delta t Q_q(f)(t, x) + \mathcal{O}\left(\frac{\Delta t^2}{\sqrt{\varepsilon}}\right). \quad (27)$$

Nevertheless, the error  $\mathcal{O}(\Delta t^2/\sqrt{\varepsilon})$  in (27) does not allow to obtain LBM schemes which are consistent with the convection-diffusion equation (21). In fact, the integration error has to be of the order of  $\Delta t^3/\sqrt{\varepsilon}$  (or lower) for reasons that we justify in §3.5: this point is important in the LBM framework and explains the classical "magic" formula (41) met in many LBM schemes. Thus, instead of the second order integration formula (27), we use the third order integration formula

$$f_q[t+\Delta t, x+(-1)^q c \Delta t] = f_q(t, x) + \frac{\Delta t}{2} [Q_q(f)(t, x) + Q_q(f)(t+\Delta t, x+(-1)^q c \Delta t)] + \mathcal{O}\left(\frac{\Delta t^3}{\sqrt{\varepsilon}}\right). \quad (28)$$

Formula (28) is equivalent to

$$g_q[t+\Delta t, x+(-1)^q c \Delta t] = g_q(t, x) + \Delta t Q_q(g)(t, x) + \mathcal{O}\left(\frac{\Delta t^3}{\sqrt{\varepsilon}}\right) \quad (29)$$

with  $g_q := f_q - \frac{\Delta t}{2} Q_q(f)$ . By using Lemma 3.1 with  $\tilde{\varepsilon} = \Delta t/2$ , we obtain that (29) is equivalent to

$$g_q[t+\Delta t, x+(-1)^q c \Delta t] = g_q(t, x) + \frac{\varepsilon}{\frac{\varepsilon}{\Delta t} + \frac{1}{2}} Q_q(g)(t, x) + \mathcal{O}\left(\frac{\Delta t^3}{\sqrt{\varepsilon}}\right).$$

We conclude by noting that  $Q_q(g) = \frac{1}{\varepsilon}(M_q - g_q)$ .  $\square$

**Proof of Lemma 3.1:** When  $\tilde{\varepsilon} \neq -\varepsilon$ , we have

$$\begin{aligned} Q(f) &= \frac{1}{\varepsilon}(M_f - f) \\ &= \frac{1}{\varepsilon}[M_f - g - \tilde{\varepsilon} Q(f)] \\ &= \frac{1}{\varepsilon + \tilde{\varepsilon}}(M_f - g). \end{aligned}$$

We conclude by noting that  $M_g = M_f$ .  $\square$

### 3.2. A first LBM scheme

Let us choose

$$\begin{cases} c = \frac{\Delta x}{\Delta t}, \\ \varepsilon = \frac{\nu}{c^2}. \end{cases} \quad (30)$$

Thus, we have  $\varepsilon = C_d \Delta t$  since  $\Delta t := C_d \frac{\Delta x^2}{\nu}$  ( $C_d \geq 0$ ). We deduce from (23) a first LBM scheme:

$$\begin{cases} g_{1,i}^{n+1} = g_{1,i+1}^n (1 - \eta) + M_{1,i+1}^n \eta, \\ g_{2,i}^{n+1} = g_{2,i-1}^n (1 - \eta) + M_{2,i-1}^n \eta, \\ \rho_i^{n+1} = g_{1,i}^{n+1} + g_{2,i}^{n+1} \end{cases} \quad \text{where} \quad \eta := \frac{1}{C_d + \frac{1}{2}} = \frac{1}{\frac{\nu \Delta t}{\Delta x^2} + \frac{1}{2}}. \quad (31)$$

And since  $M_q = \frac{g_1 + g_2}{2} \cdot \left(1 + (-1)^q \frac{\Delta t}{\Delta x} u(x)\right)$ , we see that the LBM scheme (31) is equivalent to

$$\begin{cases} g_{1,i}^{n+1} = g_{1,i+1}^n \left[1 - \frac{\eta}{2} \left(1 + \frac{\Delta t}{\Delta x} u(x_{i+1})\right)\right] + g_{2,i+1}^n \frac{\eta}{2} \left(1 - \frac{\Delta t}{\Delta x} u(x_{i+1})\right), \\ g_{2,i}^{n+1} = g_{2,i-1}^n \left[1 - \frac{\eta}{2} \left(1 - \frac{\Delta t}{\Delta x} u(x_{i-1})\right)\right] + g_{1,i-1}^n \frac{\eta}{2} \left(1 + \frac{\Delta t}{\Delta x} u(x_{i-1})\right), \\ \rho_i^{n+1} = g_{1,i}^{n+1} + g_{2,i}^{n+1} \end{cases} \quad \text{where} \quad \eta := \frac{1}{C_d + \frac{1}{2}} = \frac{1}{\frac{\nu \Delta t}{\Delta x^2} + \frac{1}{2}} \quad (32)$$

and to

$$\begin{cases} g_{1,i}^{n+1} = g_{1,i+1}^n \left(1 - \frac{\eta}{2}\right) + g_{2,i+1}^n \frac{\eta}{2} - \frac{\rho_{i+1}^n}{2} \cdot \eta \frac{\Delta t}{\Delta x} u(x_{i+1}), \\ g_{2,i}^{n+1} = g_{2,i-1}^n \left(1 - \frac{\eta}{2}\right) + g_{1,i-1}^n \frac{\eta}{2} + \frac{\rho_{i-1}^n}{2} \cdot \eta \frac{\Delta t}{\Delta x} u(x_{i-1}), \\ \rho_i^{n+1} = g_{1,i}^{n+1} + g_{2,i}^{n+1} \end{cases} \quad \text{where} \quad \eta := \frac{1}{C_d + \frac{1}{2}} = \frac{1}{\frac{\nu \Delta t}{\Delta x^2} + \frac{1}{2}} \quad (33)$$

(let us remark that  $\eta \in ]0, 2]$  when  $C_d \geq 0$ ). We will use the formulation (33) in the sequel.

Let us remark that, due to the relation (22), the LBM scheme (33) when  $u = 0$  and  $C_d \neq 0$  is equivalent to the LBM scheme (see Annex B)

$$\begin{cases} f_{1,i}^{n+1} = \frac{f_{1,i+1}^n (16C_d^2 - 1) + f_{2,i+1}^n (4C_d + 1) + f_{2,i-1}^n (4C_d - 1) + f_{1,i-1}^n}{16C_d(C_d + \frac{1}{2})}, \quad (a) \\ f_{2,i}^{n+1} = \frac{f_{1,i+1}^n (4C_d - 1) + f_{2,i+1}^n + f_{2,i-1}^n (16C_d^2 - 1) + f_{1,i-1}^n (4C_d + 1)}{16C_d(C_d + \frac{1}{2})}, \quad (b) \\ \rho_i^{n+1} = f_{1,i}^{n+1} + f_{2,i}^{n+1}. \quad (c) \end{cases} \quad (34)$$

The LBM scheme (34) is not classical. We can note that (33) is a two-points scheme and that (34) is a four-points scheme. Moreover, when  $C_d = 0$ , (22) implies that  $f_q = g_q$ : this means that (34) is not a continuous scheme with respect to the variable  $C_d$ . As a consequence, since (34) is more complex than (33) and is ill-defined when  $C_d = 0$ , we will study in the sequel the LBM schemes expressed with the distribution  $g_q$  and not with the distribution  $f_q$ . At last, let us underline that (33) and (34) are equivalent when the boundary conditions are periodic; for other boundary conditions, the LBM schemes (33) and (34) may not be equivalent. Nevertheless, we may think that (34) is better than (33) to take into account boundary conditions which are not periodic: we do not study this point in this paper.

### 3.3. A second LBM scheme

By replacing  $\Delta t$  by  $-\Delta t$  in (23) and by choosing again (30), we now deduce from (23) the second LBM scheme

$$\begin{cases} g_{1,i+1}^{n-1} = g_{1,i}^n(1 - \widehat{\eta}) + M_{1,i}^n \widehat{\eta}, \\ g_{2,i-1}^{n-1} = g_{2,i}^n(1 - \widehat{\eta}) + M_{2,i}^n \widehat{\eta}, \\ \rho_i^n = g_{1,i}^n + g_{2,i}^n \end{cases} \quad \text{where} \quad \widehat{\eta} := \frac{1}{-C_d + \frac{1}{2}} = \frac{1}{-\frac{\nu\Delta t}{\Delta x^2} + \frac{1}{2}}. \quad (35)$$

We have the property:

**Property 3.1.** *When  $C_d \neq 1/2$ , the LBM scheme (35) is equivalent to the LBM scheme*

$$\begin{cases} g_{1,i}^{n+1} = g_{1,i+1}^n \left[ 1 - \frac{\eta}{2} \left( 1 + \frac{\Delta t}{\Delta x} u(x_i) \right) \right] + g_{2,i-1}^n \frac{\eta}{2} \left( 1 - \frac{\Delta t}{\Delta x} u(x_i) \right), \\ g_{2,i}^{n+1} = g_{2,i-1}^n \left[ 1 - \frac{\eta}{2} \left( 1 - \frac{\Delta t}{\Delta x} u(x_i) \right) \right] + g_{1,i+1}^n \frac{\eta}{2} \left( 1 + \frac{\Delta t}{\Delta x} u(x_i) \right), \\ \rho_i^{n+1} = g_{1,i}^{n+1} + g_{2,i}^{n+1} \end{cases} \quad \text{where} \quad \eta := \frac{1}{C_d + \frac{1}{2}} = \frac{1}{\frac{\nu\Delta t}{\Delta x^2} + \frac{1}{2}}. \quad (36)$$

We name this scheme **LBM\*** scheme.

Let us note that when  $C_d = 1/2$ , (35) is not defined since  $|\widehat{\eta}|$  goes to the infinity when  $C_d$  goes to  $1/2$ : this comes from the fact that Lemma 3.1 is valid only when  $\widetilde{\varepsilon} \neq -\varepsilon$ . Nevertheless, (36) is defined for any  $C_d \geq 0$  since  $\eta \in ]0, 2]$ . In the sequel, we will show that the LBM\* scheme (36) is valid for any  $C_d \geq 0$ .

**Proof of Property 3.1:** The scheme (35) is equivalent to the scheme

$$\begin{cases} g_{1,i+1}^n = g_{1,i}^{n+1}(1 - \widehat{\eta}) + M_{1,i}^{n+1} \widehat{\eta}, \\ g_{2,i-1}^n = g_{2,i}^{n+1}(1 - \widehat{\eta}) + M_{2,i}^{n+1} \widehat{\eta} \end{cases}$$

that is to say to the scheme

$$\begin{cases} g_{1,i+1}^n = g_{1,i}^{n+1} \left[ 1 - \frac{\widehat{\eta}}{2} \left( 1 + \frac{\Delta t}{\Delta x} u(x_i) \right) \right] + g_{2,i-1}^{n+1} \frac{\widehat{\eta}}{2} \left( 1 - \frac{\Delta t}{\Delta x} u(x_i) \right), \\ g_{2,i-1}^n = g_{2,i}^{n+1} \left[ 1 - \frac{\widehat{\eta}}{2} \left( 1 - \frac{\Delta t}{\Delta x} u(x_i) \right) \right] + g_{1,i+1}^{n+1} \frac{\widehat{\eta}}{2} \left( 1 + \frac{\Delta t}{\Delta x} u(x_i) \right) \end{cases}$$

since  $M_{q,i} = \frac{g_{1,i} + g_{2,i}}{2} \left( 1 + (-1)^q \frac{\Delta t}{\Delta x} u(x_i) \right)$ . We end the proof by noting that

$$\begin{pmatrix} 1 - \frac{\widehat{\eta}}{2} \left( 1 + \frac{\Delta t}{\Delta x} u(x_i) \right) & \frac{\widehat{\eta}}{2} \left( 1 - \frac{\Delta t}{\Delta x} u(x_i) \right) \\ \frac{\widehat{\eta}}{2} \left( 1 + \frac{\Delta t}{\Delta x} u(x_i) \right) & 1 - \frac{\widehat{\eta}}{2} \left( 1 - \frac{\Delta t}{\Delta x} u(x_i) \right) \end{pmatrix}^{-1} = \begin{pmatrix} 1 - \frac{\eta}{2} \left( 1 + \frac{\Delta t}{\Delta x} u(x_i) \right) & \frac{\eta}{2} \left( 1 - \frac{\Delta t}{\Delta x} u(x_i) \right) \\ \frac{\eta}{2} \left( 1 + \frac{\Delta t}{\Delta x} u(x_i) \right) & 1 - \frac{\eta}{2} \left( 1 - \frac{\Delta t}{\Delta x} u(x_i) \right) \end{pmatrix}.$$

which comes from the fact that  $\widehat{\eta} + \eta = \widehat{\eta}\eta$ .  $\square$

### 3.4. First comparison between the LBM and LBM\* schemes

The LBM scheme (33) and the LBM\* scheme (36) are not equivalent *a priori* since  $u(x)$  may not be a constant and since  $g_{1,i-1}^n \neq g_{1,i+1}^n$  and  $g_{2,i-1}^n \neq g_{2,i+1}^n$  (compare (32) and (36)).

Moreover, the LBM scheme (33) with  $u(x) = 0$  is a classical LBM scheme applied to the heat equation [4, 5, 26]. But, the LBM\* scheme (36) is not a classical LBM scheme.

On the other side, it will be easier to take into account non-periodic boundary conditions with the LBM\* scheme (36) rather than with the LBM scheme (33). Indeed, for non-periodic boundary conditions in  $x_{\min}$ , we will have to define  $g_{2,i=0}^n$  in (36), but we will have to define  $g_{2,i=0}^n$  and  $g_{1,i=0}^n$  (and  $u(x_{i-1})$ ) in (33). This point explains why we will prove the results in the sequel with the LBM\* scheme (36) and not with the LBM scheme (33) although (33) with  $u(x) = 0$  is a classical LBM scheme.

Nevertheless, we will show in §4 that the LBM scheme (33) and the LBM\* scheme (36) are in fact equivalent although they do not give the same  $g_{q,i}^n$  and, thus, the same  $\rho_i^n$  (except for a particular choice of the initial condition  $g_{q,i}^{n=0}$ ). This equivalence will imply that the results obtained with the LBM\* scheme (36) will be also valid for the LBM scheme (33).

### 3.5. Justification of the use of a third order integration formula to obtain the LBM schemes

We now justify the use of the third order integration formula (28) instead of the second order integration formula (27) through a basic property and some examples.

Since  $\int_0^{\Delta t} Q_q(f)[t+s, x+(-1)^q cs] ds$  in (24) is of the order of  $\Delta t / \sqrt{\varepsilon}$  (see (26)), the error of the scheme given an estimate of  $f_q(t, x)$  has to be of the order of  $\Delta t^s / \sqrt{\varepsilon}$  with  $s > 1$ . Moreover, the LBM scheme (33) and the LBM\* scheme (36) are such that  $\Delta t = \mathcal{O}(\varepsilon)$ . Thus, the error  $\Delta t^s / \sqrt{\varepsilon}$  is of the order of  $\varepsilon^{s-1/2}$ . We now use the following property:

**Property 3.2.** *Let us suppose that  $f_q^\varepsilon$  is solution of (20) and that  $\overline{f}_q^\varepsilon$  is an approximation of  $f_q^\varepsilon$  which satisfies*

$$\overline{f}_q^\varepsilon = f_q^\varepsilon + \varepsilon^k \Psi_q(t, t/\varepsilon, x, x/\sqrt{v\varepsilon})$$

where  $\Psi_q(t_1, t_2, x_1, x_2)$  is a  $C^\infty$ -function. Thus,  $\overline{\rho}^\varepsilon := \overline{f}_1^\varepsilon + \overline{f}_2^\varepsilon$  is solution of

$$\partial_t \overline{\rho}^\varepsilon + \partial_x (u \overline{\rho}^\varepsilon) = v \partial_{xx}^2 \overline{\rho}^\varepsilon + \mathcal{O}(\varepsilon)$$

when  $k \geq 2$ .

We deduce from this property that  $s$  has to be greater than  $5/2$  which implies that  $s = 3$  since  $s \in \mathbb{N}$ . This justifies to use the third order integration formula (28) instead of the second order integration formula (27). Of course, this property gives only a necessary condition to obtain consistent LBM schemes. It remains to prove that  $s = 3$  is also a sufficient condition: when  $u = 0$ , we will prove in §4 that this is also a sufficient condition by proving that the LBM schemes (33) and (36) converge to the solution of the heat equation.

Let us note that we impose that  $\Psi_q$  is a  $C^\infty$ -function to simplify the statement of Property 3.2. Indeed, we could choose  $\Psi_q$  with less regularity. Moreover, the variables  $t/\varepsilon$  and  $x/\sqrt{v\varepsilon}$  in  $\Psi_q$  underlines that this perturbation may act at kinetic scales. Let us also note that the expansion (12) shows that  $f_q^\varepsilon$  may have variations at kinetic scales only at the order  $\varepsilon^2$ , which is coherent with the previous result.

**Proof of Property 3.2:** Let us suppose that

$$\bar{f}_q^\varepsilon = f_q^\varepsilon + \varepsilon^k \Psi_q^\varepsilon(t, t/\varepsilon, x, x/\sqrt{v\varepsilon}).$$

In that case, we have

$$\begin{cases} \partial_t \bar{\rho}^\varepsilon = \partial_t \rho^\varepsilon + O(\varepsilon^{k-1}), \\ \partial_x(u \bar{\rho}^\varepsilon) = \partial_x(u \rho^\varepsilon) + O(\varepsilon^{k-1/2}), \\ \partial_{xx}^2 \bar{\rho}^\varepsilon = \partial_{xx}^2 \rho^\varepsilon + O(\varepsilon^{k-1}) \end{cases}$$

which allows to write that

$$\partial_t \bar{\rho}^\varepsilon + \partial_x(u \bar{\rho}^\varepsilon) - v \partial_{xx}^2 \bar{\rho}^\varepsilon = \partial_t \rho^\varepsilon + \partial_x(u \rho^\varepsilon) - v \partial_{xx}^2 \rho^\varepsilon + O(\varepsilon^{k-1}).$$

Thus, we obtain that

$$\partial_t \bar{\rho}^\varepsilon + \partial_x(u \bar{\rho}^\varepsilon) = v \partial_{xx}^2 \bar{\rho}^\varepsilon + O(\varepsilon)$$

when  $k \geq 2$  by using (11).□

We now verify that the LBM schemes built by using (27) instead of (28) cannot be consistent with the convection-diffusion equation (21) when  $\Delta t = \frac{\Delta x^2}{2v}$ . When  $u = 0$ , the LBM and LBM\* schemes using (27) are respectively given by

$$\begin{cases} f_{1,i}^{n+1} = f_{1,i+1}^n \left(1 - \frac{1}{2C_d}\right) + \frac{f_{2,i+1}^n}{2C_d}, \\ f_{2,i}^{n+1} = f_{2,i-1}^n \left(1 - \frac{1}{2C_d}\right) + \frac{f_{1,i-1}^n}{2C_d}, \\ \rho_i^{n+1} = f_{1,i}^{n+1} + f_{2,i}^{n+1} \end{cases} \quad (37)$$

and

$$\begin{cases} f_{1,i}^{n+1} = f_{1,i+1}^n \left(1 - \frac{1}{2(1-C_d)}\right) + \frac{f_{2,i-1}^n}{2(1-C_d)}, \\ f_{2,i}^{n+1} = f_{2,i-1}^n \left(1 - \frac{1}{2(1-C_d)}\right) + \frac{f_{1,i+1}^n}{2(1-C_d)}, \\ \rho_i^{n+1} = f_{1,i}^{n+1} + f_{2,i}^{n+1}. \end{cases} \quad (38)$$

When  $C_d = 1/2$  that is to say  $\Delta t = \frac{\Delta x^2}{2\nu}$ , formula (37) gives

$$\begin{cases} f_{1,i}^{n+1} = f_{2,i+1}^n, \\ f_{2,i}^{n+1} = f_{1,i-1}^n, \\ \rho_i^{n+1} = f_{1,i}^{n+1} + f_{2,i}^{n+1} \end{cases}$$

which is equivalent to

$$\begin{cases} f_{1,i}^{n+1} = f_{1,i}^{n-1}, \\ f_{2,i}^{n+1} = f_{2,i}^{n-1}, \\ \rho_i^{n+1} = f_{1,i}^{n+1} + f_{2,i}^{n+1}. \end{cases}$$

Finally, we obtain that

$$\rho_i^{n+1} = \rho_i^{n-1} \quad \text{when} \quad \Delta t = \frac{\Delta x^2}{2\nu}. \quad (39)$$

In the same way, we verify that when  $C_d = 1/2$ , formula (38) implies (39). Relation (39) shows that the LBM schemes (37) and (38) cannot be consistent with the heat equation when  $\Delta t = \frac{\Delta x^2}{2\nu}$ . By continuity, we deduce that the LBM schemes built by using (27) instead of (28) cannot be consistent with the convection-diffusion equation (21) when  $\Delta t = \frac{\Delta x^2}{2\nu}$ . Let us also note that the LBM schemes (37) and (38) are not bounded when  $C_d$  converges respectively to 0 (*i.e.*  $\Delta t = 0$ ) and to 1 (*i.e.*  $\Delta t = \frac{\Delta x^2}{\nu}$ ) which is not compatible with a consistent scheme.

### 3.6. The “magic” formula

The LBM scheme (33) is equivalent to the scheme

$$\begin{cases} g_{1,i}^{n+1} = g_{1,i+1}^n \left(1 - \frac{\Delta t}{\widehat{\varepsilon}}\right) + M_{1,i+1}^n \frac{\Delta t}{\widehat{\varepsilon}}, \\ g_{2,i}^{n+1} = g_{2,i-1}^n \left(1 - \frac{\Delta t}{\widehat{\varepsilon}}\right) + M_{2,i-1}^n \frac{\Delta t}{\widehat{\varepsilon}}, \\ \rho_i^{n+1} = g_{1,i}^{n+1} + g_{2,i}^{n+1} \end{cases}$$

where  $\widehat{\varepsilon}$  is such that  $\nu = \left(\widehat{\varepsilon} - \frac{\Delta t}{2}\right) \left(\frac{\Delta x}{\Delta t}\right)^2$ . And, by taking  $\Delta x = \Delta t = 1$  and by noting  $g_{q,i}^n$  with the function  $f_q(t, x)$ , we obtain the scheme

$$\begin{cases} f_1(t+1, x-1) = f_1(t, x) \left(1 - \frac{1}{\widehat{\varepsilon}}\right) + M_1(t, x) \frac{1}{\widehat{\varepsilon}}, \\ f_2(t+1, x+1) = f_2(t, x) \left(1 - \frac{1}{\widehat{\varepsilon}}\right) + M_2(t, x) \frac{1}{\widehat{\varepsilon}} \end{cases} \quad (40)$$

where

$$\nu = \left(\widehat{\varepsilon} - \frac{1}{2}\right) c_s^2 \quad (41)$$

with  $c_s := 1$ . The scheme (40) and the “magic” formula (41) is classical in the field of LBM-type schemes [4, 9]. The velocity  $c_s$  is classically named “pseudo sound speed of the lattice” [9]. It is not always equal

to one (it depends on the type of PDE which is solved with the LBM scheme). Nevertheless, it seems that the explanation of the formula (41) is not always clear. For example, it is written p. 129 in [9] that “(...) there is a numerical-diffusion-related viscosity coefficient absorbed into  $\nu$  by modifying  $\widehat{\varepsilon} \rightarrow \widehat{\varepsilon} - \frac{1}{2}$ . This coefficient is due to the first-order accuracy of the advection operator with the expansion  $f_q(t+1, x+(-1)^q) = \sum_{k=0}^{+\infty} \frac{\widehat{\varepsilon}^k}{k!} [\partial_t + (-1)^q \partial_x]^k f_q(t, x)$ .” Formula (41) is explained in [27, 28] with a Chapman-Enskog expansion applied to the scheme (40) but not to the continuous PDE (20) which makes difficult the understanding of the expansions to our opinion. In the case of the heat equation, the explanation of the formula (41) is clear and simple: it is a direct consequence of the third order integration formula (28) which allows to take into account the stiff term  $\frac{1}{\varepsilon}(M_q - f_q)$  in (20). More precisely, by using the formula (27) instead of the formula (28), we would have the relation  $\nu = \widehat{\varepsilon}c_s^2$  (deduced from (30)) instead of (41) but the LBM scheme would not capture the asymptotic regime (21) because of Property 3.2 (see the examples in §3.5).

### 3.7. Interpretation of the LBM and LBM\* schemes with an operator splitting

We can see the LBM scheme (33) as a simple discretization of

$$\partial_t g_q + (-1)^q c \partial_x g_q = \frac{1}{\varepsilon}(M_q - g_q) \quad \text{with} \quad \begin{cases} \widehat{\varepsilon} = \frac{\Delta t}{\eta}, \\ \eta = \frac{1}{C_d + \frac{1}{2}}, \\ c = \frac{\Delta x}{\Delta t} \end{cases} \quad (42)$$

based on the following *collision-transport* splitting:

*Collision:*

$$g_q^* = g_q^n \left(1 - \frac{\Delta t}{\varepsilon}\right) + \frac{\Delta t}{\varepsilon} M_q^n = g_q^n (1 - \eta) + \eta M_q^n.$$

*Transport:*

$$\begin{cases} g_{1,i}^{n+1} = g_{1,i+1}^*, \\ g_{2,i}^{n+1} = g_{2,i-1}^*. \end{cases}$$

The LBM\* scheme (36) may also be seen as a discretization of (42) based on a *collision-transport* splitting.

### 3.8. Some questions

We have proposed the LBM scheme (33) and the LBM\* scheme (36). In the sequel, we will study the following questions:

- Are these LBM schemes identical ?
- How to choose the initial conditions  $g_{1,i}^{n=0}$  and  $g_{2,i}^{n=0}$  ?
- How to define Neumann and Dirichlet boundary conditions ?
- Are these LBM schemes unconditionally stable and are there discrete maximum principles ?

- Do these LBM schemes converge toward the solution of the convection-diffusion equation and what is the order of the error ?
- Is it possible to give a probabilistic interpretation of these LBM schemes ?

We will give clear or partial answers to each of these questions by showing that there is a deep relation of the LBM scheme (33) and of the LBM\* scheme (36) with a finite difference type scheme.

#### 4. Link with a finite difference type scheme

We now prove that the LBM scheme (33) and the LBM\* scheme (36) with the initial condition

$$\begin{cases} g_{1,i}^0 = (1 - \alpha)\rho_i^0 \cdot \left(1 - \frac{\Delta t}{\Delta x}u(x_i)\right), \\ g_{2,i}^0 = \alpha\rho_i^0 \cdot \left(1 + \frac{\Delta t}{\Delta x}u(x_i)\right) \end{cases} \quad (43)$$

are equivalent to the finite difference type scheme

$$\frac{\rho_i^{n+1} - \rho_i^{n-1}}{2\Delta t} + \frac{\Delta t}{2\Delta x}(u(x_{i+1})\rho_{i+1}^n - u(x_{i-1})\rho_{i-1}^n) = \frac{\nu}{\Delta x^2}(\rho_{i+1}^n - \rho_i^{n+1} - \rho_i^{n-1} + \rho_{i-1}^n) \quad (44)$$

when the first iterate is given by

$$\rho_i^{n=1} := \xi\rho_{i-1}^0 + (1 - \xi)\rho_{i+1}^0 - \frac{\Delta t}{\Delta x} \left[ (1 - \alpha)\rho_{i+1}^0 u(x_{i+1}) - \alpha\rho_{i-1}^0 u(x_{i-1}) \right] \quad \text{where} \quad \xi = \frac{\eta}{2} + \alpha(1 - \eta) \quad (45)$$

in the case of the LBM scheme (33) and by

$$\rho_i^{n=1} := \alpha\rho_{i-1}^0 + (1 - \alpha)\rho_{i+1}^0 - \frac{\Delta t}{\Delta x} \left[ (1 - \alpha)\rho_{i+1}^0 u(x_{i+1}) - \alpha\rho_{i-1}^0 u(x_{i-1}) \right] \quad \text{where} \quad \alpha \in \mathbb{R} \quad (46)$$

in the case of the LBM\* scheme (36). When  $u(x) = 0$ , the scheme (44) is a Du Fort-Frankel scheme [22]. We will use this property in §5 and §6 to obtain new stability and convergence results in  $L^\infty$  and discrete maximum principles. Let us underline that the first iterate (46) is not classical for the Du Fort-Frankel. For example, in [22], the first iterate is defined with

$$\frac{\rho_i^{n=1} - \rho_i^n}{\Delta t} = \frac{\nu}{\Delta x^2}(\rho_{i+1}^0 - \rho_i^0 - \rho_i^0 + \rho_{i-1}^0). \quad (47)$$

Nevertheless, the first iterates (45) and (46) are essential, firstly, to obtain the equivalence between the LBM schemes (33) and (36) with (44) and, secondly, to obtain for any  $C_d \geq 0$  stability and convergence results in  $L^\infty$  and discrete maximum principles (when  $u(x) = 0$ ).

The link between the LBM scheme (33) with the Du Fort-Frankel scheme was firstly cited in [26] in the case of periodic boundary conditions. More generally, in the LBM litterature:

- Only the LBM scheme (33) is proposed. The LBM\* scheme (36) seems to have not been proposed. Yet, the numerical analysis of the LBM\* scheme is easier than the one of the LBM scheme.



- The cases of Neumann and Dirichlet boundary conditions are not studied.
- Stability and convergence results as well as discrete maximum principles are not proposed.
- The link between the initial condition  $g_q^0$  and the order of the error of the LBM schemes is not underlined.

And, up to now, it seems that the importance of the choice of the first iterate  $\rho_i^{n=1}$  to obtain good properties in  $L^\infty$  for the Du Fort-Frankel scheme was not underlined.

In the sequel of this section, in §5 and §6, we will study all these points. In particular, we will recover in this section the *bounced-back* boundary conditions which are classical in the framework of the LBM schemes, and we will define Neumann and Dirichlet boundary conditions for the LBM schemes (33) and (36) that are not classical.

At last, we recall that  $\eta = \frac{1}{C_d + \frac{1}{2}}$  and that  $\Delta t := C_d \frac{\Delta x^2}{\nu}$  where  $C_d \geq 0$ .

#### 4.1. Periodic boundary conditions for the convection-diffusion equation

We have the following result:

**Lemma 4.1.** *In the periodic case:*

i) *The LBM scheme (33)(43) is equivalent to the finite difference type scheme (44)(45).*

ii) *The LBM\* scheme (36)(43) is equivalent to the finite difference type scheme (44)(46).*

iii) *The LBM scheme (33)(43) and the LBM\* scheme (36)(43) are identical if and only if  $\alpha = \frac{1}{2}$ .*

The proof is written in §4.4. Let us remark that  $\xi \in [0, 1] \iff \alpha \in [0, 1]$  since  $\eta \in [0, 2]$ .

#### 4.2. Neumann boundary conditions for the heat equation

We now suppose that  $u(x) = 0$ . Thus, the LBM scheme (33) is now given by

$$\left\{ \begin{array}{l} g_{1,i}^{n+1} = g_{1,i+1}^n \left(1 - \frac{\eta}{2}\right) + g_{2,i+1}^n \frac{\eta}{2}, \\ g_{2,i}^{n+1} = g_{2,i-1}^n \left(1 - \frac{\eta}{2}\right) + g_{1,i-1}^n \frac{\eta}{2}, \\ \rho_i^{n+1} = g_{1,i}^{n+1} + g_{2,i}^{n+1} \end{array} \right. \quad \text{where} \quad \eta := \frac{1}{C_d + \frac{1}{2}} = \frac{1}{\frac{\nu \Delta t}{\Delta x^2} + \frac{1}{2}} \quad (48)$$

and the LBM\* scheme (36) is now given by

$$\left\{ \begin{array}{l} g_{1,i}^{n+1} = g_{1,i+1}^n \left(1 - \frac{\eta}{2}\right) + g_{2,i-1}^n \frac{\eta}{2}, \\ g_{2,i}^{n+1} = g_{2,i-1}^n \left(1 - \frac{\eta}{2}\right) + g_{1,i+1}^n \frac{\eta}{2}, \\ \rho_i^{n+1} = g_{1,i}^{n+1} + g_{2,i}^{n+1} \end{array} \right. \quad \text{where} \quad \eta := \frac{1}{C_d + \frac{1}{2}} = \frac{1}{\frac{\nu \Delta t}{\Delta x^2} + \frac{1}{2}}. \quad (49)$$

Moreover, the initial condition (43) is now given by

$$\begin{cases} g_{1,i}^0 = (1 - \alpha)\rho_i^0, & (a) \\ g_{2,i}^0 = \alpha\rho_i^0. & (b) \end{cases} \quad (50)$$

Here, we define the mesh  $x_i = x_{\min} + (i - \frac{1}{2})\Delta x$  ( $i = 1, \dots$ ) and we apply the Neumann boundary condition  $\partial_x \rho(t, x_{\min}) = 0$ . For the sake of simplicity, we forget the boundary condition in  $x_{\max}$ .

We have the following result:

**Lemma 4.2.** *The LBM\* scheme (49)(50) with the boundary conditions*

$$\begin{cases} g_{2,i=0}^{n+1} = g_{1,i=1}^{n+1} + (g_{2,i=0}^n - g_{1,i=1}^n)(1 - \eta), & (a) \\ g_{2,i=0}^{n=0} = \alpha\rho_{i=1}^{n=0} & (b) \end{cases} \quad (51)$$

is equivalent to the Du Fort-Frankel scheme

$$\forall i \geq 1 : \quad \frac{\rho_i^{n+1} - \rho_i^{n-1}}{2\Delta t} = \frac{\nu}{\Delta x^2}(\rho_{i+1}^n - \rho_i^{n+1} - \rho_i^{n-1} + \rho_{i-1}^n) \quad (52)$$

with the Neumann boundary condition

$$\rho_{i=0}^n = \rho_{i=1}^n \quad (53)$$

when the first iterate is given by

$$\forall i \geq 1 : \quad \rho_i^{n=1} = \alpha\rho_{i-1}^0 + (1 - \alpha)\rho_{i+1}^0 \quad \text{where} \quad \alpha \in \mathbb{R}. \quad (54)$$

We have the same result for the LBM scheme (48)(50) by replacing the boundary conditions (51) with

$$\begin{cases} g_{1,i=0}^{n+1} = g_{2,i=1}^{n+1} + (g_{1,i=1}^n - g_{2,i=0}^n)(1 - \eta), & (a) \\ g_{2,i=0}^{n+1} = g_{1,i=1}^{n+1} + (g_{2,i=0}^n - g_{1,i=1}^n)(1 - \eta), & (b) \\ g_{1,i=0}^{n=0} = (1 - \alpha)\rho_{i=1}^{n=0}, & (c) \\ g_{2,i=0}^{n=0} = \alpha\rho_{i=1}^{n=0} & (d) \end{cases} \quad (55)$$

and by replacing the first iterate (54) with

$$\rho_i^{n=1} := \xi\rho_{i-1}^0 + (1 - \xi)\rho_{i+1}^0 \quad \text{where} \quad \xi = \frac{\eta}{2} + \alpha(1 - \eta). \quad (56)$$

Thus, the LBM scheme (48)(50)(55) and the LBM\* scheme (49)(50)(51) are identical if and only if  $\alpha = \frac{1}{2}$ .

The proof is written in §4.4. Let us note that when  $\alpha = \frac{1}{2}$  that is to say when

$$g_{1,i}^0 = g_{2,i}^0 = \frac{\rho_i^0}{2},$$

the boundary conditions (51) and (55) are respectively equivalent to

$$g_{2,i=0}^n = g_{1,i=1}^n \quad (57)$$

and

$$g_{1,i=0}^n = g_{2,i=1}^n \quad \text{and} \quad g_{2,i=0}^n = g_{1,i=1}^n. \quad (58)$$

The boundary conditions (57) and (58) are classical in the framework of the LBM schemes and are named *bounce-back boundary conditions*. Nevertheless, when  $\alpha \neq \frac{1}{2}$ , the boundary conditions (51) and (55) are not classical in the framework of the LBM schemes.

#### 4.3. Dirichlet boundary conditions for the heat equation

To apply the Dirichlet boundary condition  $\rho(t, x_{\min}) = \rho_{x_{\min}}$ , we now define the mesh  $x_i = x_{\min} + i\Delta x$  ( $i = 1, \dots$ ). For the sake of simplicity, we forget the boundary conditions in  $x_{\max}$ .

We have the following result:

**Lemma 4.3.** *The LBM\* scheme (49)(50) with the boundary conditions*

$$\begin{cases} g_{2,i=0}^{n+1} = \frac{\rho_{x_{\min}}}{2} + \left( \frac{\rho_{x_{\min}}}{2} - g_{1,i=1}^n \right) (1 - \eta), & (a) \\ g_{2,i=0}^{n=0} = \alpha \rho_{x_{\min}} & (b) \end{cases} \quad (59)$$

is equivalent to the Du Fort-Frankel scheme (52) with the Dirichlet boundary condition

$$\rho_{i=0}^n = \rho_{x_{\min}} \quad (60)$$

when the first iterate is given by (54). We have the same result for the LBM scheme (48)(50) by replacing the boundary conditions (59) with

$$\begin{cases} g_{1,i=0}^{n+1} = g_{1,i=1}^n \left( 1 - \frac{\eta}{2} \right) + g_{2,i=1}^n \frac{\eta}{2}, & (a) \\ g_{2,i=0}^{n+1} = \rho_{x_{\min}} - g_{1,i=0}^{n+1}, & (b) \\ g_{1,i=0}^{n=0} = (1 - \alpha) \rho_{x_{\min}}, & (c) \\ g_{2,i=0}^{n=0} = \alpha \rho_{x_{\min}} & (d) \end{cases} \quad (61)$$

and by replacing the first iterate (54) with (56). Thus, the LBM scheme (48)(50)(61) and the LBM\* scheme (49)(50)(59) are identical if and only if  $\alpha = \frac{1}{2}$ .

The proof is written in §4.4. Let us note that the boundary conditions (59) and (61) are not classical in the framework of the LBM schemes. Let us also note that (61) is equivalent to

$$\begin{cases} g_{1,i=0}^{n+1} = \frac{\rho_{i=1}^n}{2} + \left( \frac{\rho_{i=1}^n}{2} - g_{2,i=1}^n \right) (1 - \eta), & (a) \\ g_{2,i=0}^{n+1} = \rho_{x_{\min}} - \frac{\rho_{i=1}^n}{2} + \left( \frac{\rho_{i=1}^n}{2} - g_{1,i=1}^n \right) (1 - \eta), & (b) \\ g_{1,i=0}^{n=0} = (1 - \alpha) \rho_{x_{\min}}, & (c) \\ g_{2,i=0}^{n=0} = \alpha \rho_{x_{\min}} & (d) \end{cases} \quad (62)$$

which underlines that (61)(b) is not exactly equal to (59)(a). Moreover, we may think that the boundary conditions should be

$$\forall n \geq 0 : \quad g_{2,i=0}^n = \frac{\rho_{x_{\min}}}{2} \quad (63)$$

for the LBM\* scheme (49) instead of (59) and

$$\forall n \geq 0 : \quad g_{1,i=0}^n = g_{2,i=0}^n = \frac{\rho_{x_{\min}}}{2} \quad (64)$$

for the LBM scheme (48) instead of (62). In §6.2, we will explain why we should replace (59) and (61) respectively by (63) and (64) when the number of cells is low even if we lose the equivalence with the Du Fort-Frankel scheme when we use this simple boundary conditions.

#### 4.4. Proof of Lemmas 4.1, 4.2 and 4.3

In the following proof, we firstly focus on the LBM\* scheme. Then, we focus on the LBM scheme which is less easy to study.

##### Proof of Lemma 4.1:

###### • Study of the LBM\* scheme:

We deduce from the LBM\* scheme (36) that  $\rho_i^{n+1} = g_{1,i+1}^n + g_{2,i-1}^n$  ( $n \geq 0$ ). Thus, by applying again (36), we find

$$\begin{aligned} \rho_i^{n+1} &= g_{1,i+2}^{n-1} \left[ 1 - \frac{\eta}{2} \left( 1 + \frac{\Delta t}{\Delta x} u(x_{i+1}) \right) \right] + g_{2,i}^{n-1} \frac{\eta}{2} \left( 1 - \frac{\Delta t}{\Delta x} u(x_{i+1}) \right) \\ &\quad + g_{2,i-2}^{n-1} \left[ 1 - \frac{\eta}{2} \left( 1 - \frac{\Delta t}{\Delta x} u(x_{i-1}) \right) \right] + g_{1,i}^{n-1} \frac{\eta}{2} \left( 1 + \frac{\Delta t}{\Delta x} u(x_{i-1}) \right) \quad \text{with } n \geq 1. \end{aligned} \quad (65)$$

By noting that

$$\begin{cases} \rho_{i+1}^n = g_{1,i+2}^{n-1} + g_{2,i}^{n-1}, \\ \rho_{i-1}^n = g_{1,i}^{n-1} + g_{2,i-2}^{n-1} \end{cases} \quad \text{with } n \geq 1, \quad (66)$$

we deduce from (65) that

$$\begin{aligned} \rho_i^{n+1} &= (\rho_{i+1}^n - g_{2,i}^{n-1}) \left( 1 - \frac{\eta}{2} \right) + g_{2,i}^{n-1} \frac{\eta}{2} + (\rho_{i-1}^n - g_{1,i}^{n-1}) \left( 1 - \frac{\eta}{2} \right) + g_{1,i}^{n-1} \frac{\eta}{2} \\ &\quad - \frac{\eta}{2} \cdot \frac{\Delta t}{\Delta x} (u(x_{i+1}) \rho_{i+1}^n - u(x_{i-1}) \rho_{i-1}^n) \quad \text{with } n \geq 1 \end{aligned}$$

that is to say

$$\rho_i^{n+1} = \rho_{i+1}^n \left( 1 - \frac{\eta}{2} \right) + \rho_{i-1}^n \left( 1 - \frac{\eta}{2} \right) + \rho_i^{n-1} (\eta - 1) - \frac{\eta}{2} \cdot \frac{\Delta t}{\Delta x} (u(x_{i+1}) \rho_{i+1}^n - u(x_{i-1}) \rho_{i-1}^n) \quad \text{with } n \geq 1. \quad (67)$$

By using the fact that  $\eta = \frac{1}{C_d + \frac{1}{2}}$ , we obtain

$$(2C_d + 1) \rho_i^{n+1} = 2C_d (\rho_{i+1}^n + \rho_{i-1}^n) + (1 - 2C_d) \rho_i^{n-1} - \frac{\Delta t}{\Delta x} (u(x_{i+1}) \rho_{i+1}^n - u(x_{i-1}) \rho_{i-1}^n) \quad \text{with } n \geq 1$$

that is to say

$$\rho_i^{n+1} - \rho_i^{n-1} = 2C_d(\rho_{i+1}^n - \rho_i^{n+1} - \rho_i^{n-1} + \rho_{i-1}^n) - \frac{\Delta t}{\Delta x}(u(x_{i+1})\rho_{i+1}^n - u(x_{i-1})\rho_{i-1}^n) \quad \text{with } n \geq 1$$

which is equivalent to

$$\frac{\rho_i^{n+1} - \rho_i^{n-1}}{2\Delta t} = \frac{\nu}{\Delta x^2}(\rho_{i+1}^n - \rho_i^{n+1} - \rho_i^{n-1} + \rho_{i-1}^n) - \frac{\Delta t}{2\Delta x}(u(x_{i+1})\rho_{i+1}^n - u(x_{i-1})\rho_{i-1}^n) \quad \text{with } n \geq 1.$$

We conclude the proof by noting that

$$\begin{cases} g_{1,i}^0 = (1 - \alpha)\rho_i^0 \cdot \left(1 - \frac{\Delta t}{\Delta x}u(x_i)\right), \\ g_{2,i}^0 = \alpha\rho_i^0 \cdot \left(1 + \frac{\Delta t}{\Delta x}u(x_i)\right) \end{cases}$$

coupled to the LBM\* scheme (36) implies that

$$\rho_i^1 = \alpha\rho_{i-1}^0 + (1 - \alpha)\rho_{i+1}^0 - \frac{\Delta t}{\Delta x} \left[ (1 - \alpha)\rho_{i+1}^0 u(x_{i+1}) - \alpha\rho_{i-1}^0 u(x_{i-1}) \right].$$

• *Study of the LBM scheme:*

We deduce from the LBM scheme (33) that

$$\rho_i^{n+1} = (g_{1,i+1}^n + g_{2,i-1}^n) \left(1 - \frac{\eta}{2}\right) + (g_{1,i-1}^n + g_{2,i+1}^n) \frac{\eta}{2} - \frac{\eta}{2} \cdot \frac{\Delta t}{\Delta x} (u(x_{i+1})\rho_{i+1}^n - u(x_{i-1})\rho_{i-1}^n).$$

Thus, by applying again (33), we find

$$\begin{aligned} \rho_i^{n+1} &= \left[ g_{1,i+2}^{n-1} \left(1 - \frac{\eta}{2}\right) + g_{2,i+2}^{n-1} \frac{\eta}{2} - \frac{\rho_{i+2}^{n-1}}{2} \cdot \eta \frac{\Delta t}{\Delta x} u(x_{i+2}) + g_{2,i-2}^{n-1} \left(1 - \frac{\eta}{2}\right) + g_{1,i-2}^{n-1} \frac{\eta}{2} + \frac{\rho_{i-2}^{n-1}}{2} \cdot \eta \frac{\Delta t}{\Delta x} u(x_{i-2}) \right] \left(1 - \frac{\eta}{2}\right) \\ &\quad \left[ g_{1,i}^{n-1} \left(1 - \frac{\eta}{2}\right) + g_{2,i}^{n-1} \frac{\eta}{2} - \frac{\rho_i^{n-1}}{2} \cdot \eta \frac{\Delta t}{\Delta x} u(x_i) + g_{2,i}^{n-1} \left(1 - \frac{\eta}{2}\right) + g_{1,i}^{n-1} \frac{\eta}{2} + \frac{\rho_i^{n-1}}{2} \cdot \eta \frac{\Delta t}{\Delta x} u(x_i) \right] \frac{\eta}{2} \\ &\quad - \frac{\eta}{2} \cdot \frac{\Delta t}{\Delta x} (u(x_{i+1})\rho_{i+1}^n - u(x_{i-1})\rho_{i-1}^n) \quad \text{with } n \geq 1 \end{aligned}$$

which is equivalent to

$$\begin{aligned} \rho_i^{n+1} &= \left[ (g_{1,i+2}^{n-1} + g_{2,i}^{n-1}) \left(1 - \frac{\eta}{2}\right) + (g_{1,i}^{n-1} + g_{2,i+2}^{n-1}) \frac{\eta}{2} - \frac{\eta}{2} \cdot \frac{\Delta t}{\Delta x} (u(x_{i+2})\rho_{i+2}^{n-1} - u(x_i)\rho_i^{n-1}) \right] \left(1 - \frac{\eta}{2}\right) \\ &\quad + \left[ (g_{1,i}^{n-1} + g_{2,i-2}^{n-1}) \left(1 - \frac{\eta}{2}\right) + (g_{1,i-2}^{n-1} + g_{2,i}^{n-1}) \frac{\eta}{2} - \frac{\eta}{2} \cdot \frac{\Delta t}{\Delta x} (u(x_i)\rho_i^{n-1} - u(x_{i-2})\rho_{i-2}^{n-1}) \right] \left(1 - \frac{\eta}{2}\right) \quad (68) \\ &\quad + (g_{1,i}^{n-1} + g_{2,i}^{n-1})(\eta - 1) - \frac{\eta}{2} \cdot \frac{\Delta t}{\Delta x} (u(x_{i+1})\rho_{i+1}^n - u(x_{i-1})\rho_{i-1}^n) \quad \text{with } n \geq 1. \end{aligned}$$

Moreover, we have

$$\begin{cases} \rho_{i+1}^n = (g_{1,i+2}^{n-1} + g_{2,i}^{n-1}) \left(1 - \frac{\eta}{2}\right) + (g_{1,i}^{n-1} + g_{2,i+2}^{n-1}) \frac{\eta}{2} - \frac{\eta}{2} \cdot \frac{\Delta t}{\Delta x} (u(x_{i+2})\rho_{i+2}^{n-1} - u(x_i)\rho_i^{n-1}), \\ \rho_{i-1}^n = (g_{1,i}^{n-1} + g_{2,i-2}^{n-1}) \left(1 - \frac{\eta}{2}\right) + (g_{1,i-2}^{n-1} + g_{2,i}^{n-1}) \frac{\eta}{2} - \frac{\eta}{2} \cdot \frac{\Delta t}{\Delta x} (u(x_i)\rho_i^{n-1} - u(x_{i-2})\rho_{i-2}^{n-1}) \end{cases} \quad \text{with } n \geq 1$$

which allows to obtain (67) by using (68). We conclude the proof as for the LBM\* scheme by noting that

$$\begin{cases} g_{1,i}^0 = (1 - \alpha)\rho_i^0 \cdot \left(1 - \frac{\Delta t}{\Delta x} u(x_i)\right), \\ g_{2,i}^0 = \alpha\rho_i^0 \cdot \left(1 + \frac{\Delta t}{\Delta x} u(x_i)\right) \end{cases}$$

coupled to the LBM scheme (33) implies that

$$\begin{aligned} \rho_i^1 &= \left[ (1 - \alpha)\rho_{i+1}^0 \cdot \left(1 - \frac{\Delta t}{\Delta x} u(x_{i+1})\right) + \alpha\rho_{i-1}^0 \cdot \left(1 + \frac{\Delta t}{\Delta x} u(x_{i-1})\right) \right] \left(1 - \frac{\eta}{2}\right) \\ &\quad + \left[ (1 - \alpha)\rho_{i-1}^0 \cdot \left(1 - \frac{\Delta t}{\Delta x} u(x_{i-1})\right) + \alpha\rho_{i+1}^0 \cdot \left(1 + \frac{\Delta t}{\Delta x} u(x_{i+1})\right) \right] \frac{\eta}{2} \\ &\quad - \frac{\eta}{2} \cdot \frac{\Delta t}{\Delta x} (u(x_{i+1})\rho_{i+1}^0 - u(x_{i-1})\rho_{i-1}^0) \\ &= \left[ (1 - \alpha) \left(1 - \frac{\eta}{2}\right) + \alpha \frac{\eta}{2} \right] \rho_{i-1}^0 + \left[ \alpha \left(1 - \frac{\eta}{2}\right) + (1 - \alpha) \frac{\eta}{2} \right] \rho_{i+1}^0 \\ &\quad - \frac{\Delta t}{\Delta x} \rho_{i+1}^0 u(x_{i+1}) \left[ (1 - \alpha) \left(1 - \frac{\eta}{2}\right) - \alpha \frac{\eta}{2} + \frac{\eta}{2} \right] + \frac{\Delta t}{\Delta x} \rho_{i-1}^0 u(x_{i-1}) \left[ \alpha \left(1 - \frac{\eta}{2}\right) - (1 - \alpha) \frac{\eta}{2} + \frac{\eta}{2} \right] \end{aligned}$$

that is to say

$$\rho_i^1 = \xi \rho_{i-1}^0 + (1 - \xi) \rho_{i+1}^0 - \frac{\Delta t}{\Delta x} \left[ (1 - \alpha) \rho_{i+1}^0 u(x_{i+1}) - \alpha \rho_{i-1}^0 u(x_{i-1}) \right]$$

where  $\xi = \frac{\eta}{2} + \alpha(1 - \eta)$ .  $\square$

### Proof of Lemma 4.2:

- *Study of the LBM\* scheme:*

To prove Lemma 4.1 in the case of the LBM\* scheme (36), we used (65) and (66) which come from an application of the LBM\* scheme in the cells  $i$  and  $i \pm 1$ . Thus, to obtain the equivalence between the LBM\* scheme (49) (obtained when  $u(x) = 0$ ) and the Du Fort-Frankel scheme (52) in the cell  $i = 1$ , the LBM\* scheme has to be applied when  $i = 0$ ,  $i = 1$  and  $i = 2$ . When  $i = 2$ , we do not have any difficulty to apply the LBM\* scheme (49). Nevertheless, when  $i = 0$  and  $i = 1$ ,  $g_{2,-1}^n$  and  $g_{2,0}^n$  have to be defined. When the boundary conditions are periodic,  $g_{2,-1}^n$  and  $g_{2,0}^n$  are defined. But, when the boundary conditions are not

periodic,  $g_{2,-1}^n$  and  $g_{2,0}^n$  are not defined *a priori*. We will define these quantities in such a way the Neumann boundary condition

$$\rho_{i=0}^n = \rho_{i=1}^n \quad (69)$$

is satisfied. Let us apply the LBM\* scheme (49) when  $i = 0$ . We have

$$\rho_0^{n+1} = g_{1,1}^n + g_{2,-1}^n$$

which implies by using (69) at the time  $t^{n+1}$  that

$$g_{2,-1}^n = \rho_1^{n+1} - g_{1,1}^n.$$

But, we have also

$$g_{2,0}^{n+1} = g_{2,-1}^n \left(1 - \frac{\eta}{2}\right) + g_{1,1}^n \frac{\eta}{2}.$$

Thus, we have

$$g_{2,0}^{n+1} = (\rho_1^{n+1} - g_{1,1}^n) \left(1 - \frac{\eta}{2}\right) + g_{1,1}^n \frac{\eta}{2}.$$

Let us now apply the LBM\* scheme (49) when  $i = 1$ . We have

$$\rho_1^{n+1} = g_{1,2}^n + g_{2,0}^n.$$

This means that

$$\begin{aligned} g_{2,0}^{n+1} &= (g_{1,2}^n + g_{2,0}^n - g_{1,1}^n) \left(1 - \frac{\eta}{2}\right) + g_{1,1}^n \frac{\eta}{2} \\ &= g_{1,2}^n \left(1 - \frac{\eta}{2}\right) + g_{2,0}^n \frac{\eta}{2} + (g_{2,0}^n - g_{1,1}^n)(1 - \eta). \end{aligned}$$

But, we have also

$$g_{1,1}^{n+1} = g_{1,2}^n \left(1 - \frac{\eta}{2}\right) + g_{2,0}^n \frac{\eta}{2}.$$

Thus

$$g_{2,0}^{n+1} = g_{1,1}^{n+1} + (g_{2,0}^n - g_{1,1}^n)(1 - \eta)$$

which gives (51)(a). We conclude by noting that (51)(b) is a consequence of (50)(b) and (53).

• *Study of the LBM scheme:* Let us apply the LBM scheme (48) when  $i = 0$  and  $i = 1$ . We have

$$\rho_0^{n+1} = (g_{1,1}^n + g_{2,-1}^n) \left(1 - \frac{\eta}{2}\right) + (g_{1,-1}^n + g_{2,1}^n) \frac{\eta}{2}$$

and

$$\rho_1^{n+1} = (g_{1,2}^n + g_{2,0}^n) \left(1 - \frac{\eta}{2}\right) + (g_{1,0}^n + g_{2,2}^n) \frac{\eta}{2}.$$

Thus, by taking into account (69) at the time  $t^{n+1}$ , we obtain

$$(g_{1,1}^n + g_{2,-1}^n) \left(1 - \frac{\eta}{2}\right) + (g_{1,-1}^n + g_{2,1}^n) \frac{\eta}{2} = (g_{1,2}^n + g_{2,0}^n) \left(1 - \frac{\eta}{2}\right) + (g_{1,0}^n + g_{2,2}^n) \frac{\eta}{2}. \quad (70)$$

We have also

$$g_{1,1}^{n+1} = g_{1,2}^n \left(1 - \frac{\eta}{2}\right) + g_{2,2}^n \frac{\eta}{2}$$

and

$$g_{2,0}^{n+1} = g_{2,-1}^n \left(1 - \frac{\eta}{2}\right) + g_{1,-1}^n \frac{\eta}{2}.$$

Thus, we deduce from (70) that

$$g_{2,0}^{n+1} = g_{1,1}^{n+1} + (g_{2,0}^n - g_{1,1}^n) \left(1 - \frac{\eta}{2}\right) + (g_{1,0}^n - g_{2,1}^n) \frac{\eta}{2}$$

that is to say

$$\begin{aligned} g_{2,0}^{n+1} &= g_{1,1}^{n+1} + (g_{2,0}^n - g_{1,1}^n)(1 - \eta) + [(g_{2,0}^n - g_{1,1}^n) + (g_{1,0}^n - g_{2,1}^n)] \frac{\eta}{2} \\ &= g_{1,1}^{n+1} + (g_{2,0}^n - g_{1,1}^n)(1 - \eta) + (\rho_0^n - \rho_1^n) \frac{\eta}{2} \end{aligned}$$

which gives (55)(b) by taking into account (69). By using (55)(b), we obtain

$$g_{1,0}^{n+1} + g_{2,0}^{n+1} = g_{1,0}^{n+1} + g_{1,1}^{n+1} + (g_{2,0}^n - g_{1,1}^n)(1 - \eta).$$

Thus, by using (69) at the time  $t^{n+1}$ , we obtain

$$g_{1,1}^{n+1} + g_{2,1}^{n+1} = g_{1,0}^{n+1} + g_{1,1}^{n+1} + (g_{2,0}^n - g_{1,1}^n)(1 - \eta)$$

which gives (55)(a). Moreover, (55)(c,d) is a consequence of (50) and (53). At last, we obtain that

$$\rho_i^1 = \xi \rho_{i-1}^0 + (1 - \xi) \rho_{i+1}^0$$

as in the periodic case.  $\square$

**Proof of Lemma 4.3:** The proof is similar to the one of Lemma 4.2.

• *Study of the LBM\* scheme:*

Let us apply the LBM\* scheme (49) when  $i = 0$ . We have

$$\rho_0^{n+1} = g_{1,1}^n + g_{2,-1}^n.$$

Thus, by applying the boundary condition

$$\rho_{i=0}^n = \rho_{x_{\min}} \tag{71}$$

at the time  $t^{n+1}$ , we obtain that

$$g_{2,-1}^n = \rho_{x_{\min}} - g_{1,1}^n.$$

But, we have also

$$g_{2,0}^{n+1} = g_{2,-1}^n \left(1 - \frac{\eta}{2}\right) + g_{1,1}^n \frac{\eta}{2}.$$

Thus, we have

$$g_{2,0}^{n+1} = (\rho_{x_{\min}} - g_{1,1}^n) \left(1 - \frac{\eta}{2}\right) + g_{1,1}^n \frac{\eta}{2}$$

that is to say

$$g_{2,0}^{n+1} = \frac{\rho_{x_{\min}}}{2} + \left(\frac{\rho_{x_{\min}}}{2} - g_{1,1}^n\right)(1 - \eta)$$



which gives (59)(a). We conclude the proof as in the periodic case.

• *Study of the LBM scheme:*

Let us apply the LBM scheme (48) when  $i = 0$ . We have

$$g_{1,0}^{n+1} = g_{1,1}^n \left(1 - \frac{\eta}{2}\right) + g_{2,1}^n \frac{\eta}{2}$$

which gives (61)(a). We obtain (61)(b) by applying (71) at the time  $t^{n+1}$ . We conclude the proof as in the periodic case.  $\square$

### 5. Stability and convergence in $L^\infty$ for the LBM schemes applied to the heat equation

In the periodic, Neumann and Dirichlet cases, the LBM scheme (48)(50) and the LBM\* scheme (49)(50) are equivalent to the Du Fort-Frankel scheme (52) when the first iterate is given by (54) that is to say by

$$\rho_i^{n=1} := \alpha \rho_{i-1}^0 + (1 - \alpha) \rho_{i+1}^0 \quad \text{where} \quad \alpha \in \mathbb{R}$$

(see Lemmae 4.1, 4.2 and 4.3). This will allow us, firstly, to obtain the stability in  $L^\infty$  for any  $C_d \geq 0$  of the LBM and Du Fort-Frankel schemes and, secondly, to prove the convergence in  $L^\infty$  of these schemes also for any  $C_d \geq 0$ . This will also allow us to obtain discrete maximum principles for the LBM and Du Fort-Frankel schemes for any  $C_d \geq 0$  (we study this point in §6). Let us recall that the first iterate (54) of the Du Fort-Frankel scheme is not classical; in [22], it is defined with the classical three-points scheme

$$\frac{\rho_i^{n=1} - \rho_i^n}{\Delta t} = \frac{\nu}{\Delta x^2} (\rho_{i+1}^0 - \rho_i^0 - \rho_i^0 + \rho_{i-1}^0). \quad (72)$$

The first iterate (72) is more natural than (54). Nevertheless, when we do not use (54), we obtain that the Du Fort-Frankel scheme is stable for any  $C_d \geq 0$  in  $L^2$  (at least when  $n \geq 2$ ) [22] and, thus, not in  $L^\infty$ . Moreover, it seems difficult to obtain discrete maximum principles for any  $C_d \geq 0$  without using (54).

For the sake of simplicity, we forget the boundary condition in  $x = x_{\max}$  in the cases of Neumann and Dirichlet boundary conditions. Moreover, we recall that  $\Delta t := C_d \frac{\Delta x^2}{\nu}$  and that  $\eta := \frac{1}{C_d + \frac{1}{2}} \in ]0, 2]$  where  $C_d \geq 0$ . We have the following result:

**Proposition 5.1.**

*i) The LBM\* scheme (49)(50) with periodic, Neumann or Dirichlet boundary conditions converge in  $L^\infty$  and*

verifies:

$$\left\{ \begin{array}{l}
\text{Periodic case: } \max_i |\rho_i^n| \leq 2 \max(|1 - \alpha|, |\alpha|) \cdot \max_i |\rho_i^0| \quad \text{when } \begin{cases} C_d \geq 0, \\ \alpha \in \mathbb{R}. \end{cases} \quad (a) \\
\text{Neumann case: } \begin{cases} \max_{i \geq 1} |\rho_i^{n+1}| \leq 2 \max(|1 - \alpha|, |\alpha|) \cdot \max_{i \geq 1} |\rho_i^0| + 2|2\alpha - 1| \frac{|1 - \eta|}{1 - |1 - \eta|} |\rho_1^0| \\ \max_{i \geq 1} |\rho_i^{n+1}| \leq 2 \max(|1 - \alpha|, |\alpha|) \cdot \max_{i \geq 1} |\rho_i^0| \\ \max_{i \geq 1} |\rho_i^{n+1}| \leq 2 \max(|1 - \alpha|, |\alpha|) \cdot \max_{i \geq 1} |\rho_i^0| \end{cases} \quad \text{when } \begin{cases} C_d > 0, \\ \alpha \in \mathbb{R}. \\ C_d \geq 0, \\ \alpha = \frac{1}{2}. \\ C_d = 0, \\ \alpha \in \mathbb{R}. \end{cases} \quad (b) \\
\text{Dirichlet case: } \max_{i \geq 1} |\rho_i^{n+1}| \leq 2 \max(|1 - \alpha|, |\alpha|) \cdot \max\left(\max_{i \geq 1} |\rho_i^0|, |\rho_{x_{\min}}|\right) + \frac{2\left(1 - \frac{\eta}{2}\right)}{1 - |\eta - 1|} |\rho_{x_{\min}}| \quad \text{when } \begin{cases} C_d \geq 0, \\ \alpha \in \mathbb{R}. \end{cases} \quad (c)
\end{array} \right. \quad (73)$$

We have the same results for the LBM scheme (48)(50) by replacing  $\alpha$  with  $\xi = \frac{\eta}{2} + \alpha(1 - \eta)$  in (73).

ii) The Du Fort-Frankel scheme (52) with periodic, Neumann or Dirichlet boundary conditions converges in  $L^\infty$  when the first iterate is given by (54), and verifies (73).

iii) The error of the LBM schemes and of the Du Fort-Frankel scheme is of order  $\Delta x$  when  $\alpha \neq \frac{1}{2}$  and is of order  $\Delta x^2$  if and only if  $\alpha = \frac{1}{2}$ .

When the boundary conditions is a Dirichlet boundary condition in  $x = x_{\min}$  and a Neumann boundary condition in  $x = x_{\max}$ , due to the linearity of the scheme, we easily deduce from the proof of Proposition 5.1 that we simply have to replace (73)(b,c) by

$$\max_{1 \leq i \leq N} |\rho_i^{n+1}| \leq 2 \max(|1 - \alpha|, |\alpha|) \cdot \max\left(\max_{1 \leq i \leq N} |\rho_i^0|, |\rho_{x_{\min}}|\right) + \frac{2\left(1 - \frac{\eta}{2}\right)}{1 - |\eta - 1|} |\rho_{x_{\min}}| + 2|2\alpha - 1| \frac{|1 - \eta|}{1 - |1 - \eta|} |\rho_N^0|$$

(when  $C_d > 0$  and  $\alpha \in \mathbb{R}$ ) where  $N$  is the number of cells. The other possible cases are similar. It is known since 1953 that the Du Fort-Frankel scheme with periodic boundary conditions is stable – and, thus, is convergent – in  $L^2$  for any  $C_d \geq 0$  (this result is obtained *via* a Fourier analysis). Since the Du Fort-Frankel scheme may be written with

$$\rho_i^{n+1} = \rho_{i+1}^n \left(1 - \frac{\eta}{2}\right) + \rho_{i-1}^n \left(1 - \frac{\eta}{2}\right) + \rho_i^{n-1} (\eta - 1)$$

(see (67) with  $u(x) = 0$ ), we have also the stability in  $L^\infty$  under the stability condition  $\eta \in [1, 2]$  that is to say when  $0 \leq C_d \leq 1/2$  (for a reasonable choice of the first iterate: with (47) for example). Here, we obtain the stability in  $L^\infty$  of the Du Fort-Frankel scheme – and, thus, the convergence in  $L^\infty$  – for any  $C_d \geq 0$  when the first iterate is defined with (54).

At last, let us remark that (73)(b) with  $C_d = 0$  (that is to say when  $\Delta t = 0$ ) seems strange in the sense that we do not write  $\rho_i^n = \rho_i^0$  when  $C_d = 0$ : we will discuss about this question in §7.1.

**Proof of Proposition 5.1:**

Firstly, we prove the stability in  $L^\infty$  for any  $C_d \geq 0$  of the LBM\* scheme (49). Indeed, it is more simple to analyze this scheme than the LBM scheme (48). Then, by applying Lemmae 4.1, 4.2 and 4.3 (and the Lax Theorem), we easily obtain the other results.

- *Stability in  $L^\infty$  of the LBM\* scheme with periodic boundary conditions:*

Since  $\eta \in ]0, 2]$ , we deduce from (49) that

$$\max_i (|g_{1,i}^{n+1}|, |g_{2,i}^{n+1}|) \leq \max_i (|g_{1,i}^n|, |g_{2,i}^n|) \quad (74)$$

which proves the unconditionnal stability in  $L^\infty$  as soon as the initial condition is bounded. Moreover, since  $\rho_i^{n+1} = g_{1,i}^{n+1} + g_{2,i}^{n+1}$ , we have

$$\max_i |\rho_i^n| \leq 2 \max_i (|g_{1,i}^{n+1}|, |g_{2,i}^{n+1}|).$$

Thus, we deduce from (74) that

$$\max_i |\rho_i^n| \leq 2 \max_i (|g_{1,i}^0|, |g_{2,i}^0|)$$

that is to say

$$\max_i |\rho_i^n| \leq 2 \max(|1 - \alpha|, |\alpha|) \cdot \max_i |\rho_i^0| \quad (75)$$

by using the initial condition (50).

- *Stability in  $L^\infty$  of the LBM\* scheme with Neumann boundary conditions:*

Since  $\eta \in ]0, 2]$ , we deduce from (49) that

$$\max_{i \geq 1} (|g_{1,i}^{n+1}|, |g_{2,i}^{n+1}|) \leq \max[|g_{2,0}^n|, \max_{i \geq 1} (|g_{1,i}^n|, |g_{2,i}^n|)]. \quad (76)$$

Inequalities (74) and (76) are different because of the boundary term  $|g_{2,0}^n|$  in (76) which does not exist when the boundary conditions are periodic. The difficulty to obtain the stability in  $L^\infty$  comes from this term. We deduce from the boundary condition (51)(a) that

$$\begin{aligned} g_{2,0}^{n+1} &= g_{1,1}^{n+1} + (1 - \eta)g_{2,0}^n - (1 - \eta)g_{1,1}^n \\ &= g_{1,1}^{n+1} + (1 - \eta)[g_{1,1}^n + (1 - \eta)g_{2,0}^{n-1} - (1 - \eta)g_{1,1}^{n-1}] - (1 - \eta)g_{1,1}^n \\ &= g_{1,1}^{n+1} + (1 - \eta)^2 g_{2,0}^{n-1} - (1 - \eta)^2 g_{1,1}^{n-1} \\ &= \dots \\ &= g_{1,1}^{n+1} + (1 - \eta)^{n+1} g_{2,0}^0 - (1 - \eta)^{n+1} g_{1,1}^0 \end{aligned}$$

that is to say

$$g_{2,0}^{n+1} = g_{1,1}^{n+1} + (1 - \eta)^{n+1} (g_{2,0}^0 - g_{1,1}^0). \quad (77)$$

On the other side, we have

$$g_{1,1}^{n+1} = g_{1,2}^n \left(1 - \frac{\eta}{2}\right) + g_{2,0}^n \frac{\eta}{2}.$$

Thus, by using (77), we obtain

$$g_{2,0}^{n+1} \leq \max(|g_{1,2}^n|, |g_{2,0}^n|) + |1 - \eta|^{n+1} \cdot |g_{2,0}^0 - g_{1,1}^0|.$$

By injecting this inequality in (76), we find

$$\max[|g_{2,0}^{n+1}|, \max_{i \geq 1}(|g_{1,i}^{n+1}|, |g_{2,i}^{n+1}|)] \leq \max \left[ \max(|g_{1,2}^n|, |g_{2,0}^n|) + |1 - \eta|^{n+1} \cdot |g_{2,0}^0 - g_{1,1}^0|, \max_{i \geq 1}(|g_{1,i}^n|, |g_{2,i}^n|) \right]. \quad (78)$$

Let us now define

$$G^n := \max[|g_{2,0}^n|, \max_{i \geq 1}(|g_{1,i}^n|, |g_{2,i}^n|)]. \quad (79)$$

We deduce from (78) that

$$G^{n+1} \leq G^n + |1 - \eta|^{n+1} \cdot |g_{2,0}^0 - g_{1,1}^0|$$

that is to say

$$G^{n+1} \leq G^0 + |1 - \eta| S_n \cdot |g_{2,0}^0 - g_{1,1}^0| \quad (80)$$

where

$$S_n := \sum_{k=0}^n |1 - \eta|^k. \quad (81)$$

Let us now suppose that  $\eta \in ]0, 2[$  that is to say  $C_d > 0$ . By noting that  $S_n \leq \frac{1}{1 - |\eta - 1|}$  when  $\eta \in ]0, 2[$ , we obtain

$$G^{n+1} \leq G^0 + \frac{|1 - \eta|}{1 - |1 - \eta|} |g_{2,0}^0 - g_{1,1}^0| \quad (82)$$

which proves the unconditionnal stability in  $L^\infty$  as soon as the initial condition is bounded. Moreover, by applying the arguments used to obtain (75) in the periodic case, we deduce from (82) that

$$\max_{i \geq 0} |\rho_i^{n+1}| \leq 2 \max(|1 - \alpha|, |\alpha|) \cdot \max_{i \geq 0} |\rho_i^0| + 2|2\alpha - 1| \frac{|1 - \eta|}{1 - |1 - \eta|} |\rho_1^0|$$

that is to say

$$\max_{i \geq 1} |\rho_i^{n+1}| \leq 2 \max(|1 - \alpha|, |\alpha|) \cdot \max_{i \geq 1} |\rho_i^0| + 2|2\alpha - 1| \frac{|1 - \eta|}{1 - |1 - \eta|} |\rho_1^0|$$

when  $\eta \in ]0, 2[$  since  $\rho_0^n = \rho_1^n$ . Let us now suppose that  $\eta = 2$  that is to say  $C_d = 0$ . We deduce from (49) and (51) that  $g_{q,i}^{n+1} = g_{q,i}^{n-1}$  for any  $i \geq 1$  and  $q \in \{1, 2\}$ , and that  $g_{2,0}^{n+1} = g_{2,0}^{n-1}$  which allows to obtain

$$\max_{i \geq 1} |\rho_i^{n+1}| \leq 2 \max(|1 - \alpha|, |\alpha|) \cdot \max_{i \geq 1} |\rho_i^0|. \quad (83)$$

At last, when  $\alpha = \frac{1}{2}$  and for any  $\eta \in ]0, 2[$ , we have  $g_{2,0}^0 = g_{1,1}^0$  which implies that  $G^{n+1} \leq G^0$  by using (80). Thus, (83) is also satisfied.

- *Stability in  $L^\infty$  of the LBM\* scheme with Dirichlet boundary conditions:*

Inequality (76) is still satisfied. Moreover, we deduce from the boundary condition (59)(a) that

$$|g_{2,0}^{n+1}| \leq \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| + |\eta - 1| \cdot |g_{1,1}^n|.$$

Thus, by using (76), we obtain

$$\max[|g_{2,0}^{n+1}|, \max_{i \geq 1} (|g_{1,i}^{n+1}|, |g_{2,i}^{n+1}|)] \leq \max \left[ \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| + |\eta - 1| \cdot |g_{1,1}^n|, |g_{2,0}^n|, \max_{i \geq 1} (|g_{1,i}^n|, |g_{2,i}^n|) \right]. \quad (84)$$

We deduce from (84) that

$$G^{n+1} \leq \max \left[ \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| + |\eta - 1| G^n, G^n \right]. \quad (85)$$

where  $G^n$  is defined with (79). Thus, we have also

$$G^{n+1} \leq \max \left[ \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| + |\eta - 1| \max \left[ \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| + |\eta - 1| G^{n-1}, G^{n-1} \right], \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| + |\eta - 1| G^{n-1}, G^{n-1} \right]$$

that is to say

$$G^{n+1} \leq \max \left[ \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| \cdot (1 + |\eta - 1|) + |\eta - 1|^2 G^{n-1}, \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| + |\eta - 1| G^{n-1}, G^{n-1} \right].$$

The previous inequalities incite us to prove that

$$\begin{aligned} G^{n+1} &\leq \max \left[ \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| S_m + |\eta - 1|^{m+1} G^{n-m}, \right. \\ &\quad \left. \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| S_{m-1} + |\eta - 1|^m G^{n-m}, \right. \\ &\quad \dots, \\ &\quad \left. \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| S_0 + |\eta - 1| G^{n-m}, \right. \\ &\quad \left. G^{n-m} \right] \end{aligned} \quad (86)$$

where  $S_m$  is defined with (81). We know that (86) is verified when  $m = 0$  and  $m = 1$ . Let us now suppose that (86) is verified at the rank  $m$ . By injecting (85) in (86), we obtain

$$\begin{aligned} G^{n+1} &\leq \max \left\{ \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| S_m + |\eta - 1|^{m+1} \max \left[ \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| + |\eta - 1| G^{n-m-1}, G^{n-m-1} \right], \right. \\ &\quad \left. \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| S_{m-1} + |\eta - 1|^m \max \left[ \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| + |\eta - 1| G^{n-m-1}, G^{n-m-1} \right], \right. \\ &\quad \dots, \\ &\quad \left. \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| S_0 + |\eta - 1| \max \left[ \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| + |\eta - 1| G^{n-m-1}, G^{n-m-1} \right], \right. \\ &\quad \left. \max \left[ \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| + |\eta - 1| G^{n-m-1}, G^{n-m-1} \right] \right\} \end{aligned}$$

which gives

$$\begin{aligned}
G^{n+1} \leq \max & \left[ \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| (S_m + |\eta - 1|^{m+1}) + |\eta - 1|^{m+2} G^{n-m-1}, \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| S_m + |\eta - 1|^{m+1} G^{n-m-1} \right. \\
& \left. \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| (S_{m-1} + |\eta - 1|^m) + |\eta - 1|^{m+1} G^{n-m-1}, \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| S_{m-1} + |\eta - 1|^m G^{n-m-1} \right. \\
& \dots, \\
& \left. \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| (S_0 + |\eta - 1|) + |\eta - 1|^2 G^{n-m-1}, \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| S_0 + |\eta - 1| G^{n-m-1} \right. \\
& \left. \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| + |\eta - 1| G^{n-m-1}, G^{n-m-1} \right]
\end{aligned}$$

that is to say

$$\begin{aligned}
G^{n+1} \leq \max & \left[ \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| S_{m+1} + |\eta - 1|^{m+2} G^{n-m-1}, \right. \\
& \left. \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| S_m + |\eta - 1|^{m+1} G^{n-m-1}, \right. \\
& \dots, \\
& \left. \left(1 - \frac{\eta}{2}\right) |\rho_{x_{\min}}| S_0 + |\eta - 1| G^{n-m-1}, \right. \\
& \left. G^{n-m-1} \right].
\end{aligned}$$

Thus, (86) is also verified at the rank  $m + 1$ , which proves (86) for any  $m \in \{0, \dots, n - 1\}$ . By applying (86) at the rank  $n - 1$ , by noting that  $S_m \leq \frac{1}{1-|\eta-1|}$  and that  $|\eta - 1|^m \leq 1$  for any  $m \in \mathbb{N}$  (we recall that  $\eta \in ]0, 2[$ ), we obtain that

$$G^{n+1} \leq \frac{1 - \frac{\eta}{2}}{1 - |\eta - 1|} |\rho_{x_{\min}}| + G^0 \quad (87)$$

which proves the unconditionnal stability in  $L^\infty$  as soon as the initial condition is bounded. Moreover, by applying the arguments used to obtain (75) in the periodic case, we deduce from (87) that

$$\max_{i \geq 0} |\rho_i^{n+1}| \leq 2 \max(|1 - \alpha|, |\alpha|) \max_{i \geq 0} |\rho_i^0| + \frac{2 \left(1 - \frac{\eta}{2}\right)}{1 - |\eta - 1|} |\rho_{x_{\min}}|$$

that is to say

$$\max_{i \geq 1} |\rho_i^{n+1}| \leq 2 \max(|1 - \alpha|, |\alpha|) \cdot \max \left( \max_{i \geq 1} |\rho_i^0|, |\rho_{x_{\min}}| \right) + \frac{2 \left(1 - \frac{\eta}{2}\right)}{1 - |\eta - 1|} |\rho_{x_{\min}}|$$

since  $\rho_i^n = \rho_{x_{\min}}$ .

• *Stability in  $L^\infty$  of the Du Fort-Frankel scheme:*

By using the unconditionnal stability in  $L^\infty$  of the LBM\* scheme (49)(50) and by using Lemmae 4.1, 4.2 and 4.3, we obtain the unconditionnal stability in  $L^\infty$  of the Du Fort-Frankel scheme (52)(54).

- *Stability in  $L^\infty$  of the LBM scheme:*

By using the unconditionnal stability in  $L^\infty$  of the Du Fort-Frankel scheme (52)(56) and by using again Lemmae 4.1, 4.2 and 4.3, we obtain the unconditionnal stability in  $L^\infty$  of the LBM scheme (48)(50).

- *Consistency and order of the error:*

When  $n \geq 2$  and when  $\Delta t = C_d \frac{\Delta x^2}{\nu}$  ( $C_d \geq 0$ ), the Du Fort-Frankel scheme (52) is consistent and its error is of order  $\Delta x^2$  [22]. Let us study the first iterate (54). We have

$$\begin{aligned}\rho_i^1 &= \alpha \rho_{i-1}^0 + (1 - \alpha) \rho_{i+1}^0 \\ &= \rho_{exact}(0, x_i) + \mathcal{O}(\Delta x^\beta) \\ &= \rho_{exact}(\Delta t, x_i) + \mathcal{O}(\Delta t, \Delta x^\beta)\end{aligned}$$

with

$$\begin{cases} \alpha \neq 1/2 \implies \beta = 1, \\ \alpha = 1/2 \implies \beta = 2 \end{cases}$$

where  $\rho_{exact}$  is the exact solution of the heat equation. Thus, we have the consistency for any  $\alpha \in \mathbb{R}$ . Moreover, the error is of order  $\Delta x$  when  $\alpha \neq \frac{1}{2}$  and is of order  $\Delta x^2$  if and only if  $\alpha = \frac{1}{2}$ .

- *Convergence in  $L^\infty$ :*

When  $\Delta t = C_d \frac{\Delta x^2}{\nu}$ , we obtain the convergence in  $L^\infty$  of the Du Fort-Frankel scheme for any  $C_d \geq 0$  by applying the Lax Theorem. Thus, by using again Lemmae 4.1, 4.2 and 4.3, we also obtain the convergence in  $L^\infty$  of the LBM and LBM\* schemes for any  $C_d \geq 0$ .  $\square$

## 6. Discrete maximum principles for the LBM schemes applied to the heat equation

It is easy to obtain a discrete maximum principle for the Du Fort-Frankel scheme (52) when  $C_d \in [0, \frac{1}{2}]$  (we recall that  $\Delta t := C_d \frac{\Delta x^2}{\nu}$ ). Indeed, this scheme can be rewritten with

$$\rho_i^{n+1} = \rho_{i+1}^n \left(1 - \frac{\eta}{2}\right) + \rho_{i-1}^n \left(1 - \frac{\eta}{2}\right) + \rho_i^{n-1} (\eta - 1)$$

(see (67) with  $u(x) = 0$ ) which allows to obtain discrete maximum principles when  $\eta \in [1, 2]$  that is to say when  $C_d \in [0, \frac{1}{2}]$  since  $\eta = \frac{1}{C_d + \frac{1}{2}}$ .

On the other side, we proved in Proposition 5.1 the stability in  $L^\infty$  for any  $C_d \geq 0$ . Thus, we may think that we could also obtain discrete maximum principles for any  $C_d \geq 0$ . Unfortunately, Inequalities (73) do not

allow to conclude. Moreover, when  $C_d$  goes to the infinity (that is to say when  $\eta = 0$ ), the constants in the right hand sides of (73)(b,c) go to the infinity (except when  $\alpha = \frac{1}{2}$  in the Neumann case).

Moreover, the LBM schemes are often applied in complex porous media which may contain areas where the number of cells is low. Thus, it is important to obtain discrete maximum principles (to preserve for example the positivity of the temperature or of the mass fraction when these quantities are solution of a heat equation) and, by the same time, to have  $C_d$  at least greater than  $\frac{1}{2}$  to justify the use of the LBM schemes (or of the Du Fort-Frankel scheme) instead of the classical three-points finite difference type scheme (which satisfies discrete maximum principles when  $C_d \in [0, \frac{1}{2}]$ ).

We show below that it is possible to obtain discrete maximum principles for any  $C_d \geq 0$  with the LBM scheme (48)(50) and with the LBM\* scheme (49)(50) in the periodic and Neumann cases. Thus, this is also the case for the Du Fort-Frankel scheme. In the Dirichlet case, we will show that we have to change the boundary conditions (59) and (61) to obtain a discrete maximum principle for any  $C_d \geq 0$ . Unfortunately, we will lose in that case the equivalence between the LBM schemes and the Du Fort-Frankel scheme, and the error of the LBM schemes will not be of order  $\Delta x^2$  but should be of order  $\Delta x$ . As a consequence, this modified Dirichlet boundary conditions will have to be applied only in areas where the number of cells is low. This point underlines the utility of the LBM schemes to obtain robust schemes.

As before, for the sake of simplicity, we forget the boundary condition in  $x = x_{\max}$  in the cases of Neumann and Dirichlet boundary conditions.

### 6.1. Periodic and Neumann boundary conditions

We have the following result:

**Proposition 6.1.** *For any  $C_d \geq 0$ :*

*i) When  $\alpha \in [0, 1]$ , the LBM scheme (48)(50) and the LBM\* scheme (49)(50) with periodic boundary conditions verify the discrete maximum principle*

$$\min_j \rho_j^0 \leq \rho_i^n \leq \max_j \rho_j^0. \quad (88)$$

*ii) When  $\alpha = \frac{1}{2}$ , the LBM scheme (48)(50) and the LBM\* scheme (49)(50) with Neumann boundary conditions verify the discrete maximum principle*

$$\forall i \geq 1 : \min_{j \geq 1} \rho_j^0 \leq \rho_i^n \leq \max_{j \geq 1} \rho_j^0. \quad (89)$$

*Thus, this is also the case for the Du Fort-Frankel scheme (52) with periodic or Neumann boundary condition when the first iterate is given by (54).*

The proof is written in §6.3. Let us note that the Du Fort-Frankel scheme is equivalent to

$$\rho_i^{n+1} = \rho_{i+1}^n \left(1 - \frac{\eta}{2}\right) + \rho_{i-1}^n \left(1 - \frac{\eta}{2}\right) + \rho_i^{n-1} (\eta - 1)$$



(see (67) with  $u(x) = 0$ ). Thus, when  $\rho_i^{n=1} := \alpha\rho_{i-1}^0 + (1-\alpha)\rho_{i+1}^0$ , we obtain

$$\begin{aligned}\rho_i^2 &= [\alpha\rho_i^0 + (1-\alpha)\rho_{i+2}^0]\left(1 - \frac{\eta}{2}\right) + [\alpha\rho_{i-2}^0 + (1-\alpha)\rho_i^0]\left(1 - \frac{\eta}{2}\right) + \rho_i^0(\eta - 1) \\ &= [\alpha\rho_{i-2}^0 + (1-\alpha)\rho_{i+2}^0]\left(1 - \frac{\eta}{2}\right) + \rho_i^0\frac{\eta}{2}.\end{aligned}$$

This proves that  $\min_j \rho_j^0 \leq \rho_i^2 \leq \max_j \rho_j^0$  for any  $C_d \geq 0$  in the periodic case when  $\alpha \in [0, 1]$ . Nevertheless, it is *a priori* more difficult to obtain a similar result for  $\rho_i^{n \geq 3}$  without using the equivalence between the LBM\* scheme and the Du Fort-Frankel scheme. This remark shows that the LBM schemes may also be seen as a numerical analysis tool to study properties of classical finite difference schemes.

## 6.2. Modified Dirichlet boundary conditions

We have the following result:

**Lemma 6.1.** *For any  $C_d \in [0, \frac{1}{2}]$  and when  $\alpha = \frac{1}{2}$ , the LBM scheme (48)(50)(61) and the LBM\* scheme (49)(50)(59) verify the maximum principle*

$$\forall i \geq 1 : \quad \min(\rho_{x_{\min}}, \min_{j \geq 1} \rho_j^0) \leq \rho_i^n \leq \max(\rho_{x_{\min}}, \max_{j \geq 1} \rho_j^0). \quad (90)$$

Thus, this is also the case for the Du Fort-Frankel scheme (52) with Dirichlet boundary conditions when the first iterate is given by (54).

The proof is written in §6.3. Lemma 6.1 is less interesting than Proposition 6.1 since the discrete maximum principle (90) is satisfied under the condition  $C_d \in [0, \frac{1}{2}]$ . Nevertheless, by modifying the Dirichlet boundary conditions (59) and (61), we obtain the following result:

**Proposition 6.2.** *For any  $C_d \geq 0$  and when  $\alpha = \frac{1}{2}$ , the LBM\* scheme (49)(50) with the modified Dirichlet boundary condition*

$$\forall n \geq 0 : \quad g_{2,i=0}^n = \frac{\rho_{x_{\min}}}{2} \quad (91)$$

verifies the maximum principle

$$\forall i \geq 1 : \quad \min(\rho_{x_{\min}}, \min_{j \geq 1} \rho_j^0) \leq \rho_i^n \leq \max(\rho_{x_{\min}}, \max_{j \geq 1} \rho_j^0). \quad (92)$$

We have the same result for the LBM scheme (48)(50) with the modified Dirichlet boundary conditions

$$\forall n \geq 0 : \quad g_{1,i=0}^n = g_{2,i=0}^n = \frac{\rho_{x_{\min}}}{2}. \quad (93)$$

The proof is written in §6.3. Let us remark that when  $C_d = \alpha = \frac{1}{2}$ , the modified Dirichlet boundary condition (91) is equivalent to the Dirichlet boundary conditions (59) firstly proposed and which make equivalent the LBM\* scheme and the Du Fort-Frankel scheme (see Lemma 4.2). This is coherent with the fact that it is possible to easily prove that the Du Fort-Frankel scheme with Dirichlet boundary condition satisfies the maximum principle when  $\alpha \in [0, 1]$  and  $0 \leq C_d \leq 1/2$ .

By supposing that Expansion (16) is valid near the boundary  $x = x_{\min}$  – which is not proven since the boundary conditions are periodic in Corollary 2.1 –, we obtain that

$$\frac{\rho}{2} - f_q = O(\sqrt{\Delta t}) = O(\Delta x)$$

since  $\varepsilon = O(\Delta t)$  (cf. §3.2) and  $\Delta t = O(\Delta x^2)$ . In the same way, we obtain that

$$\frac{\Delta t}{2} Q_q(f) = O(\Delta x).$$

As a consequence, by using (22) and since  $\rho_{x_{\min}} - \rho_{i=1}^n = O(\Delta x)$ , we obtain that

$$\left( \frac{\rho_{x_{\min}}}{2} - g_{1,i=1}^n \right) (1 - \eta) = (1 - \eta) O(\Delta x). \quad (94)$$

Although this term goes to zero when  $\Delta x$  goes to zero, it is important in the Dirichlet boundary conditions (59) to obtain the equivalence between the LBM\* scheme (49)(50)(59) and the Du Fort-Frankel scheme (52)(54) with Dirichlet boundary condition. Moreover, when  $\alpha = \frac{1}{2}$ , the error of the LBM\* scheme (49)(50)(59) is of the order of  $\Delta x^2$  (see point *iii* of Proposition 5.1).

Thus, when we replace (59) by (91) in the LBM\* scheme:

- The error of the LBM\* scheme with  $\alpha = \frac{1}{2}$  should be of the order of  $\Delta x$  instead of  $\Delta x^2$ .
- Near the boundary  $x = x_{\min}$ , we lose the equivalence between the LBM\* scheme and the Du Fort-Frankel scheme. This avoids to obtain the convergence in  $L^\infty$  for any  $C_d \geq 0$  of the LBM\* scheme with modified Dirichlet boundary condition *by using the Lax Theorem*.

Of course, we have the same remarks when we replace (61) by (93) in the LBM scheme. Nevertheless, Proposition 6.2, estimation (94) (which remains to be proven) and the fact that the equivalence with the Du Fort-Frankel scheme remains valid far from the boundary  $x = x_{\min}$  incite us to conjecture the following result:

**Conjecture 6.1.** *For any  $C_d \geq 0$  and when  $\alpha = \frac{1}{2}$ , the LBM\* scheme (49)(50) with the modified Dirichlet boundary conditions (91) converges in  $L^\infty$  with an error of the order of  $\Delta x$ . We have the same result for the LBM scheme (48)(50) with the modified Dirichlet boundary conditions (93).*

Numerical results proposed in §9.1 will justify this conjecture.

### 6.3. Proof of Propositions 6.1 and 6.2, and of Lemma 6.1

#### Proof of Proposition 6.1:

We focus on the LBM\* scheme (49) since this scheme is more simple than the LBM scheme (48). Then, by applying Lemmae 4.1 and 4.2, we obtain the results for the Du Fort-Frankel scheme and, then, for the LBM scheme (48) (this approach was also used for the proof of Proposition 5.1).

- *Discrete Maximum principle with periodic boundary conditions for the LBM\* scheme when  $\alpha = \frac{1}{2}$ :*

The LBM\* scheme (49) implies that

$$\min_j(g_{1,j}^n, g_{2,j}^n) \leq g_{q,i}^{n+1} \leq \max_j(g_{1,j}^n, g_{2,j}^n) \quad (q \in \{1, 2\})$$

since  $\eta \in ]0, 2]$ . Thus, we have

$$\min_j(g_{1,j}^0, g_{2,j}^0) \leq g_{q,i}^{n+1} \leq \max_j(g_{1,j}^0, g_{2,j}^0) \quad (q \in \{1, 2\}). \quad (95)$$

Thus, by using (50), we obtain

$$\min[(1 - \alpha), \alpha] \cdot \min_j \rho_j^0 \leq g_{q,i}^n \leq \max[(1 - \alpha), \alpha] \cdot \max_j \rho_j^0 \quad (q \in \{1, 2\}) \quad (96)$$

when  $\alpha \in [0, 1]$ . Since  $\rho_i^n = g_{1,i}^n + g_{2,i}^n$ , we deduce from (96) that

$$2 \min[(1 - \alpha), \alpha] \cdot \min_j \rho_j^0 \leq \rho_i^n \leq 2 \max[(1 - \alpha), \alpha] \cdot \max_j \rho_j^0 \quad (q \in \{1, 2\}). \quad (97)$$

Thus, we deduce from (97) that the discrete maximum principle (88) is verified when  $\alpha = \frac{1}{2}$ .

• *Discrete Maximum principle with periodic boundary conditions for the LBM\* scheme when  $\alpha \in [0, 1]$ :*

The discrete maximum principle (88) cannot be deduced from (97) when  $\alpha \neq \frac{1}{2}$ . Nevertheless, we now prove that (88) is still satisfied when  $\alpha \in [0, 1]$ . To obtain this result, we prove that

$$\left\{ \begin{array}{l} g_{1,i}^n = \sum_k \Gamma_k^n g_{1,i_k^1}^0 + \sum_k \tilde{\Gamma}_k^n g_{2,i_k^2}^0, \quad (a) \\ g_{2,i}^n = \sum_k \tilde{\Gamma}_k^n g_{1,i_k^1}^0 + \sum_k \Gamma_k^n g_{2,i_k^2}^0, \quad (b) \\ \sum_k (\Gamma_k^n + \tilde{\Gamma}_k^n) = 1, \quad (c) \\ \Gamma_k^n \geq 0, \quad (d) \\ \tilde{\Gamma}_k^n \geq 0 \quad (e) \end{array} \right. \quad (98)$$

where  $\{i_k^1\}_k$  et  $\{i_k^2\}_k$  are two sequences which depend on  $i$ , and where  $\{\Gamma_k^n\}_k$  and  $\{\tilde{\Gamma}_k^n\}_k$  are two positive real sequences. It is obvious that (98) is verified when  $n = 1$  since

$$\left\{ \begin{array}{l} g_{1,i}^1 = g_{1,i+1}^0 \left(1 - \frac{\eta}{2}\right) + g_{2,i-1}^0 \frac{\eta}{2}, \\ g_{2,i}^1 = g_{2,i-1}^0 \left(1 - \frac{\eta}{2}\right) + g_{1,i+1}^0 \frac{\eta}{2}. \end{array} \right.$$

Let us suppose that (98) is satisfied at the rank  $n$ . Then, the LBM\* scheme (49) can be written with

$$\left\{ \begin{array}{l} g_{1,i}^{n+1} = \left(1 - \frac{\eta}{2}\right) \left( \sum_k \Gamma_k^n g_{1,i_k^1+1}^0 + \sum_k \tilde{\Gamma}_k^n g_{2,i_k^2+1}^0 \right) + \frac{\eta}{2} \left( \sum_k \tilde{\Gamma}_k^n g_{1,i_k^1-1}^0 + \sum_k \Gamma_k^n g_{2,i_k^2-1}^0 \right), \\ g_{2,i}^{n+1} = \frac{\eta}{2} \left( \sum_k \Gamma_k^n g_{1,i_k^1+1}^0 + \sum_k \tilde{\Gamma}_k^n g_{2,i_k^2+1}^0 \right) + \left(1 - \frac{\eta}{2}\right) \left( \sum_k \tilde{\Gamma}_k^n g_{1,i_k^1-1}^0 + \sum_k \Gamma_k^n g_{2,i_k^2-1}^0 \right) \end{array} \right.$$

that is to say with

$$\begin{cases} g_{1,i}^{n+1} = \sum_k \left[ \left(1 - \frac{\eta}{2}\right) \Gamma_k^n g_{1,i_k+1}^0 + \frac{\eta}{2} \tilde{\Gamma}_k^n g_{1,i_k-1}^0 \right] + \sum_k \left[ \left(1 - \frac{\eta}{2}\right) \tilde{\Gamma}_k^n g_{2,i_k+1}^0 + \frac{\eta}{2} \Gamma_k^n g_{2,i_k-1}^0 \right], \\ g_{2,i}^{n+1} = \sum_k \left[ \frac{\eta}{2} \Gamma_k^n g_{1,i_k+1}^0 + \left(1 - \frac{\eta}{2}\right) \tilde{\Gamma}_k^n g_{1,i_k-1}^0 \right] + \sum_k \left[ \frac{\eta}{2} \tilde{\Gamma}_k^n g_{2,i_k+1}^0 + \left(1 - \frac{\eta}{2}\right) \Gamma_k^n g_{2,i_k-1}^0 \right]. \end{cases} \quad (99)$$

But, (99) can be written with (98)(a,b) at the rank  $n + 1$  after a reorganization of the sequences. Moreover, we have

$$\sum_k \left[ \left(1 - \frac{\eta}{2}\right) \Gamma_k^n + \frac{\eta}{2} \tilde{\Gamma}_k^n \right] + \sum_k \left[ \frac{\eta}{2} \Gamma_k^n + \left(1 - \frac{\eta}{2}\right) \tilde{\Gamma}_k^n \right] = \sum_k (\Gamma_k^n + \tilde{\Gamma}_k^n) = 1$$

and

$$\begin{cases} \left(1 - \frac{\eta}{2}\right) \Gamma_k^n \geq 0, \\ \frac{\eta}{2} \tilde{\Gamma}_k^n \geq 0, \\ \frac{\eta}{2} \Gamma_k^n \geq 0, \\ \left(1 - \frac{\eta}{2}\right) \tilde{\Gamma}_k^n \geq 0 \end{cases}$$

since  $\eta \in ]0, 2]$ . Thus, (98) is satisfied for any  $n \geq 1$ . By using the fact that  $\rho_i^n = g_{1,i}^n + g_{2,i}^n$  and by using (50), (98)(a,b) implies that

$$\begin{aligned} \rho_i^n &= \sum_k (\Gamma_k^n + \tilde{\Gamma}_k^n) (g_{1,i_k}^0 + g_{2,i_k}^0) \\ &= \sum_k (\Gamma_k^n + \tilde{\Gamma}_k^n) [(1 - \alpha) \rho_{i_k}^0 + \alpha \rho_{i_k}^0] \end{aligned}$$

since  $\rho_i^n = g_{1,i}^n + g_{2,i}^n$ . Thus, because of (98)(c,d,e), we obtain that  $\rho_i^n$  is a convex combination of  $\{\rho_j^0\}_j$  when  $\alpha \in [0, 1]$  which allows to obtain (88).

• *Discrete Maximum principle with Neumann boundary conditions for the LBM\* scheme when  $\alpha = \frac{1}{2}$ :*

*A priori*, the proof in the periodic case when  $\alpha \in [0, 1]$  is not valid in the Neumann case because of the boundary conditions (51) in  $x = x_{\min}$ . Nevertheless, when  $\alpha = \frac{1}{2}$ , the boundary conditions (51) are given by

$$\forall n \geq 0 : \quad g_{2,0}^n = g_{1,1}^n \quad (100)$$

since  $\alpha = \frac{1}{2} \implies g_{1,1}^0 = g_{2,1}^0 = \frac{\rho_1^0}{2}$  and  $g_{2,0}^0 = g_{1,1}^0 = \frac{\rho_1^0}{2}$  that is to say  $g_{2,0}^0 = g_{1,1}^0$ . As a consequence, the proof in the periodic case with  $\alpha = \frac{1}{2}$  becomes valid in the Neumann case.  $\square$

**Proof of Lemma 6.1:** In the Dirichlet case, the boundary conditions (59) in  $x = x_{\min}$  can be rewritten with

$$\begin{cases} g_{2,i=0}^{n+1} = \frac{\rho_{x_{\min}}}{2} (2 - \eta) + g_{1,i=1}^n (\eta - 1), & \text{(a)} \\ g_{2,i=0}^{n=0} = \alpha \rho_{x_{\min}}. & \text{(b)} \end{cases} \quad (101)$$

We deduce from (101) that when  $\eta \in [1, 2]$  that is to say when  $C_d \in [0, \frac{1}{2}]$ , we have

$$\min \left[ \frac{\rho_{x_{\min}}}{2}, g_{1,i=1}^n \right] \leq g_{2,i=0}^{n+1} \leq \max \left[ \frac{\rho_{x_{\min}}}{2}, g_{1,i=1}^n \right].$$

Thus, the proof in the periodic case with  $\alpha = \frac{1}{2}$  can be applied.  $\square$

**Proof of Proposition 6.2:** The proof is identical to the periodic case with  $\alpha = \frac{1}{2}$  by replacing (95) with

$$\min \left[ \frac{\rho_{x_{\min}}}{2}, \min_{j \geq 1} (g_{1,j}^n, g_{2,j}^n) \right] \leq g_{1,i}^{n+1} \leq \max \left[ \frac{\rho_{x_{\min}}}{2}, \max_{j \geq 1} (g_{1,j}^n, g_{2,j}^n) \right].$$

$\square$

## 7. Limitations of the LBM schemes

### 7.1. Preservation of the initial condition

We have the following result:

**Lemma 7.1.** *When  $C_d = 0$ , the LBM\* scheme (36)(43) with periodic boundary conditions preserve the initial condition in the sense*

$$\forall n \in \mathbb{N} : \quad \rho_i^{n+2} = \rho_i^n.$$

*Thus, this is also the case for the LBM scheme (33)(43) and for the finite difference type scheme (44) when the first iterate is given by (46).*

In the case of the heat equation with Neumann or Dirichlet boundary conditions, we obtain the following lemma:

**Lemma 7.2.** *When  $C_d = 0$ , the LBM\* scheme (49)(50) with periodic, Neumann, Dirichlet or modified Dirichlet boundary conditions preserve the initial condition in the sense*

$$\forall n \in \mathbb{N} : \quad \rho_i^{n+2} = \rho_i^n.$$

*Thus, this is also the case for the LBM scheme (48)(50) and for the Du Fort-Frankel scheme (52) when the first iterate is given by (54).*

These lemmata show that the proposed LBM schemes do not satisfy  $\rho_i^{n+1} = \rho_i^n$  when  $C_d = 0$  i.e. when  $\Delta t = 0$ . Nevertheless, we deduce from (46) that  $\rho_i^1 - \rho_{exact}(\Delta t, x_i) = \mathcal{O}(\Delta x^\beta)$  with  $\beta = 1$  when  $\alpha \neq \frac{1}{2}$  and with  $\beta = 2$  when  $\alpha = \frac{1}{2}$ . Thus, the proposed LBM schemes preserve the initial condition when  $\Delta t = 0$  with an error of order  $\Delta x^\beta$ . As a consequence, we cannot say that this property is an important limitation of the proposed LBM schemes.

**Proof of Lemma 7.1:** When  $C_d = 0$ , we deduce from the LBM\* scheme (36) that

$$g_{1,i}^{n+1} = g_{2,i-1}^n \quad \text{and} \quad g_{2,i}^{n+1} = g_{1,i+1}^n.$$

As a consequence, we have

$$g_{1,i}^{n+1} = g_{1,i}^{n-1} \quad \text{and} \quad g_{2,i}^{n+1} = g_{2,i}^{n-1}$$

which concludes the proof. We obtain the result for the LBM scheme and for the finite difference type scheme (44) by using Lemma 4.1.  $\square$

**Proof of Lemma 7.2:** The proof in the case of periodic boundary conditions is a direct application of Lemma 7.1.

• *The case of Neumann boundary conditions:*

For the LBM\* scheme, we deduce from (51)(a) that  $g_{2,0}^{n+1} = g_{1,1}^{n+1} - (g_{2,0}^n - g_{1,1}^n)$  when  $C_d = 0$ . On the other side, we have also  $g_{1,1}^{n+1} = g_{2,0}^n$  for any  $i \geq 1$  by using (49) with  $C_d = 0$ . Thus, we obtain  $g_{2,0}^{n+1} = g_{1,1}^n$  that is to say  $g_{2,0}^{n+1} = g_{1,1}^{n-2} = g_{2,0}^{n-1}$  which allows to obtain the result. We obtain the result for the LBM and Du Fort-Frankel schemes by applying Lemma 4.2.

• *The case of Dirichlet boundary conditions:*

For the LBM\* scheme, we deduce from (59)(a) that  $g_{2,0}^{n+1} = g_{1,1}^n$  when  $C_d = 0$ . We conclude as in the Neumann case. We obtain the result for the LBM and Du Fort-Frankel schemes by applying Lemma 4.3.

• *The case of modified Dirichlet boundary conditions for the LBM and LBM\* schemes:*

Since the boundary conditions (91) and (93) do not depend on the time, we obtain the result as in the other cases.  $\square$

## 7.2. Consistency condition

We proved in Lemma 4.1 that the LBM scheme (33)(43) and the LBM\* scheme (36)(43) are equivalent to the finite difference type scheme (44) (when the first iterate is defined with (44)(46)). On the other side, we know that the consistency error  $\mathbf{E}$  of the Du Fort-Frankel scheme (52) is given by [22]

$$\mathbf{E} = -v \frac{\Delta t^2}{\Delta x^2} \partial_{tt}^2 \rho + O(\Delta x^2).$$

As a consequence, the equivalent equation of the Du Fort-Frankel scheme is the telegraph equation

$$\partial_t \rho = v \left( \partial_{xx}^2 \rho - \frac{1}{c} \partial_{tt}^2 \rho \right) \quad \text{with} \quad c = \frac{\Delta x}{\Delta t} \quad (102)$$

which implies that the Du Fort-Frankel scheme is consistent with the heat equation if and only if

$$\Delta t = O(\Delta x^\beta) \quad \text{with} \quad \beta > 1. \quad (103)$$

As a consequence, the LBM scheme (33)(43) and the LBM\* scheme (36)(43) cannot be consistent with the convection-diffusion equation (1) when  $O(C_d \Delta x) \geq 1$ .

The consistency condition (103) limits the range of the unconditional stability in  $L^\infty$  of the LBM schemes (48) and (49) obtained in the case of the heat equation (see Proposition 5.1; see also the discrete maximum

principles obtained in §6) and which makes robust these LBM schemes. Let us note that the LBM schemes (48) and (49) are equivalent to

$$\begin{cases} g_{1,i}^{n+1} = g_{1,i+1}^n, & \text{(a)} \\ g_{2,i}^{n+1} = g_{2,i-1}^n, & \text{(b)} \\ \rho_i^{n+1} = g_{1,i}^{n+1} + g_{2,i}^{n+1} & \text{(c)} \end{cases} \quad (104)$$

when  $\eta := \frac{1}{C_d + \frac{1}{2}} = 0$  that is to say when  $C_d \rightarrow +\infty$ . This confirms the fact that the LBM schemes (48) and (49) cannot be consistent with the heat equation when  $O(C_d \Delta x) \geq 1$  since (104)(a,b) are two convective schemes with  $CFL = 1$ .

### 7.3. High Reynolds flows

The discrete convection operator in (44) is obtained with an explicit centered scheme. This should impact the stability of the LBM schemes (33) and (36) when  $u(x) \neq 0$  and when  $\nu$  is low that is to say when the Reynolds number  $Re := \frac{L\bar{u}}{\nu}$  is high (we use the definitions  $\bar{u} := \max_{\Omega} |u(x)|$ ,  $L := x_{\max} - x_{\min}$  where  $\Omega := [x_{\min}, x_{\max}]$ ) and when  $\Delta t = O(\Delta x)$  independently of the consistency condition (103). We do not study this point in this paper. This remark underlines that the LBM schemes applied to the incompressible Navier-Stokes system may present numerical instabilities and consistency errors for high Reynolds number flows when  $\Delta t = O(\Delta x)$ .

## 8. Probabilistic interpretation of the LBM schemes

We now propose two Monte-Carlo algorithms deduced from the LBM scheme (48) and from the LBM\* scheme (49) in the case of periodic boundary conditions. To obtain these Monte-Carlo algorithms, we define

$$g^n(x, v) = w \sum_{k=1}^{\mathcal{K}} \delta(x - X_k^n) \cdot \delta(v - V_k^n)$$

where the particles  $k \in \{1, \dots, \mathcal{K}\}$  are characterized by the position  $X_k^n \in \Omega$ , the velocity  $V_k^n \in \mathbb{R}$  and the weight  $w$  supposed to be constant, and where  $\delta(\cdot)$  is the Dirac distribution,  $(\{X_k^n\}_k, \{V_k^n\}_k)$  being a random process which will be defined below. Thus, we approach  $g_{q,i}^n$  and  $\rho_i^n$  with

$$\begin{cases} g_{1,i}^n = \frac{w}{\Delta x} \cdot \text{Card} \left( \left\{ k / X_k^n = x_i \text{ and } v = -\frac{\Delta x}{\Delta t} \right\} \right), \\ g_{2,i}^n = \frac{w}{\Delta x} \cdot \text{Card} \left( \left\{ k / X_k^n = x_i \text{ and } v = \frac{\Delta x}{\Delta t} \right\} \right), \\ \rho_i^n = \frac{w}{\Delta x} \cdot \text{Card} \left( \{ k / X_k^n = x_i \} \right). \end{cases}$$

Moreover, we initialize the particles with the random process

$$\left\{ \begin{array}{l} X_k^0 = x_i \text{ with the discrete probability } P(X_k^0 = x_i) = \frac{\rho(0, x_i) - \min_l \rho(0, x_l)}{\sum_j [\rho(0, x_j) - \min_l \rho(0, x_l)]}, \\ V_k^0 = \frac{\Delta x}{\Delta t} \text{ with the probability } \alpha, \\ \quad = -\frac{\Delta x}{\Delta t} \text{ with the probability } 1 - \alpha \end{array} \right. \quad (105)$$

which is a consequence of the initial condition (50),  $\rho(0, x)$  being the initial condition (due to the random nature of (105), we only have  $\rho_i^0 \simeq \rho(0, x_i)$ ). The random process (105) implies that we have to impose

$$\alpha \in [0, 1].$$

At last, the weight  $w$  is defined with

$$w = \frac{\sum_i \rho_i^0}{\mathcal{K}} \Delta x$$

which comes from the conservation constraint

$$\int_{\Omega \times \mathbb{R}} g^n(x, v) dx dv = \int_{\Omega} \rho(0, x) dx = \sum_i \rho_i^0 \Delta x.$$

### 8.1. Monte-Carlo algorithm for the LBM scheme

The LBM scheme (48) can be written with the following splitting *collision-transport*:

*Collision:*

$$\left\{ \begin{array}{l} g_{1,i}^* = g_{1,i}^n \left(1 - \frac{\eta}{2}\right) + g_{2,i}^n \frac{\eta}{2}, \\ g_{2,i}^* = g_{2,i}^n \left(1 - \frac{\eta}{2}\right) + g_{1,i}^n \frac{\eta}{2}. \end{array} \right. \quad (106)$$

*Transport:*

$$\left\{ \begin{array}{l} g_{1,i}^{n+1} = g_{1,i+1}^*, \\ g_{2,i}^{n+1} = g_{2,i-1}^*. \end{array} \right. \quad (107)$$

This incites us to approach (106)(107) with the random algorithm

$$\left\{ \begin{array}{l} V_k^{n+1} = V_k^n \text{ with the probability } 1 - \frac{\eta}{2}, \\ \quad = -V_k^n \text{ with the probability } \frac{\eta}{2}, \\ X_k^{n+1} = X_k^n + \Delta t V_k^{n+1} \end{array} \right. \quad (108)$$

where

$$\eta = \frac{1}{C_d + \frac{1}{2}}.$$

We recall that  $\Delta t := C_d \frac{\Delta x^2}{\nu}$  with  $C_d \geq 0$ . Let us underline that since  $\eta \in ]0, 2]$ , the random process (108) is always defined. Let us note that a similar Monte-Carlo algorithm has been proposed in [29] for the telegraph equation (102).



## 8.2. Monte-Carlo algorithm for the LBM\* scheme

In the same way, the LBM\* scheme (49) can be written with the following splitting *transport-collision*:

*Transport:*

$$\begin{cases} g_{1,i}^* = g_{1,i+1}^n, \\ g_{2,i}^* = g_{2,i-1}^n. \end{cases} \quad (109)$$

*Collision:*

$$\begin{cases} g_{1,i}^{n+1} = g_{1,i}^* \left(1 - \frac{\eta}{2}\right) + g_{2,i}^* \frac{\eta}{2}, \\ g_{2,i}^{n+1} = g_{2,i}^* \left(1 - \frac{\eta}{2}\right) + g_{1,i}^* \frac{\eta}{2}. \end{cases} \quad (110)$$

This incites us to approach (109)(110) with the random algorithm

$$\begin{cases} X_k^{n+1} = X_k^n + \Delta t V_k^n, \\ V_k^{n+1} = V_k^n \text{ with the probability } 1 - \frac{\eta}{2}, \\ \quad = -V_k^n \text{ with the probability } \frac{\eta}{2}. \end{cases} \quad (111)$$

We show below the relation between the Monte-Carlo algorithms (105)(108) and (105)(111).

## 8.3. Some properties of the Monte-Carlo algorithms

We present some properties satisfied by the Monte-Carlo algorithms (105)(108) and (105)(111).

### 8.3.1. Discrete maximum principle

We have the following result:

**Lemma 8.1.** *For any  $C_d \geq 0$ , the Monte-Carlo algorithms (105)(108) and (105)(111) verify the discrete maximum principle*

$$\min_j \rho_j^0 \leq \rho_i^n \leq \max_j \rho_j^0. \quad (112)$$

We recall that the Monte-Carlo algorithms (105)(108) and (105)(111) are defined when  $\alpha \in [0, 1]$ . Lemma 8.1 is coherent with the fact that the LBM schemes (48)(50) and (49)(50) with periodic boundary conditions verify the discrete maximum principle (112) when  $\alpha \in [0, 1]$  (see point  $i$  of Proposition 6.1).

**Proof of Lemma 8.1:** We have  $\rho_i^n = N_i^n \frac{w}{\Delta x}$  where  $N_i^n$  is the number of particles in the cell  $i$  at the time  $t^n$ . Since  $w = \frac{\sum_j \rho_j^0}{\mathcal{K}} \Delta x$ , we obtain  $\rho_i^n = \frac{N_i^n}{\mathcal{K}} \sum_j \rho_j^0$  that is to say

$$\rho_i^n = \frac{N_i^n}{\sum_i N_i^n} \sum_j \rho_j^0$$

since  $\mathcal{K} = \sum_i N_i^n$ . Thus,  $\rho_i^n$  is a convex combination of  $\{\rho_j^0\}_j$  which allows to conclude.  $\square$

### 8.3.2. Link between the Monte-Carlo algorithms

We can remark that the Monte-Carlo algorithms (105)(108) and (105)(111) are similar. More precisely, the LBM scheme (105)(108) can be rewritten with

$$\left\{ \begin{array}{l} X_k^0 = x_i \text{ with the discrete probability } P(X_k^0 = x_i) = \frac{\rho(0, x_i) - \min_l \rho(0, x_l)}{\sum_j [\rho(0, x_j) - \min_l \rho(0, x_l)]}, \\ \bar{V}_k^0 = \frac{\Delta x}{\Delta t} \text{ with the probability } \alpha, \\ \quad = -\frac{\Delta x}{\Delta t} \text{ with the probability } 1 - \alpha, \\ V_k^0 = \bar{V}_k^0 \text{ with the probability } 1 - \frac{\eta}{2}, \\ \quad = -\bar{V}_k^0 \text{ with the probability } \frac{\eta}{2} \end{array} \right. \quad (113)$$

and

$$\left\{ \begin{array}{l} X_k^{n+1} = X_k^n + \Delta t V_k^n, \\ V_k^{n+1} = V_k^n \text{ with the probability } 1 - \frac{\eta}{2}, \\ \quad = -V_k^n \text{ with the probability } \frac{\eta}{2}. \end{array} \right. \quad (114)$$

But, the random process

$$\left\{ \begin{array}{l} \bar{V}_k^0 = \frac{\Delta x}{\Delta t} \text{ with the probability } \alpha, \\ \quad = -\frac{\Delta x}{\Delta t} \text{ with the probability } 1 - \alpha, \\ V_k^0 = \bar{V}_k^0 \text{ with the probability } 1 - \frac{\eta}{2}, \\ \quad = -\bar{V}_k^0 \text{ with the probability } \frac{\eta}{2} \end{array} \right.$$

is equivalent to the random process

$$\left\{ \begin{array}{l} V_k^0 = \frac{\Delta x}{\Delta t} \text{ with the probability } \xi, \\ \quad = -\frac{\Delta x}{\Delta t} \text{ with the probability } 1 - \xi \end{array} \right.$$

with  $\xi = \alpha \left(1 - \frac{\eta}{2}\right) + (1 - \alpha) \frac{\eta}{2}$  that is to say with

$$\xi = \frac{\eta}{2} + \alpha(1 - \eta)$$

which belongs to  $[0, 1]$  since  $\alpha \in [0, 1]$  and  $\eta \in ]0, 2]$ . To summarize, the LBM scheme (105)(108) is equivalent to the LBM\* scheme (105)(111) by replacing  $\alpha$  with  $\xi$  in (105). This result is coherent with the fact that the LBM schemes (48)(50) and (49)(50) are equivalent to the Du Fort-Frankel scheme whose the first iterate is respectively given by

$$\rho_i^{n=1} := \xi \rho_{i-1}^0 + (1 - \xi) \rho_{i+1}^0$$

and by

$$\rho_i^{n=1} := \alpha \rho_{i-1}^0 + (1 - \alpha) \rho_{i+1}^0$$

(see Lemma 4.1).

### 8.3.3. Other properties

Let us suppose that  $C_d = 0$ . Thus, we have  $\eta = 2$  which implies that the Monte-Carlo algorithms (108) and (111) are deterministic and verify  $V_k^{n+1} = -V_k^n$ . As a consequence, we obtain

$$\forall n \in \mathbb{N} : \rho_i^{n+2} = \rho_i^n$$

which corresponds to Lemma 7.1.

We now suppose that  $C_d \rightarrow +\infty$ . In that case, we have  $\eta = 0$ . Again, the Monte-Carlo algorithms (108) and (111) are deterministic but verify now  $V_k^{n+1} = V_k^n$ . Thus, the particles move to the left or to the right without changing their initial velocity: in that case, the Monte-Carlo algorithms (105)(108) and (105)(111) do not converge toward the solution of the heat equation. This situation is related to the consistency condition of the LBM schemes described in §7.2.

At last, let us suppose that  $C_d = \frac{1}{2}$ . In that case, we easily verify that the Du Fort-Frankel scheme is equivalent to the classical three points finite difference scheme for the heat equation (see (67) with  $\eta = 1$  and  $u(x) = 0$ ). On the other side, the Monte-Carlo algorithms (108) and (111) describe a discrete brownian motion which is the Monte-Carlo version of the three points scheme for the heat equation. These remarks are coherent with the fact that the LBM schemes (48) and (49) are equivalent to the Du Fort-Frankel scheme and, thus, are equivalent to the three points scheme when  $C_d = \frac{1}{2}$ .

### 8.4. Convergence of the Monte-Carlo algorithms

It remains to prove that the Monte-Carlo algorithms (105)(108) and (105)(111) converge to the solution of the heat equation with probabilistic tools, which would be a probabilistic version of Proposition 5.1 in the periodic case. More generally, it would be interesting to extend the Monte-Carlo algorithms (105)(108) and (105)(111) to the Neumann and Dirichlet cases, and to verify the convergence of these schemes with probabilistic tools. Moreover, it would be also interesting to prove the convergence of the LBM schemes (48) and (49) with modified Dirichlet boundary conditions (see Conjecture 6.1) by using a probabilistic approach. At last, the case of the LBM schemes (33) and (36) with  $u(x) \neq 0$  should be also studied with a probabilistic approach. A starting point could be [29, 30].

## 9. Numerical results

We now present numerical results which illustrate some of the results presented before in the case of the heat equation. In the following test-cases, we choose  $x_{\max} = -x_{\min} = 10$  and  $\nu = 1$ . Moreover,  $N$  is the number of cells: in the periodic or Neumann cases, we have  $N\Delta x = x_{\max} - x_{\min}$  and in the Dirichlet case, we have  $(N + 1)\Delta x = x_{\max} - x_{\min}$ . At last, we recall that  $\Delta t = C_d \frac{\Delta x^2}{\nu}$  and that  $\eta = \frac{1}{C_d + \frac{1}{2}}$ .

### 9.1. LBM\* scheme

- *Test-case 1: Discrete maximum principle with Dirichlet boundary conditions*

We test the the LBM\* scheme (49)(50) with  $\alpha = \frac{1}{2}$  when we apply the Dirichlet boundary conditions  $\rho(t, x_{\min}) = \rho_{x_{\min}}$  and  $\rho(t, x_{\max}) = \rho_{x_{\max}}$ . At the discrete level, we use the Dirichlet boundary conditions (59)

in  $x = x_{\min}$  and its extension in  $x = x_{\max}$  that is to say

$$\left\{ \begin{array}{l} g_{2,i=0}^{n+1} = \frac{\rho_{x_{\min}}}{2} + \left( \frac{\rho_{x_{\min}}}{2} - g_{1,i=1}^n \right) (1 - \eta), \\ g_{2,i=0}^{n=0} = \frac{\rho_{x_{\min}}}{2}, \\ g_{1,i=N+1}^{n+1} = \frac{\rho_{x_{\max}}}{2} + \left( \frac{\rho_{x_{\max}}}{2} - g_{2,i=N}^n \right) (1 - \eta), \\ g_{1,i=N+1}^{n=0} = \frac{\rho_{x_{\max}}}{2}. \end{array} \right. \quad (115)$$

We also use the modified Dirichlet boundary conditions (59) in  $x = x_{\min}$  and its extension in  $x = x_{\max}$  that is to say

$$\forall n \geq 0 : \left\{ \begin{array}{l} g_{2,i=0}^n = \frac{\rho_{x_{\min}}}{2}, \\ g_{1,i=N+1}^n = \frac{\rho_{x_{\max}}}{2}. \end{array} \right. \quad (116)$$

We recall that the boundary conditions (116) allow to satisfy a discrete maximum principle for any  $C_d \geq 0$  which is not the case of (115): see Lemma 6.1 and Proposition 6.2. To illustrate this result, we choose  $N = 10$  – that is to say a low number of cells –, we define the following initial condition

$$\begin{aligned} \rho_i^0 &= \frac{1}{4} \text{ if } i \notin \{5, 6\}, \\ &= \frac{3}{4} \text{ if } i \in \{5, 6\} \end{aligned}$$

and we choose  $C_d = 4$ . Figures 1-2 show the results respectively with  $\rho_{x_{\min}} = \rho_{x_{\max}} = 1$  and  $\rho_{x_{\min}} = \rho_{x_{\max}} = 0$  when we use (115) (Figures 1-2 show also the initial condition and the stationary solution). Figures 3-4 show these results when we replace (115) by (116). We see on Figures 1-2 that the discrete maximum principle

$$\forall i \in \{1, \dots, N\} : \min(\rho_{x_{\min}}, \rho_{x_{\max}}, \min_{1 \leq j \leq N} \rho_j^0) \leq \rho_i^n \leq \max(\rho_{x_{\min}}, \rho_{x_{\max}}, \max_{1 \leq j \leq N} \rho_j^0)$$

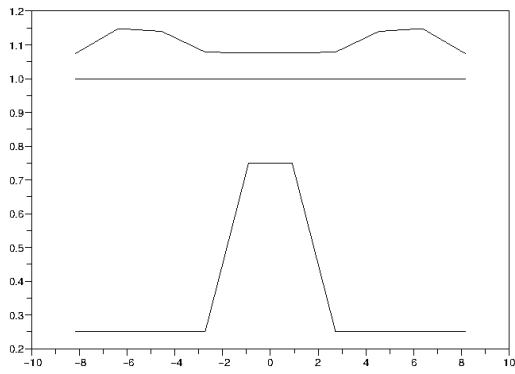
is not satisfied, and that it is satisfied on Figures 3-4: this is coherent with Lemma 6.1 and Proposition 6.2.

Let us underline that although the discrete maximum principle is not satisfied on Figures 1-2, these figures show that the LBM\* scheme (49)(50)(115) is stable in  $L^\infty$  although  $C_d = 4$ , which is coherent with Proposition 5.1.

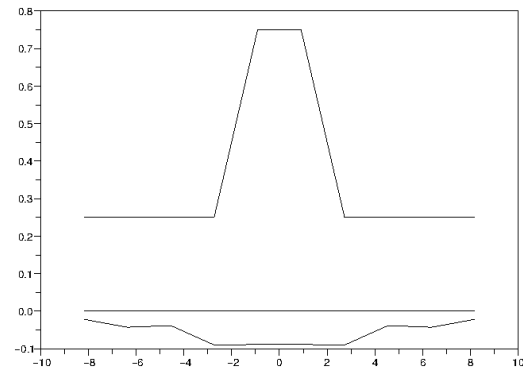
• *Test-case 2: Convergence order of the modified Dirichlet boundary conditions (116)*

The test-case 1 shows that to make robust the LBM\* scheme when the number of cells is low, it is better to use (116) than (115). Nevertheless, we may think that (115) is more accurate than (116). Indeed, the error of the LBM\* scheme using (115) is in  $\Delta x^2$  since  $\alpha = \frac{1}{2}$  (see Proposition 5.1) and we conjectured that the order of the LBM\* scheme using (116) is in  $\Delta x$  (see Conjecture 6.1). To verify these convergence orders, we use the exact solution  $\rho_{exact}(t, x)$  of the heat equation

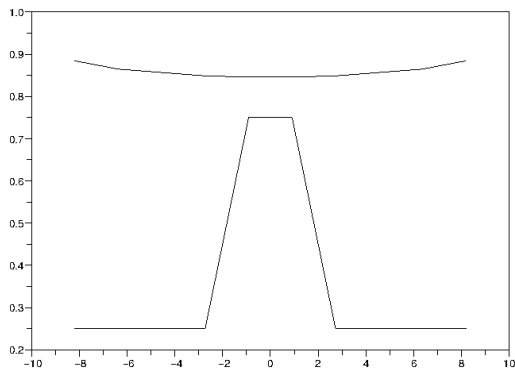
$$\rho_{exact}(t, x) = erf \left[ \frac{x_i - x_{\min}}{\sqrt{4\nu(t+1)}} \right]$$



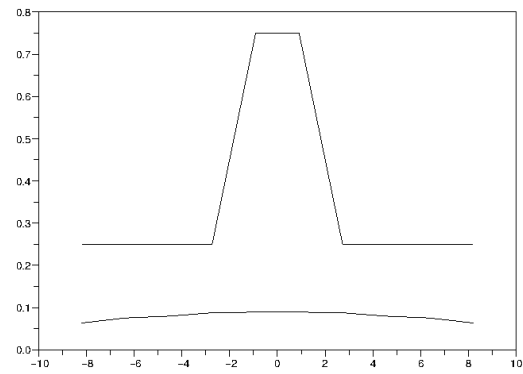
*Fig. 1: LBM\* scheme with (115)  
when  $\rho_{x_{\min}} = \rho_{x_{\max}} = 1$*



*Fig. 2: LBM\* scheme with (115)  
when  $\rho_{x_{\min}} = \rho_{x_{\max}} = 0$*



*Fig. 3: LBM\* scheme with (116)  
when  $\rho_{x_{\min}} = \rho_{x_{\max}} = 1$*



*Fig. 4: LBM\* scheme with (116)  
when  $\rho_{x_{\min}} = \rho_{x_{\max}} = 0$*

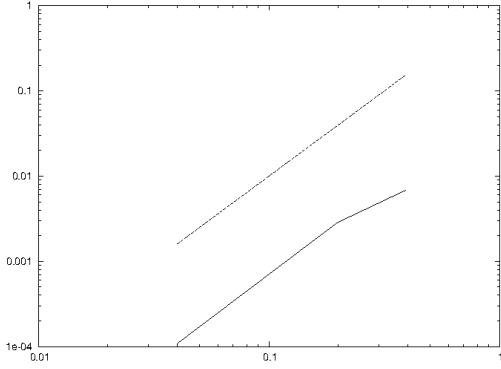


Fig. 5: LBM\* scheme with (115)

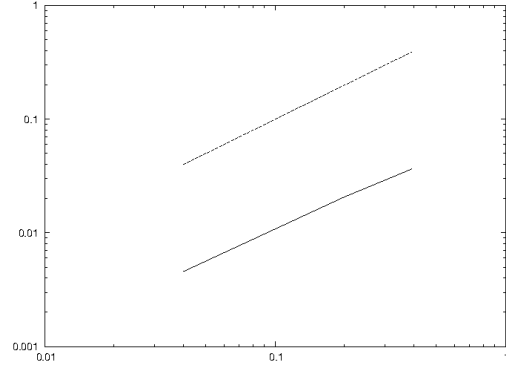


Fig. 6: LBM\* scheme with (116)

with the unstationary Dirichlet boundary conditions

$$\begin{cases} \rho_{x_{\min}}^n = \rho_{exact}(t^n, x_{\min}), \\ \rho_{x_{\max}}^n = \rho_{exact}(t^n, x_{\max}). \end{cases}$$

Moreover, we choose  $C_d = 2$ ,  $t_{final} = 15$  and the number of cells  $N \in \{50, 100, 200\}$ . Figure 5 shows the function  $y = x^2$  and the normalized  $L^2$  error

$$e(\Delta x) := \frac{\sqrt{\sum_i |\rho_i^n - \rho_{exact}(t^n, x_i)|^2 \Delta x}}{\sqrt{\sum_i |\rho_{exact}(t^n, x_i)|^2 \Delta x}}$$

in function of  $\Delta x$  in (log-log scale) when we use (115); Figure 6 shows the function  $y = x$  and  $e(\Delta x)$  when we use (116). These figures confirm that the error is in  $\Delta x^2$  when we use (115) and that it is in  $\Delta x$  when we use (116).

- *Test-case 3: Influence of the first iterate  $\rho_i^{n=1}$  on the Du Fort-Frankel scheme in the periodic case*

We know that the LBM\* scheme (49)(50) and the Du Fort-Frankel scheme (52) are equivalent when the first iterate  $\rho_i^{n=1}$  of the Du Fort-Frankel scheme is given by

$$\rho_i^{n=1} := \alpha \rho_{i-1}^0 + (1 - \alpha) \rho_{i+1}^0 \quad \text{where} \quad \alpha \in \mathbb{R} \quad (117)$$

(see Lemma 4.1). Moreover, these schemes verify the discrete maximum principle

$$\min_j \rho_j^0 \leq \rho_i^n \leq \max_j \rho_j^0$$

when  $\alpha \in [0, 1]$  in the periodic case (see Proposition 6.1). Here, we verify the influence of the choice of (117) when  $\alpha \in [0, 1]$  on the Du Fort-Frankel scheme by comparing with the results obtained by replacing (117) with

$$\rho_i^{n=1} := \rho_i^0. \quad (118)$$

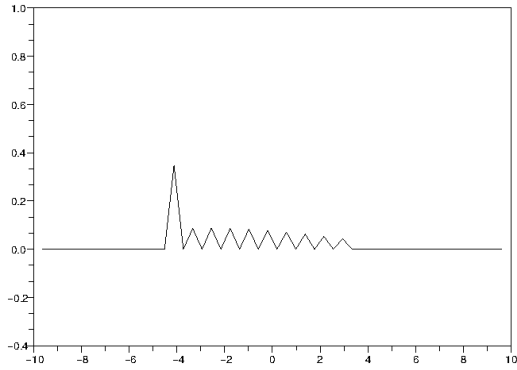


Fig. 7: Du Fort Frankel scheme with (117) and  $\alpha = 0$

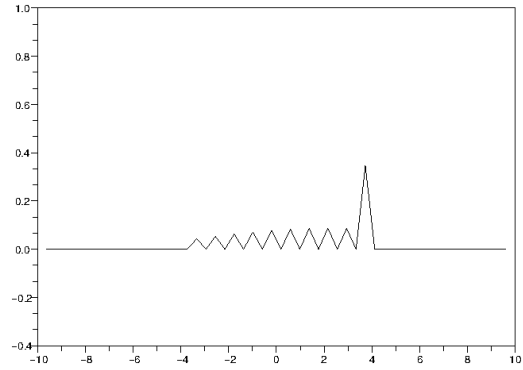


Fig. 8: Du Fort Frankel scheme with (117) and  $\alpha = 1$

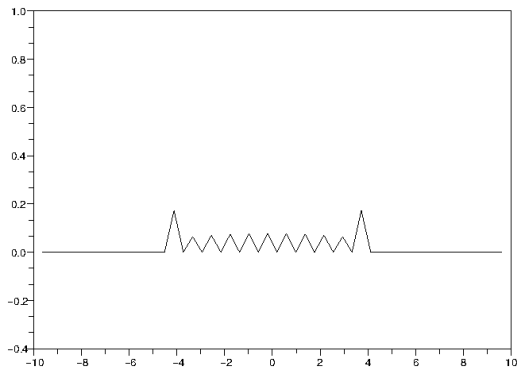


Fig. 9: Du Fort Frankel scheme with (117) and  $\alpha = \frac{1}{2}$

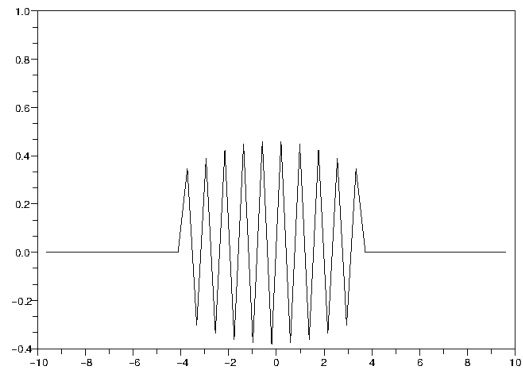


Fig. 10: Du Fort Frankel scheme with (118)

Let us underline that the Du Fort-Frankel scheme (52) is not equivalent to the LBM\* scheme (49)(50) when the first iterate is given by (118) instead of (117). As a consequence, the discrete maximum principle may not be satisfied when we use (118). To verify this, we choose  $C_d = 4$  and a number of cells  $N$  equal to 100, and we define the initial condition with the discrete Dirac distribution

$$\begin{aligned} \rho_i^0 &= 0 \text{ if } i \neq 50 \\ &= 1 \text{ if } i = 50. \end{aligned}$$

Figures 7-9 show the results after some time steps when we use the Du Fort-Frankel scheme (52) with (117) by choosing respectively  $\alpha = 0$ ,  $\alpha = 1$  and  $\alpha = \frac{1}{2}$ : these figures confirm Proposition 6.1. Figure 10 shows the result when we replace (117) by (118): this figure shows that the discrete maximum principle is not satisfied by the Du Fort-Frankel scheme.

These results underline the importance of the choice of the first iterate  $\rho_i^{n=1}$  to obtain for any  $C_d \geq 0$  the stability in  $L^\infty$  and a discrete maximum principle with the Du Fort-Frankel scheme.

### 9.2. Monte-Carlo algorithm

We now test the Monte-Carlo algorithm (105)(111) which is the random version of the LBM\* scheme (49)(50). The initial condition  $\rho(t = 0, x)$  is a gaussian function centered in  $x = 0$ , the boundary conditions are periodic and we choose  $\alpha = \frac{1}{2}$ .

Figures 11-14 show the result after some time steps obtained with 100, 1000, 5000 and 10000 particles when  $C_d = 2$  and when the number of cells  $N$  is equal to 100 (we also represent on these figures the initial condition and the result obtained with the LBM\* scheme). These results confirm that the Monte-Carlo algorithm converges to the LBM\* scheme when the number of particles goes to the infinity.

Figure 15 shows the result when  $C_d = 2$ , when the number of cells  $N$  and the number of particles  $\mathcal{K}$  are equal to 1000: by comparing Figure 12 ( $N = 100$  and  $\mathcal{K} = 1000$ ) and Figure 15 ( $N = \mathcal{K} = 1000$ ), we see that  $\mathcal{K}$  has to be greater than  $N$  to obtain a good convergence of the Monte-Carlo algorithm. This behaviour is classical and can be justified by the fact that when  $\mathcal{K} < N$ , there exists at any time  $t^n$  at least one cell where the number of particles is equal to zero.

### 9.3. On the consistency condition

Figure 16 shows the result of the test-case presented in §9.2 when  $C_d = 100$ ,  $N = 100$  and  $\mathcal{K} = 1000$  (we also represent on these figures the initial condition and the result obtained with the LBM\* scheme when  $C_d = 2$ ). Figure 17 show the result obtained with the LBM\* scheme when  $C_d = 1000$ .

Figures 16 and 17 show that when  $C_d \rightarrow +\infty$ , the Monte-Carlo algorithm and the LBM\* scheme do not approach the solution of the heat equation. This confirms the importance of the consistency condition  $\Delta t = C_d \frac{\Delta x^2}{\nu}$  (see §7.2 and §8.3.3).

## 10. Conclusion

In order to construct and to justify LBM schemes for the 1D convection-diffusion equation, we have firstly studied the fluid limit of a discrete velocity kinetic system whose kinetic velocities belong to a discrete and finite set  $\{v_q^\varepsilon\}_{q \in \{1,2\}}$  and whose the collision term is a BGK-type operator characterized by the collision time  $\varepsilon$ . This fluid limit – which is the 1D convection-diffusion equation – has been formally obtained with a Chapman-Enskog expansion and with a Hilbert expansion. The originality of this kinetic system relies on the fact that the kinetic velocity  $v_q^\varepsilon$  is proportional to  $1/\sqrt{\varepsilon}$ . We have imposed this constraint by previously noting that all LBM schemes use a discrete and finite set of velocities  $\{v_q\}_q$  (that can be assigned to virtual particles) and that the discrete velocity  $v_q$  is proportional to  $\frac{\Delta x}{\Delta t}$  (where  $\Delta x$  and  $\Delta t$  are respectively the mesh size and the time step) and, thus, is proportional to  $1/\sqrt{\Delta t}$  in the case of the heat equation (for which  $\Delta t = O(\Delta x^2)$ ).

Then, we have constructed two LBM schemes for the 1D convection-diffusion equation by discretizing the kinetic system with a third order integration formula. We have also underlined that a second order integration formula cannot capture the fluid limit because of the dependency of  $v_q^\varepsilon$  with  $\varepsilon$ . This third integration formula explains the classical "magic" formula  $\nu = \left(\widehat{\varepsilon} - \frac{\Delta t}{2}\right) \times c_s^2$  which relates the diffusion coefficient  $\nu$  to  $c_s := C \times \frac{\Delta x}{\Delta t}$  (named "pseudo sound speed of the lattice") where  $C$  is a constant and to a corrected collision time  $\widehat{\varepsilon}$ . Then, for periodic, Neumann and Dirichlet boundary conditions, we have shown that theses LBM



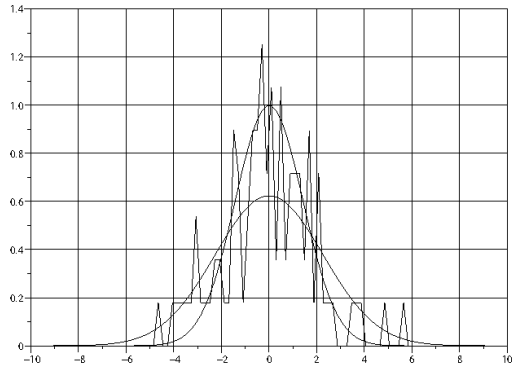


Fig. 11: 100 particles

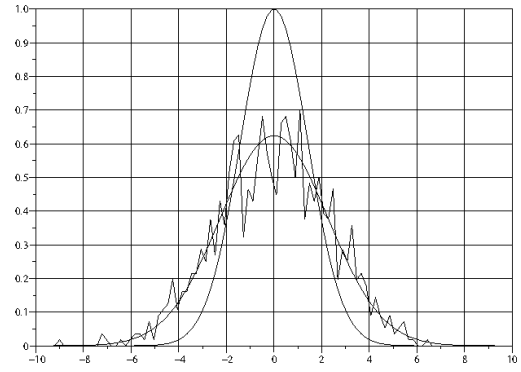


Fig. 12: 1000 particles

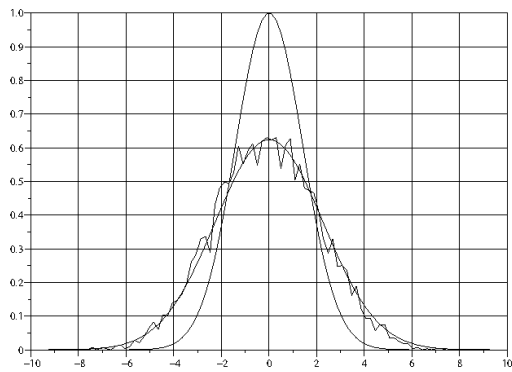


Fig. 13: 5000 particles

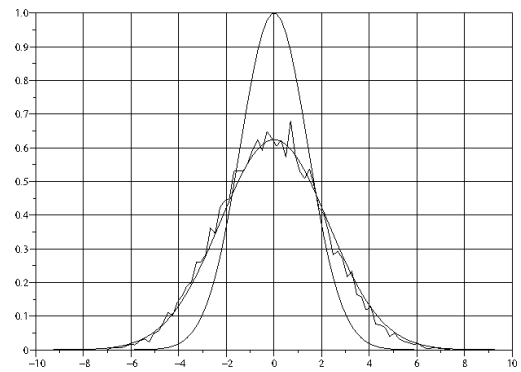


Fig. 14: 10000 particles

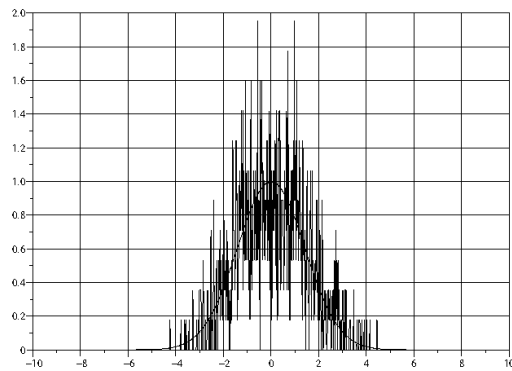


Fig. 15: 1000 cells and 1000 particles

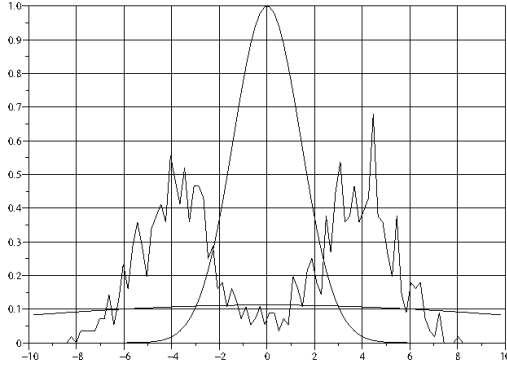


Fig. 16: 100 cells, 1000 particles and  $C_d = 100$

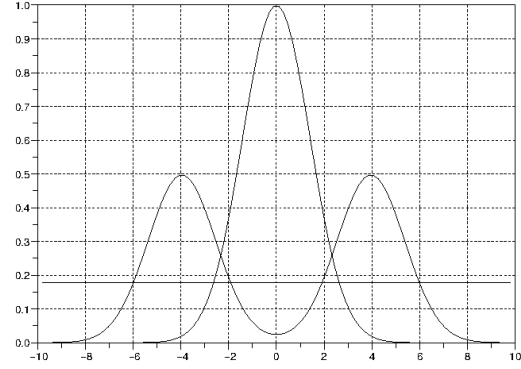


Fig. 17: LBM<sup>\*</sup> scheme, 100 cells and  $C_d = 1000$

schemes are equivalent to a finite difference type scheme. In the case of the heat equation, this finite difference type scheme is a Du Fort-Frankel scheme initiated by a particular first iterate. This equivalence has allowed us to obtain for these schemes the convergence in  $L^\infty$  for any  $\Delta t$  of the order of  $\Delta x^2$ .

These results are new for the LBM schemes but also for the Du Fort-Frankel scheme (which has been known for a long time to converge in  $L^2$  when  $\Delta t = O(\Delta x^2)$  [22]). Moreover, we have also obtained discrete maximum principles for the LBM schemes with periodic and Neumann boundary conditions for any  $\Delta t = O(\Delta x^2)$ , which are thus also verified by this particular Du Fort-Frankel scheme. Nevertheless, in the case of the Dirichlet boundary conditions, the discrete maximum principle is verified only under the classical stability condition  $\Delta t \leq C\Delta x^2$  (where  $C$  is a constant). Thus, we have modified the Dirichlet boundary conditions applied to the LBM schemes in such a way the discrete maximum principle is verified for any  $\Delta t = O(\Delta x^2)$ . The price to pay is that these LBM schemes cannot be equivalent to the Du Fort-Frankel scheme and that their convergence error should be only of the order of  $\Delta x$  (instead of  $\Delta x^2$ ). As a consequence, the proposed LBM schemes with these modified Dirichlet boundary conditions should be used only in areas where the number of cells are low to make robust the algorithm, and not in areas where the number of cells is high.

To summarize, the LBM schemes have been used as a tool to give new results for a finite difference type scheme and, at the same time, the classical theory of finite difference type schemes has allowed us to obtain convergence results for the LBM schemes.

In the same spirit, we have proposed two Monte-Carlo algorithms for the resolution of the heat equation coming from a probabilistic interpretation of the proposed LBM schemes in the periodic case. Thus, we expect that it will be possible to justify the modified Dirichlet boundary conditions and the order of convergence in  $\Delta x$  by using probabilistic tools.

We also expect that in the case of the convection-diffusion equation, it will be possible to extend the previous LBM schemes, firstly, to 2D/3D cartesian meshes and, secondly, to non-cartesian meshes (let us underline that we cannot extend the previous LBM schemes to the 2D/3D case on cartesian meshes by using a simple directional splitting). The case of non-isotropic diffusion matrix should be also studied. Moreover, we also expect that it will be possible to propose high order LBM schemes by using a larger set of kinetic

velocities and by using other integration formulae for the resolution of the discrete velocity kinetic system and, then, to eventually obtain similarities with the generalization of Du Fort-Frankel schemes proposed in [31]. The case of boundary conditions of the type  $\alpha(t)\rho + \beta(t)\partial_x\rho = \gamma(t)$  should be also studied to see connections with [32].

At last, we expect that it will be possible to analyze the properties of LBM schemes applied to more complicate equations as non-linear equations of the type  $\partial_t\rho = \Phi(t, x, \rho, \partial_x\rho, \partial_{xx}^2\rho)$  where  $\Phi(\cdot)$  is a given function (let us note that the Du Fort-Frankel scheme is generalized to this type of equation in [22]) by using an approach similar to the one proposed in this paper. Beyond the potential existence of links between LBM schemes, finite difference type schemes and Monte-Carlo algorithms for simple PDEs, we may also expect to find links between LBM schemes applied to the incompressible Navier-Stokes system and theoretical works on discrete velocity kinetic systems [33].

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### A. Proof of Proposition 2.1

We now give two (formal) proofs which allow to write that the fluid limit of the kinetic system

$$\forall q \in \{1, 2\} : \quad \partial_t f_q^\varepsilon + v_q^\varepsilon \partial_x f_q^\varepsilon = \frac{1}{\varepsilon} (M_q^\varepsilon - f_q^\varepsilon) \quad \text{with} \quad v_q^\varepsilon := (-1)^q \sqrt{\frac{v}{\varepsilon}} \quad (119)$$

is the convection-diffusion equation

$$\partial_t \rho^\varepsilon + \partial_x(u\rho^\varepsilon) = \nu \partial_{xx}^2 \rho^\varepsilon + \mathcal{O}(\varepsilon). \quad (120)$$

One of the difficulties is linked to the fact that the kinetic velocity  $v_q^\varepsilon := (-1)^q \sqrt{\frac{v}{\varepsilon}}$  depends on the collision time  $\varepsilon$  which is not at all classical in the framework of the kinetic theory. This characteristic is a constraint imposed by the LBM schemes that we want to obtain or to justify through an *ad hoc* discretization of (119).

The first proof is based on a Chapman-Enskog expansion; the second proof is based on a Hilbert expansion. The proof based on the Chapman-Enskog expansion is easier than the one based on the Hilbert expansion. Moreover, the Chapman-Enskog expansion allows to obtain

$$\begin{aligned} f_q^\varepsilon(t, x) &= \frac{\rho^\varepsilon}{2} \left[ 1 + (-1)^q \sqrt{\varepsilon} \left( \frac{u}{\sqrt{v}} - \sqrt{v} \frac{\partial_x \rho^\varepsilon}{\rho^\varepsilon} \right) \right. \\ &\quad \left. + (-1)^q \varepsilon^{3/2} \left( \frac{u}{\sqrt{v}} \cdot \frac{\partial_x(u\rho^\varepsilon) - \nu \partial_{xx}^2 \rho^\varepsilon}{\rho^\varepsilon} - \sqrt{v} \frac{\partial_{xx}^2(u\rho^\varepsilon)}{\rho^\varepsilon} + \nu^{3/2} \frac{\partial_{xxx}^3 \rho^\varepsilon}{\rho^\varepsilon} \right) \right] + \mathcal{O}(\varepsilon^2). \end{aligned} \quad (121)$$

With the Hilbert expansion, we only obtain

$$f_q^\varepsilon(t, x) = \frac{\rho^\varepsilon}{2} \left[ 1 + (-1)^q \sqrt{\varepsilon} \left( \frac{u}{\sqrt{v}} - \sqrt{v} \frac{\partial_x \rho^\varepsilon}{\rho^\varepsilon} \right) \right] + \mathcal{O}(\varepsilon^{3/2}) \quad (122)$$

which is less accurate than (121).

The fact that the Chapman-Enskog approach is easier than the Hilbert approach is classical in the kinetic theory. In fact, the compressible Navier-Stokes system – which is the fluid limit of the classical Boltzmann equation – is obtained with a Chapman-Enskog expansion and not with a Hilbert expansion which is too complicated to give the result. Here, it is possible to obtain the fluid limit with a Hilbert expansion because the kinetic velocity set is a discrete and finite set, which implies that the linear operators are simple  $2 \times 2$  matrix. Moreover, it seems to us that the Hilbert expansion is more adapted than the Chapman-Enskog expansion to clearly justify the fluid limit (120) of the kinetic system (119) because the Hilbert approach is based on a sequence of PDEs that we can study *a posteriori* (we do not try to do such theoretical study in the present paper). At last, the Hilbert expansion can also be seen as a (formal) justification of the Chapman-Enskog expansion since both expansions give the same result. That is why we also write the proof based on the Hilbert expansion.

At last, let us note that in the following analysis, we forget any possible influence of boundary conditions on  $\partial\Omega$ : that is why we suppose that  $\Omega \subseteq \mathbb{R}^3$  is periodic. An analysis of the influence of boundary conditions on  $\partial\Omega$  which are not periodic on the fluid limit of (119) is really complicated because of possible Knudsen layers in the vicinity of  $\partial\Omega$  where the distribution  $f_q^\varepsilon(t, x)$  is not close to the Maxwellian  $M_q^\varepsilon$  even when  $\varepsilon \ll 1$ . As a consequence, here, we can only expect that the fluid limit (120) is valid far from the boundary  $\partial\Omega$  when the boundary conditions are not periodic.

#### A.1. Proof based on a Chapman-Enskog expansion

Let us suppose that the solution  $f_q^\varepsilon$  of (119) can be expanded with the Chapman-Enskog expansion

$$f_q^\varepsilon = M_q^\varepsilon \cdot \left( 1 + \sqrt{\varepsilon} g_{1,q}^\varepsilon + \varepsilon g_{2,q}^\varepsilon + \varepsilon^{3/2} g_{3,q}^\varepsilon \right) + \mathcal{O}(\varepsilon^2) \quad (123)$$

under the constraints

$$\sum_{q \in \{1,2\}} M_q^\varepsilon (g_{1,q}^\varepsilon + \sqrt{\varepsilon} g_{2,q}^\varepsilon) = 0 \quad (124)$$

and

$$\sum_{q \in \{1,2\}} M_q^\varepsilon g_{3,q}^\varepsilon = 0 \quad (125)$$

where  $g_{k,q}^\varepsilon$  is supposed to be of order one. We recall that the Maxwellian  $M_q^\varepsilon$  is given by

$$M_q^\varepsilon := \frac{\rho^\varepsilon}{2} \left[ 1 + \frac{u}{v_q^\varepsilon} \right] = \frac{\rho^\varepsilon}{2} \left[ 1 + (-1)^q \sqrt{\frac{\varepsilon}{v}} \cdot u \right]$$

where  $\rho^\varepsilon := f_1^\varepsilon + f_2^\varepsilon$  and verifies

$$\sum_{q \in \{1,2\}} \begin{pmatrix} 1 \\ v_q^\varepsilon \end{pmatrix} M_q^\varepsilon = \begin{pmatrix} \rho^\varepsilon \\ \rho^\varepsilon u \end{pmatrix}. \quad (126)$$

It is important to note that the constraint (124) is not classical in the framework of Chapman-Enskog expansions. Indeed, we should *a priori* impose

$$\sum_{q \in \{1,2\}} M_q^\varepsilon g_{1,q}^\varepsilon = 0 \quad \text{and} \quad \sum_{q \in \{1,2\}} M_q^\varepsilon g_2^\varepsilon = 0. \quad (127)$$

Here, we replace (127) by (124) because the set of kinetic velocities  $\{v_q^\varepsilon\}_{q \in \{1,2\}}$  depends on  $\sqrt{\varepsilon}$  which implies that  $M_q^\varepsilon g_{1,q}^\varepsilon$  has a term of order  $\sqrt{\varepsilon}$  (and, thus, of order  $\sqrt{\varepsilon} g_{2,q}^\varepsilon$ ) since  $g_{1,q}^\varepsilon$  (and  $g_{2,q}^\varepsilon$ ) is of order one.

By injecting expansion (123) into (119), we obtain:

- *Order  $\sqrt{\varepsilon}^{-1}$* : We obtain the equality

$$M_q^\varepsilon g_{1,q}^\varepsilon = -\sqrt{\varepsilon} v_q^\varepsilon \partial_x M_q^\varepsilon = -(-1)^q \sqrt{v} \partial_x M_q^\varepsilon \quad (128)$$

that is to say

$$M_q^\varepsilon g_{1,q}^\varepsilon = -(-1)^q \sqrt{v} \frac{\partial_x \rho^\varepsilon}{2} - \sqrt{\varepsilon} \frac{\partial_x (u \rho^\varepsilon)}{2} \quad (129)$$

since  $M_q^\varepsilon = \frac{\rho^\varepsilon}{2} \left[ 1 + (-1)^q \sqrt{\frac{\varepsilon}{v}} \cdot u \right]$ .

- *Order  $\sqrt{\varepsilon}^0$* : We obtain the equality

$$M_q^\varepsilon g_{2,q}^\varepsilon = - \left[ \partial_t M_q^\varepsilon + \sqrt{\varepsilon} v_q^\varepsilon \partial_x (M_q^\varepsilon g_{1,q}^\varepsilon) \right]. \quad (130)$$

- *Order  $\sqrt{\varepsilon}$* : We obtain the equality

$$M_q^\varepsilon g_{3,q}^\varepsilon = - \left[ \partial_t (M_q^\varepsilon g_{1,q}^\varepsilon) + \sqrt{\varepsilon} v_q^\varepsilon \partial_x (M_q^\varepsilon g_{2,q}^\varepsilon) \right]. \quad (131)$$

Moreover, by summing (119) over the set  $\{v_q^\varepsilon\}_{q \in \{1,2\}}$  and by injecting the expansion (123), we obtain

$$\begin{aligned} \partial_t \rho^\varepsilon + \partial_x (u \rho^\varepsilon) &= -\partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) f_q^\varepsilon \right] \quad \left( \text{since } \sum_{q \in \{1,2\}} u f_q^\varepsilon = u \rho^\varepsilon \text{ and } \sum_{q \in \{1,2\}} \frac{1}{\varepsilon} (M_q^\varepsilon - f_q^\varepsilon) = 0 \right) \\ &= -\partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) M_q^\varepsilon \right] - \sqrt{\varepsilon} \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) M_q^\varepsilon g_{1,q}^\varepsilon \right] - \varepsilon \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) M_q^\varepsilon g_{2,q}^\varepsilon \right] + \mathcal{O}(\varepsilon) \\ &= -\partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) M_q^\varepsilon \right] - \sqrt{\varepsilon} \partial_x \left[ \sum_{q \in \{1,2\}} v_q^\varepsilon M_q^\varepsilon g_{1,q}^\varepsilon \right] - \varepsilon \partial_x \left[ \sum_{q \in \{1,2\}} v_q^\varepsilon M_q^\varepsilon g_{2,q}^\varepsilon \right] \\ &\quad + \sqrt{\varepsilon} \partial_x \left[ u \sum_{q \in \{1,2\}} M_q^\varepsilon (g_{1,q}^\varepsilon + \sqrt{\varepsilon} g_{2,q}^\varepsilon) \right] + \mathcal{O}(\varepsilon). \end{aligned} \quad (132)$$

By taking into account (126), (128) and (130), we obtain

$$\begin{aligned}
\varepsilon \partial_x \left[ \sum_{q \in \{1,2\}} v_q^\varepsilon M_q^\varepsilon g_{2,q}^\varepsilon \right] &= -\varepsilon \partial_x \left\{ \sum_{q \in \{1,2\}} v_q^\varepsilon \left[ \partial_t M_q^\varepsilon + \sqrt{\varepsilon} v_q^\varepsilon \partial_x (M_q^\varepsilon g_{1,q}^\varepsilon) \right] \right\} \\
&= -\varepsilon \partial_{xt}^2 (u \rho^\varepsilon) + \varepsilon \partial_x \left[ \sum_{q \in \{1,2\}} v_q^\varepsilon \sqrt{\varepsilon} v_q^\varepsilon \partial_x (\sqrt{\varepsilon} v_q^\varepsilon \partial_x M_q^\varepsilon) \right] \\
&= -\varepsilon \partial_{xt}^2 (u \rho^\varepsilon) + \varepsilon v \partial_{xxx}^3 (u \rho^\varepsilon) \\
&= O(\varepsilon).
\end{aligned}$$

Thus, by also taking into account (124), we obtain

$$\begin{aligned}
\partial_t \rho^\varepsilon + \partial_x (u \rho^\varepsilon) &= -\sqrt{\varepsilon} \partial_x \left[ \sum_{q \in \{1,2\}} v_q^\varepsilon M_q^\varepsilon g_{1,q}^\varepsilon \right] + O(\varepsilon) \\
&= \varepsilon \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon)^2 \partial_x M_q^\varepsilon \right] + O(\varepsilon) \\
&= v \partial_{xx}^2 \left( \sum_{q \in \{1,2\}} M_q^\varepsilon \right) + O(\varepsilon) \\
&= v \partial_{xx}^2 \rho^\varepsilon + O(\varepsilon)
\end{aligned}$$

which gives (120) that is to say

$$\partial_t \rho^\varepsilon + \partial_x (u \rho^\varepsilon) = v \partial_{xx}^2 \rho^\varepsilon + O(\varepsilon). \quad (133)$$

We deduce from (129), (130) and (133) that

$$\begin{aligned}
M_q^\varepsilon g_{2,q}^\varepsilon &= -\partial_t M_q^\varepsilon + v \partial_{xx}^2 M_q^\varepsilon \\
&= -\frac{\partial_t \rho^\varepsilon}{2} - (-1)^q \sqrt{\frac{\varepsilon}{v}} \cdot \frac{\partial_t (u \rho^\varepsilon)}{2} + v \frac{\partial_{xx}^2 \rho^\varepsilon}{2} + (-1)^q \sqrt{\varepsilon v} \cdot \frac{\partial_{xx}^2 (u \rho^\varepsilon)}{2} \\
&= \frac{\partial_x (u \rho^\varepsilon)}{2} + (-1)^q \sqrt{\frac{\varepsilon}{v}} u \cdot \frac{\partial_x (u \rho^\varepsilon) - v \partial_{xx}^2 \rho^\varepsilon}{2} + (-1)^q \sqrt{\varepsilon v} \cdot \frac{\partial_{xx}^2 (u \rho^\varepsilon)}{2} + O(\varepsilon)
\end{aligned} \quad (134)$$

(we also use the fact that  $u(x)$  does not depend on the time  $t$ ). This last equality encourages us to take

$$M_q^\varepsilon g_{2,q}^\varepsilon = \frac{\partial_x (u \rho^\varepsilon)}{2} + (-1)^q \sqrt{\frac{\varepsilon}{v}} u \cdot \frac{\partial_x (u \rho^\varepsilon) - v \partial_{xx}^2 \rho^\varepsilon}{2} + (-1)^q \sqrt{\varepsilon v} \cdot \frac{\partial_{xx}^2 (u \rho^\varepsilon)}{2} \quad (135)$$

since the term of order  $\varepsilon$  in (134) is a term of order  $\varepsilon^2$  in (123) and, thus, of order  $\varepsilon$  in (133). We deduce from (129) and (135) that

$$M_q^\varepsilon \cdot (\sqrt{\varepsilon} g_{1,q}^\varepsilon + \varepsilon g_{2,q}^\varepsilon) = \frac{\rho^\varepsilon}{2} \left[ -(-1)^q \sqrt{\varepsilon v} \frac{\partial_x \rho^\varepsilon}{\rho^\varepsilon} + (-1)^q \frac{\varepsilon^{3/2}}{\sqrt{v}} u \cdot \frac{\partial_x (u \rho^\varepsilon) - v \partial_{xx}^2 \rho^\varepsilon}{\rho^\varepsilon} + (-1)^q \varepsilon^{3/2} \sqrt{v} \cdot \frac{\partial_{xx}^2 (u \rho^\varepsilon)}{\rho^\varepsilon} \right]$$

which verifies the constraint (124). We deduce from (129), (131) and (135) that

$$M_q^\varepsilon g_{3,q}^\varepsilon = (-1)^q \sqrt{v} \frac{\partial_{xx}^2 \rho^\varepsilon}{2} - (-1)^q \sqrt{v} \frac{\partial_{xx}^2 (u \rho^\varepsilon)}{2} + \mathcal{O}(\sqrt{\varepsilon})$$

which allows to obtain

$$\begin{aligned} M_q^\varepsilon g_{3,q}^\varepsilon &= (-1)^q \sqrt{v} \frac{v \partial_{xxx}^3 \rho^\varepsilon - \partial_{xx}^2 (u \rho^\varepsilon)}{2} - (-1)^q \sqrt{v} \frac{\partial_{xx}^2 (u \rho^\varepsilon)}{2} + \mathcal{O}(\sqrt{\varepsilon}) \\ &= (-1)^q v^{3/2} \frac{\partial_{xxx}^3 \rho^\varepsilon}{2} - (-1)^q \sqrt{v} \partial_{xx}^2 (u \rho^\varepsilon) + \mathcal{O}(\sqrt{\varepsilon}) \end{aligned} \quad (136)$$

by using (133). This last equality encourages us to take

$$M_q^\varepsilon g_{3,q}^\varepsilon = (-1)^q v^{3/2} \frac{\partial_{xxx}^3 \rho^\varepsilon}{2} - (-1)^q \sqrt{v} \partial_{xx}^2 (u \rho^\varepsilon) \quad (137)$$

since the term of order  $\sqrt{\varepsilon}$  in (136) is a term of order  $\varepsilon^2$  in (123) and, thus, of order  $\varepsilon$  in (133). Let us note that (137) verifies the constraint (125). Thus, by taking into account (133), we obtain

$$\begin{aligned} M_q^\varepsilon \cdot (\sqrt{\varepsilon} g_{1,q}^\varepsilon + \varepsilon g_{2,q}^\varepsilon + \varepsilon^{3/2} g_{3,q}^\varepsilon) &= \frac{\rho^\varepsilon}{2} \left[ 1 + (-1)^q \sqrt{\varepsilon} \left( \frac{u}{\sqrt{v}} - \sqrt{v} \frac{\partial_x \rho^\varepsilon}{\rho^\varepsilon} \right) \right. \\ &\quad \left. + (-1)^q \frac{\varepsilon^{3/2}}{\sqrt{v}} u \cdot \frac{\partial_x (u \rho^\varepsilon) - v \partial_{xx}^2 \rho^\varepsilon}{\rho^\varepsilon} + (-1)^q \varepsilon^{3/2} \sqrt{v} \frac{\partial_{xx}^2 (u \rho^\varepsilon)}{\rho^\varepsilon} \right. \\ &\quad \left. + (-1)^q \varepsilon^{3/2} v^{3/2} \frac{\partial_{xxx}^3 \rho^\varepsilon}{\rho^\varepsilon} - 2(-1)^q \varepsilon^{3/2} \sqrt{v} \frac{\partial_{xx}^2 (u \rho^\varepsilon)}{\rho^\varepsilon} \right] \end{aligned}$$

that is to say

$$\begin{aligned} M_q^\varepsilon \cdot (\sqrt{\varepsilon} g_{1,q}^\varepsilon + \varepsilon g_{2,q}^\varepsilon + \varepsilon^{3/2} g_{3,q}^\varepsilon) &= \frac{\rho^\varepsilon}{2} \left[ 1 + (-1)^q \sqrt{\varepsilon} \left( \frac{u}{\sqrt{v}} - \sqrt{v} \frac{\partial_x \rho^\varepsilon}{\rho^\varepsilon} \right) \right. \\ &\quad \left. + (-1)^q \varepsilon^{3/2} \left( \frac{u}{\sqrt{v}} \cdot \frac{\partial_x (u \rho^\varepsilon) - v \partial_{xx}^2 \rho^\varepsilon}{\rho^\varepsilon} - \sqrt{v} \frac{\partial_{xx}^2 (u \rho^\varepsilon)}{\rho^\varepsilon} + v^{3/2} \frac{\partial_{xxx}^3 \rho^\varepsilon}{\rho^\varepsilon} \right) \right] \end{aligned}$$

which gives (121) by using (123).

## A.2. Proof based on a Hilbert expansion

Let us suppose that the solution  $f_q^\varepsilon$  of (119) can be expanded with the Hilbert expansion

$$f_q^\varepsilon = m_q^\varepsilon \cdot (g_{0,q}^\varepsilon + \sqrt{\varepsilon} g_{1,q}^\varepsilon + \sqrt{\varepsilon^2} g_{2,q}^\varepsilon + \dots) \quad (138)$$

where

$$m_q^\varepsilon := 1 + \frac{u}{v_q^\varepsilon} = 1 + (-1)^q \sqrt{\frac{\varepsilon}{v}} \cdot u.$$

The density  $\rho^\varepsilon := f_1^\varepsilon + f_2^\varepsilon$  is given by

$$\rho^\varepsilon = \rho_0 + \sqrt{\varepsilon} \rho_1^\varepsilon + \sqrt{\varepsilon^2} \rho_2^\varepsilon + \dots$$

with

$$\forall n : \rho_n^\varepsilon = \sum_{q \in \{1,2\}} m_q^\varepsilon g_{n,q}^\varepsilon. \quad (139)$$

And, the maxwellian  $M_q^\varepsilon$  defined with

$$M_q^\varepsilon := \frac{\rho^\varepsilon}{2} \left[ 1 + \frac{u}{v_q^\varepsilon} \right] = \frac{\rho^\varepsilon}{2} \left[ 1 + (-1)^q \sqrt{\frac{\varepsilon}{v}} \cdot u \right]$$

whose density is equal to  $\rho^\varepsilon$  is given by

$$M_q^\varepsilon = m_q^\varepsilon \cdot (\rho_0^\varepsilon + \sqrt{\varepsilon} \rho_1^\varepsilon + \sqrt{\varepsilon}^2 \rho_2^\varepsilon + \dots).$$

In the sequel, we will prove that when the Hilbert expansion (138) is valid, the density  $\rho^\varepsilon$  is necessarily solution of (120). Moreover, by computing  $g_{0,q}^\varepsilon$ ,  $g_{1,q}^\varepsilon$  and  $g_{2,q}^\varepsilon$ , we will obtain (122).

Let us note that the difference between the Chapman-Enskog expansion (123) and the Hilbert expansion (138) can be underlined by comparing the constraints (124)(125) and the relations (139) which are not constraints,  $\rho_n^\varepsilon$  being unknowns which are solution of a sequence of PDEs (see below).

By injecting expansion (138) into (119), we obtain:

- *Order  $\varepsilon^{-1}$* : We obtain the equality

$$g_{0,1}^\varepsilon = g_{0,2}^\varepsilon = \rho_0^\varepsilon(t, x). \quad (140)$$

- *Order  $(\sqrt{\varepsilon})^{n-1/2}$  ( $n \in \mathbb{N}$ )*: We obtain the following PDEs whose  $\{g_{n,q}^\varepsilon\}_{n \geq 0}$  is solution:

$$(\sqrt{\varepsilon})^n [\partial_t (m_q^\varepsilon g_{n,q}^\varepsilon) + v_q^\varepsilon \partial_x (m_q^\varepsilon g_{n,q}^\varepsilon)] = m_q^\varepsilon (\sqrt{\varepsilon})^{n-1} \left( \sum_{k \in \{1,2\}} m_k^\varepsilon g_{n+1,k}^\varepsilon - g_{n+1,q}^\varepsilon \right). \quad (141)$$

We recall that  $O(|v_q^\varepsilon|) = 1/\sqrt{\varepsilon}$  which implies that  $(\sqrt{\varepsilon})^n v_q^\varepsilon \partial_x (m_q^\varepsilon g_{n,q}^\varepsilon)$  and  $m_q^\varepsilon (\sqrt{\varepsilon})^{n-1} \left( \sum_{k \in \{1,2\}} m_k^\varepsilon g_{n+1,k}^\varepsilon - g_{n+1,q}^\varepsilon \right)$  are formally of the same order. Moreover, we keep the unstationary term  $(\sqrt{\varepsilon})^n \partial_t (m_q^\varepsilon g_{n,q}^\varepsilon)$  to obtain an initial value problem for  $m_q^\varepsilon g_{n,q}^\varepsilon$ . PDEs (141) can be written with the equivalent formulation

$$\forall n \geq 0 : \mathbf{A}^\varepsilon \cdot \mathcal{G}_{n+1} = \mathcal{B}^\varepsilon(\mathcal{G}_n) \quad (142)$$

where  $\mathcal{G}_n^\varepsilon = (g_{n,1}^\varepsilon, g_{n,2}^\varepsilon)^T$ ,  $\mathcal{B}^\varepsilon = (b_1^\varepsilon, b_2^\varepsilon)^T$  and where

$$\begin{cases} \mathbf{A}^\varepsilon = \begin{pmatrix} -m_2^\varepsilon & m_2^\varepsilon \\ m_1^\varepsilon & -m_1^\varepsilon \end{pmatrix}, & \text{(a)} \\ b_q^\varepsilon(\mathcal{G}_n^\varepsilon) = \frac{\sqrt{\varepsilon}}{m_q^\varepsilon} \cdot [\partial_t (m_q^\varepsilon g_{n,q}^\varepsilon) + v_q^\varepsilon \partial_x (m_q^\varepsilon g_{n,q}^\varepsilon)]. & \text{(b)} \end{cases} \quad (143)$$

Since the matrix  $\mathbf{A}^\varepsilon$  is not invertible, we have to study carefully linear system (142). By applying the Fredholm alternative, we obtain the following result:



**Lemma A.1.** Let  $\mathcal{G}_{-1}^\varepsilon = 0$  and

$$\mathcal{G}_0^\varepsilon = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \rho_0^\varepsilon. \quad (144)$$

Then, Equation (142) has an unique solution under the constraints

$$\forall n \geq 0: \quad \partial_t \rho_n^\varepsilon + \partial_x(u \rho_n^\varepsilon) = \mathcal{F}^\varepsilon(\mathcal{G}_{n-1}^\varepsilon) \quad (145)$$

where

$$\forall n \geq 0: \quad \mathcal{F}^\varepsilon(\mathcal{G}_{n-1}^\varepsilon) := \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) m_q^\varepsilon b_q^\varepsilon(\mathcal{G}_{n-1}^\varepsilon) \right]. \quad (146)$$

Moreover,  $\{\mathcal{G}_n^\varepsilon\}_{n \geq 1}$  is given by the recurrence relation

$$\forall n \geq 1: \quad \mathcal{G}_n^\varepsilon = -\mathcal{B}^\varepsilon(\mathcal{G}_{n-1}^\varepsilon) + \rho_n^\varepsilon \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \quad (147)$$

Thus, the construction process to obtain  $\{\mathcal{G}_n^\varepsilon\}_{n \geq 0}$  is the following:

$$\left\{ \begin{array}{l} \text{Firstly, we note that } \mathcal{F}^\varepsilon(\mathcal{G}_{-1}^\varepsilon) = 0 \text{ since } \mathcal{G}_{-1}^\varepsilon = 0; \\ \text{secondly, we compute } \rho_0^\varepsilon \text{ with (145);} \\ \text{thirdly, we compute } \mathcal{G}_0^\varepsilon \text{ with (144).} \end{array} \right. \rightarrow \left\{ \begin{array}{l} \text{Firstly, we compute } \mathcal{F}^\varepsilon(\mathcal{G}_0^\varepsilon) \text{ with (146);} \\ \text{secondly, we compute } \rho_1^\varepsilon \text{ with (145);} \\ \text{thirdly, we compute } \mathcal{G}_1^\varepsilon \text{ with (147).} \end{array} \right. \rightarrow \dots$$

$$\dots \rightarrow \left\{ \begin{array}{l} \text{Firstly, we compute } \mathcal{F}^\varepsilon(\mathcal{G}_{n-1}^\varepsilon) \text{ with (146);} \\ \text{secondly, we compute } \rho_n^\varepsilon \text{ with (145);} \\ \text{thirdly, we compute } \mathcal{G}_n^\varepsilon \text{ with (147).} \end{array} \right. \rightarrow \dots \quad (148)$$

By using (145), we obtain that

$$\left\{ \begin{array}{l} \partial_t \rho_0^\varepsilon + \partial_x(u \rho_0^\varepsilon) = 0 \quad (\text{constraint (145) with } n = 0), \quad (a) \\ \partial_t \rho_1^\varepsilon + \partial_x(u \rho_1^\varepsilon) = \mathcal{F}^\varepsilon(\mathcal{G}_0^\varepsilon) \quad (\text{constraint (145) with } n = 1) \quad (b) \\ \partial_t \rho_2^\varepsilon + \partial_x(u \rho_2^\varepsilon) = \mathcal{F}^\varepsilon(\mathcal{G}_1^\varepsilon) \quad (\text{constraint (145) with } n = 2) \quad (c) \end{array} \right. \quad (149)$$

that is to say

$$\partial_t \rho^\varepsilon + \partial_x(u \rho^\varepsilon) = \sqrt{\varepsilon} \mathcal{F}^\varepsilon(\mathcal{G}_0^\varepsilon) + \varepsilon \mathcal{F}^\varepsilon(\mathcal{G}_1^\varepsilon) + \mathcal{O}(\varepsilon) \quad (150)$$

since  $\rho^\varepsilon = \rho_0 + \sqrt{\varepsilon} \rho_1 + \varepsilon \rho_2 + \mathcal{O}(\varepsilon^{3/2})$ . Let us note that the term of order  $\varepsilon$  in (150) is obtained by supposing that  $\mathcal{F}^\varepsilon(\mathcal{G}_n^\varepsilon) = \mathcal{O}(1/\sqrt{\varepsilon})$  ( $\forall n \geq 0$ ) because of the velocity  $v_q^\varepsilon$  in (146). Thus, we obtain (120) by using the following lemma:

**Lemma A.2.** We have

$$\left\{ \begin{array}{l} \mathcal{F}^\varepsilon(\mathcal{G}_0^\varepsilon) = \frac{v}{\sqrt{\varepsilon}} \partial_{xx}^2 \rho_0^\varepsilon + \mathcal{O}(\sqrt{\varepsilon}), \quad (a) \\ \mathcal{F}^\varepsilon(\mathcal{G}_1^\varepsilon) = \frac{v}{\sqrt{\varepsilon}} \partial_{xx}^2 \rho_1^\varepsilon + \mathcal{O}(1). \quad (b) \end{array} \right. \quad (151)$$

Moreover, we have the following result which will allow us to obtain (122):

**Lemma A.3.** *We have*

$$\begin{cases} g_{1,q}^\varepsilon = \sqrt{\varepsilon} \partial_x (u \rho_0^\varepsilon) - (-1)^q \sqrt{v} \frac{\partial_x (m_q^\varepsilon \rho_0^\varepsilon)}{m_q^\varepsilon} + \rho_1^\varepsilon, & (a) \\ g_{2,q}^\varepsilon = -v \left[ \partial_{xx}^2 \rho_0^\varepsilon - \frac{\partial_{xx}^2 (m_q^\varepsilon \rho_0^\varepsilon)}{m_q^\varepsilon} \right] - (-1)^q \sqrt{v} \frac{\partial_x (m_q^\varepsilon \rho_1^\varepsilon)}{m_q^\varepsilon} + \rho_2^\varepsilon + \mathcal{O}(\sqrt{\varepsilon}). & (b) \end{cases} \quad (152)$$

Thus, by using (152), we obtain

$$\begin{aligned} m_q^\varepsilon (g_{0,q}^\varepsilon + \sqrt{\varepsilon} g_{1,q}^\varepsilon + \varepsilon g_{2,q}^\varepsilon) &= \frac{1}{2} \left( 1 + (-1)^q \sqrt{\frac{\varepsilon}{v}} u \right) \times \\ &\times \left\{ \rho_0^\varepsilon + \sqrt{\varepsilon} \rho_1^\varepsilon + \varepsilon \rho_2^\varepsilon - (-1)^q \frac{\sqrt{\varepsilon v}}{m_q^\varepsilon} \partial_x \left[ m_q^\varepsilon (\rho_0^\varepsilon + \sqrt{\varepsilon} \rho_1^\varepsilon) \right] \right. \\ &\left. + \varepsilon \partial_x (u \rho_0^\varepsilon) - \varepsilon v \left[ \partial_{xx}^2 \rho_0^\varepsilon - \frac{\partial_{xx}^2 (m_q^\varepsilon \rho_0^\varepsilon)}{m_q^\varepsilon} \right] \right\} + \mathcal{O}(\varepsilon^{3/2}). \end{aligned}$$

By noting that  $\partial_x m_q^\varepsilon = (-1)^q \sqrt{\frac{\varepsilon}{v}} \cdot \frac{u'(x)}{2}$ , we deduce from the previous equality that

$$\begin{aligned} m_q^\varepsilon (g_{0,q}^\varepsilon + \sqrt{\varepsilon} g_{1,q}^\varepsilon + \varepsilon g_{2,q}^\varepsilon) &= \frac{1}{2} \left( 1 + (-1)^q \sqrt{\frac{\varepsilon}{v}} u \right) \times \\ &\times \left[ \rho_0^\varepsilon + \sqrt{\varepsilon} \rho_1^\varepsilon + \varepsilon \rho_2^\varepsilon - (-1)^q \sqrt{\varepsilon v} \partial_x (\rho_0^\varepsilon + \sqrt{\varepsilon} \rho_1^\varepsilon) - \varepsilon \rho_0^\varepsilon \frac{u'(x)}{2m_q^\varepsilon} + \varepsilon \partial_x (u \rho_0^\varepsilon) \right] + \mathcal{O}(\varepsilon^{3/2}) \\ &= \frac{1}{2} (\rho_0^\varepsilon + \sqrt{\varepsilon} \rho_1^\varepsilon + \varepsilon \rho_2^\varepsilon) \left( 1 + (-1)^q \sqrt{\frac{\varepsilon}{v}} u \right) \\ &\quad - (-1)^q \frac{\sqrt{\varepsilon v}}{2} \partial_x (\rho_0^\varepsilon + \sqrt{\varepsilon} \rho_1^\varepsilon) - \frac{\varepsilon}{2} \left[ \rho_0^\varepsilon \frac{u'(x)}{2m_q^\varepsilon} + u \partial_x \rho_0^\varepsilon + \partial_x (u \rho_0^\varepsilon) \right] + \mathcal{O}(\varepsilon^{3/2}) \end{aligned}$$

that is to say

$$f_q^\varepsilon = \frac{\rho^\varepsilon}{2} \left( 1 + (-1)^q \sqrt{\frac{\varepsilon}{v}} u \right) - (-1)^q \frac{\sqrt{\varepsilon v}}{2} \partial_x \rho^\varepsilon - \frac{\varepsilon}{2} \left[ \rho_0^\varepsilon \frac{u'(x)}{2m_q^\varepsilon} + u \partial_x \rho_0^\varepsilon - \partial_x (u \rho_0^\varepsilon) \right] + \mathcal{O}(\varepsilon^{3/2}).$$

Since  $\rho_0^\varepsilon \frac{u'(x)}{2m_q^\varepsilon} + u \partial_x \rho_0^\varepsilon = \partial_x (u \rho_0^\varepsilon) + \mathcal{O}(\sqrt{\varepsilon})$ , we obtain

$$f_q^\varepsilon(t, x) = \frac{\rho^\varepsilon}{2} \left[ 1 + (-1)^q \sqrt{\varepsilon} \left( \frac{u(x)}{\sqrt{v}} - \sqrt{v} \frac{\partial_x \rho^\varepsilon}{\rho^\varepsilon} \right) \right] + \mathcal{O}(\varepsilon^{3/2}) \quad (153)$$

which is exactly the expansion (122).

It remains to prove Lemmae A.1, A.2 and A.3:

**Proof of lemma A.1:** The matrix  $\mathbf{A}^\varepsilon$  is not invertible and its kernel is given by

$$\text{Ker} \mathbf{A}^\varepsilon = \left\{ X \in \mathbb{R}^2 \quad \text{such that} \quad X = \mu(1, 1)^T, \quad \mu \in \mathbb{R} \right\}.$$

Moreover,  $\mathbf{A}^\varepsilon$  admits the eigenvalue  $\lambda = -1$  whose eigenspace is given by

$$\begin{aligned} \mathcal{E}^{\varepsilon, \lambda=-1} &= \left\{ X \in \mathbb{R}^2 \quad \text{such that} \quad X = \mu(m_2^\varepsilon, -m_1^\varepsilon)^T, \quad \mu \in \mathbb{R} \right\} \quad (\text{a}) \\ &= \left\{ X \in \mathbb{R}^2 \quad \text{such that} \quad \sum_{q \in \{1,2\}} X_q m_q^\varepsilon = 0 \right\}. \quad (\text{b}) \end{aligned} \quad (154)$$

Let us note that  $\mathcal{E}^{\varepsilon, \lambda=-1}$  depends on  $\varepsilon$  – which is not the case of  $\text{Ker} \mathbf{A}^\varepsilon$  –, that  $\text{Ker} \mathbf{A}^\varepsilon \oplus \mathcal{E}^{\varepsilon, \lambda=-1} = \mathbb{R}^2$  and that  $\mathcal{E}^{\varepsilon, \lambda=-1} \perp (m_1^\varepsilon, m_2^\varepsilon)^T$ . The linear application  $\mathbf{A}^\varepsilon : X \mapsto \mathbf{A}^\varepsilon \cdot X$  defines a bijection from  $\mathcal{E}^{\varepsilon, \lambda=-1}$  into  $\mathcal{E}^{\varepsilon, \lambda=-1}$ . Thus, we can solve linear system (142) if and only if

$$\forall n \geq 0 : \quad \mathcal{B}^\varepsilon(\mathcal{G}_n^\varepsilon) \in \mathcal{E}^{\varepsilon, \lambda=-1}. \quad (155)$$

This corresponds to the Fredholm alternative in finite dimension. Thus, by using (154)(b), the vector  $\mathcal{B}^\varepsilon(\mathcal{G}_n^\varepsilon)$  has to verify the constraint

$$\forall n \geq 0 : \quad \sum_{q \in \{1,2\}} m_q^\varepsilon b_q^\varepsilon(\mathcal{G}_n^\varepsilon) = 0 \quad (156)$$

that is to say

$$\forall n \geq 0 : \quad \sum_{q \in \{1,2\}} \left[ \partial_t(m_q^\varepsilon g_{n,q}^\varepsilon) + v_q^\varepsilon \partial_x(m_q^\varepsilon g_{n,q}^\varepsilon) \right] = 0$$

which is equivalent to

$$\forall n \geq 0 : \quad \partial_t \rho_n^\varepsilon + \partial_x(u \rho_n^\varepsilon) = -\partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) m_q^\varepsilon g_{n,q}^\varepsilon \right] \quad (157)$$

by using (139). Moreover, we have

$$\forall n \geq 0 : \quad \mathbf{A}^\varepsilon \cdot \mathcal{G}_{n+1}^\varepsilon = \mathcal{B}^\varepsilon(\mathcal{G}_n^\varepsilon) \quad \text{and} \quad \mathcal{B}^\varepsilon(\mathcal{G}_n^\varepsilon) \in \mathcal{E}^{\varepsilon, \lambda=-1} \implies \mathcal{G}_{n+1}^\varepsilon = -\mathcal{B}^\varepsilon(\mathcal{G}_n^\varepsilon) + \mu_{n+1} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

where  $\mu_{n+1} \in \mathbb{R}$ . Thus, by using (139) and (156), we obtain  $\rho_{n+1}^\varepsilon = \sum_{q \in \{1,2\}} m_q^\varepsilon g_{n+1,q}^\varepsilon = 0 + \mu_{n+1}$  which implies that  $\mathcal{G}_{n+1}^\varepsilon$  is given by (147). As a consequence, we have

$$\begin{aligned} -\partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) m_q^\varepsilon g_{n,q}^\varepsilon \right] &= -\partial_x \left\{ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) m_q^\varepsilon \left[ -b_q^\varepsilon(\mathcal{G}_{n-1}^\varepsilon) + \rho_n^\varepsilon \right] \right\} \\ &= \mathcal{F}^\varepsilon(\mathcal{G}_{n-1}^\varepsilon) + 0 \end{aligned}$$

by using the fact that

$$\sum_{q \in \{1,2\}} \begin{pmatrix} 1 \\ v_q^\varepsilon \end{pmatrix} m_q^\varepsilon = \begin{pmatrix} 1 \\ u \end{pmatrix}$$

and Definition (146), which allows to obtain (145) by taking into account (157). Finally, we have proven that (142) admits a solution  $\{\mathcal{G}_n^\varepsilon\}_{n \geq 0}$  under the constraints (145). Moreover, this solution is unique since (145) are linear PDEs which admit an unique solution.  $\square$

**Proof of Lemmae A.2 and A.3:** We firstly prove (151)(a) and (152)(a); then, we prove (151)(b) and (152)(b). We have

$$\begin{aligned}
\mathcal{F}^\varepsilon(\mathcal{G}_0) &= \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) m_q^\varepsilon b_q^\varepsilon(\mathcal{G}_0^\varepsilon) \right] \\
&= \sqrt{\varepsilon} \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) m_q^\varepsilon \partial_t \rho_0^\varepsilon \right] + \sqrt{\varepsilon} \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) v_q^\varepsilon \partial_x (m_q^\varepsilon \rho_0^\varepsilon) \right] \\
&= 0 + \sqrt{\varepsilon} \partial_x \left[ \sum_{q \in \{1,2\}} v_q^{\varepsilon 2} \partial_x (m_q^\varepsilon \rho_0^\varepsilon) \right] - \sqrt{\varepsilon} \partial_x \left[ u \partial_x \left( \sum_{q \in \{1,2\}} v_q^\varepsilon m_q^\varepsilon \rho_0^\varepsilon \right) \right] \\
&= \frac{v}{\sqrt{\varepsilon}} \partial_x \left[ \sum_{q \in \{1,2\}} \partial_x (m_q^\varepsilon \rho_0^\varepsilon) \right] - \sqrt{\varepsilon} \partial_x [u \partial_x (u \rho_0^\varepsilon)] \\
&= \frac{v}{\sqrt{\varepsilon}} \partial_{xx}^2 \rho_0^\varepsilon + \mathcal{O}(\sqrt{\varepsilon})
\end{aligned}$$

which gives (151)(a). Moreover, we have

$$\begin{aligned}
b_q^\varepsilon(\mathcal{G}_0^\varepsilon) &= \sqrt{\varepsilon} \frac{\partial_t (m_q^\varepsilon \rho_0^\varepsilon)}{m_q^\varepsilon} + \sqrt{\varepsilon} v_q^\varepsilon \frac{\partial_x (m_q^\varepsilon \rho_0^\varepsilon)}{m_q^\varepsilon} \\
&= \sqrt{\varepsilon} \partial_t \rho_0^\varepsilon + (-1)^q \sqrt{v} \frac{\partial_x (m_q^\varepsilon \rho_0^\varepsilon)}{m_q^\varepsilon} \\
&= -\sqrt{\varepsilon} \partial_x (u \rho_0^\varepsilon) + (-1)^q \sqrt{v} \frac{\partial_x (m_q^\varepsilon \rho_0^\varepsilon)}{m_q^\varepsilon}
\end{aligned}$$

by using (149)(a). We obtain (152)(a) by using (147). In the same way, we have

$$\begin{aligned}
\mathcal{F}^\varepsilon(\mathcal{G}_1^\varepsilon) &= \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) m_q^\varepsilon b_q^\varepsilon(\mathcal{G}_1) \right] \\
&= \sqrt{\varepsilon} \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) m_q^\varepsilon \partial_t g_{1,q}^\varepsilon \right] + \sqrt{\varepsilon} \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) v_q^\varepsilon \partial_x (m_q^\varepsilon g_{1,q}^\varepsilon) \right] \\
&= \sqrt{\varepsilon} \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) m_q^\varepsilon \partial_t g_{1,q}^\varepsilon \right] + \sqrt{\varepsilon} \partial_x \left[ \sum_{q \in \{1,2\}} v_q^{\varepsilon 2} \partial_x (m_q^\varepsilon g_{1,q}^\varepsilon) \right] - \sqrt{\varepsilon} \partial_x \left[ u \partial_x \left( \sum_{q \in \{1,2\}} v_q^\varepsilon m_q^\varepsilon g_{1,q}^\varepsilon \right) \right] \\
&= \sqrt{\varepsilon} \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) m_q^\varepsilon \partial_t g_{1,q}^\varepsilon \right] + \frac{\nu}{\sqrt{\varepsilon}} \partial_x \left[ \sum_{q \in \{1,2\}} \partial_x (m_q^\varepsilon g_{1,q}^\varepsilon) \right] + \mathcal{O}(1) \\
&= \sqrt{\varepsilon} \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) m_q^\varepsilon \partial_t g_{1,q}^\varepsilon \right] + \frac{\nu}{\sqrt{\varepsilon}} \partial_{xx}^2 \rho_1^\varepsilon + \mathcal{O}(1).
\end{aligned}$$

But, by using (152)(a), we have also

$$\begin{aligned}
\sqrt{\varepsilon} \partial_x \left[ \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) m_q^\varepsilon \partial_t g_{1,q}^\varepsilon \right] &= \sqrt{\varepsilon} \partial_{tx}^2 \sum_{q \in \{1,2\}} (v_q^\varepsilon - u) m_q^\varepsilon \left[ \sqrt{\varepsilon} \partial_x (u \rho_0^\varepsilon) - (-1)^q \sqrt{\nu} \frac{\partial_x (m_q^\varepsilon \rho_0^\varepsilon)}{m_q^\varepsilon} + \rho_1^\varepsilon \right] \\
&= 0 - \sqrt{\varepsilon} \nu \partial_{tx}^2 \sum_{q \in \{1,2\}} (-1)^q (v_q^\varepsilon - u) \partial_x (m_q^\varepsilon \rho_0^\varepsilon) \\
&= \mathcal{O}(1).
\end{aligned}$$

Thus, we can write that

$$\mathcal{F}^\varepsilon(\mathcal{G}_1^\varepsilon) = \frac{\nu}{\sqrt{\varepsilon}} \partial_{xx}^2 \rho_1^\varepsilon + \mathcal{O}(1)$$

which gives (151)(b). Moreover, by taking into account (152)(a), we obtain

$$\begin{aligned}
b_q^\varepsilon(\mathcal{G}_1^\varepsilon) &= \sqrt{\varepsilon} \frac{\partial_t (m_q^\varepsilon g_{1,q}^\varepsilon)}{m_q^\varepsilon} + \sqrt{\varepsilon} v_q^\varepsilon \frac{\partial_x (m_q^\varepsilon g_{1,q}^\varepsilon)}{m_q^\varepsilon} \\
&= \sqrt{\varepsilon} \partial_t \left( \sqrt{\varepsilon} \partial_x (u \rho_0^\varepsilon) - (-1)^q \sqrt{v} \frac{\partial_x (m_q^\varepsilon \rho_0^\varepsilon)}{m_q^\varepsilon} + \rho_1^\varepsilon \right) \\
&\quad + (-1)^q \sqrt{v} \frac{\partial_x \left[ m_q^\varepsilon \left( \sqrt{\varepsilon} \partial_x (u \rho_0^\varepsilon) - (-1)^q \sqrt{v} \frac{\partial_x (m_q^\varepsilon \rho_0^\varepsilon)}{m_q^\varepsilon} + \rho_1^\varepsilon \right) \right]}{m_q^\varepsilon} \\
&= \sqrt{\varepsilon} \partial_t \rho_1^\varepsilon - v \frac{\partial_{xx}^2 (m_q^\varepsilon \rho_0^\varepsilon)}{m_q^\varepsilon} + (-1)^q \sqrt{v} \frac{\partial_x (m_q^\varepsilon \rho_1^\varepsilon)}{m_q^\varepsilon} + \mathcal{O}(\sqrt{\varepsilon}) \\
&= v \partial_{xx}^2 \rho_0^\varepsilon - v \frac{\partial_{xx}^2 (m_q^\varepsilon \rho_0^\varepsilon)}{m_q^\varepsilon} + (-1)^q \sqrt{v} \frac{\partial_x (m_q^\varepsilon \rho_1^\varepsilon)}{m_q^\varepsilon} + \mathcal{O}(\sqrt{\varepsilon})
\end{aligned}$$

by also using (149)(b) and (151)(a). Then, we obtain (152)(b) by using (147).  $\square$

## B. The LBM scheme written in function of $f_q$ when $u(x) = 0$

When  $u(x) = 0$ , the LBM scheme (33) is given by

$$\begin{cases} g_{1,i}^{n+1} = g_{1,i+1}^n \left(1 - \frac{\eta}{2}\right) + g_{2,i+1}^n \frac{\eta}{2}, \\ g_{2,i}^{n+1} = g_{2,i-1}^n \left(1 - \frac{\eta}{2}\right) + g_{1,i-1}^n \frac{\eta}{2}, \\ \rho_i^{n+1} = g_{1,i}^{n+1} + g_{2,i}^{n+1} \end{cases} \quad \text{where} \quad \eta := \frac{1}{C_d + \frac{1}{2}} = \frac{1}{\frac{v \Delta t}{\Delta x^2} + \frac{1}{2}}. \quad (158)$$

On the other side, by using (22), we have  $g_q = f_q - \frac{\Delta t}{2\varepsilon} (M_q - f_q)$  that is to say

$$\begin{cases} g_1 = f_1 \left(1 + \frac{1}{4C_d}\right) - \frac{f_2}{4C_d}, \\ g_2 = f_2 \left(1 + \frac{1}{4C_d}\right) - \frac{f_1}{4C_d} \end{cases} \quad (159)$$

since  $\varepsilon = C_d \Delta t$  and  $M_1 = \frac{f_1 + f_2}{2}$ . By injecting (159) in (158), we obtain

$$A \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}_i^{n+1} = b$$

with

$$A = \begin{pmatrix} 1 + \frac{1}{4C_d} & -\frac{1}{4C_d} \\ -\frac{1}{4C_d} & 1 + \frac{1}{4C_d} \end{pmatrix}$$

and

$$b = \begin{pmatrix} \left[ f_{1,i+1}^n \left( 1 + \frac{1}{4C_d} \right) - \frac{f_{2,i+1}^n}{4C_d} \right] \cdot \left( 1 - \frac{\eta}{2} \right) + \left[ f_{2,i+1}^n \left( 1 + \frac{1}{4C_d} \right) - \frac{f_{1,i+1}^n}{4C_d} \right] \cdot \frac{\eta}{2} \\ \left[ f_{2,i-1}^n \left( 1 + \frac{1}{4C_d} \right) - \frac{f_{1,i-1}^n}{4C_d} \right] \cdot \left( 1 - \frac{\eta}{2} \right) + \left[ f_{1,i-1}^n \left( 1 + \frac{1}{4C_d} \right) - \frac{f_{2,i-1}^n}{4C_d} \right] \cdot \frac{\eta}{2} \end{pmatrix}.$$

By using the fact that

$$A^{-1} = \frac{1}{C_d + 1/2} \begin{pmatrix} C_d + 1/4 & 1/4 \\ 1/4 & C_d + 1/4 \end{pmatrix}$$

and that  $\eta = \frac{1}{C_d + 1/2}$ , we obtain

$$\begin{aligned} f_{1,i}^{n+1} &= \frac{C_d + 1/4}{(C_d + 1/2)^2} \left\{ C_d \left[ f_{1,i+1}^n \left( 1 + \frac{1}{4C_d} \right) - \frac{f_{2,i+1}^n}{4C_d} \right] + \frac{1}{2} \left[ f_{2,i+1}^n \left( 1 + \frac{1}{4C_d} \right) - \frac{f_{1,i+1}^n}{4C_d} \right] \right\} \\ &\quad + \frac{1}{4(C_d + 1/2)^2} \left\{ C_d \left[ f_{2,i-1}^n \left( 1 + \frac{1}{4C_d} \right) - \frac{f_{1,i-1}^n}{4C_d} \right] + \frac{1}{2} \left[ f_{1,i-1}^n \left( 1 + \frac{1}{4C_d} \right) - \frac{f_{2,i-1}^n}{4C_d} \right] \right\} \end{aligned}$$

that is to say

$$\begin{aligned} f_{1,i}^{n+1} &= \frac{4C_d + 1}{4(C_d + 1/2)^2} \left\{ f_{1,i+1}^n \cdot \frac{8C_d^2 + 2C_d - 1}{8C_d} + f_{2,i+1}^n \cdot \frac{C_d + 1/2}{4C_d} \right\} \\ &\quad + \frac{1}{4(C_d + 1/2)^2} \left\{ f_{2,i-1}^n \cdot \frac{8C_d^2 + 2C_d - 1}{8C_d} + f_{1,i-1}^n \cdot \frac{C_d + 1/2}{4C_d} \right\}. \end{aligned}$$

By noting that  $8C_d^2 + 2C_d - 1 = 2(4C_d - 1) \cdot (C_d + 1/2)$ , we finally obtain

$$f_{1,i}^{n+1} = \frac{f_{1,i+1}^n (16C_d^2 - 1) + f_{2,i+1}^n (4C_d + 1) + f_{2,i-1}^n (4C_d - 1) + f_{1,i-1}^n}{16C_d(C_d + \frac{1}{2})}$$

which gives (34)(a). We obtain (34)(b) by symmetry.

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