A Lattice Boltzmann Method applied to the heat equation

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Outlines:

1 - Introduction

2 - Fluid limit of a simple kinetic system

3 - Two LBM schemes

4 - Links with a finite-difference type scheme

5 - Some properties: convergence and maximum principle

6 - Numerical results

7 - Two strange properties

8 - Conclusion

1 - Introduction

The LBM method is said to be :

1) simple and explicit;

2) unconditionally stable and accurate;

3) adapted to model porous medium;

4) parallelisable.

Nevertheless, the LBM method is not really known in the applied math. community.

WHY ?

In fact, the LBM scheme is often presented ...

• **Point 1)** ... as a physical model that is more general than the EDPs it is supposed to solve. For example:

"It is known that existence-uniqueness-regularity problems are very hard at the Navier-Stokes level (...). However, at the lattice Boltzmann level, [there is] *no existence, uniqueness and regularity problems."* **In :** U. Frisch, Phycica D, **47**, p. 231-232, 1991.

Or: *"It may appear unusual that (...) in the LBM approach, the approximation of the flow equation is only shown after the method is already postulated."*

In : Mishra et al, Journal of Heat and Mass Transfer, **48**, p. 3648-3659, 2005.

As a consequence, the LBM scheme is often described with:

LBM scheme → continuous EDPs

(as it is the case for the Boltzmann equation) instead of

continuous EDPs → discretization → LBM scheme.

• **Point 2)** ... as a miraculous numerical method:

Example : *" (...) the Lattice Boltzmann technique may be regarded as a new* [explicit] *finite-difference technique for the Navier-Stokes equation having the property of unconditionnal stability." (Mishra et al.).*

The aim of this talk is to give **precise math. justifications** of all these assertions in the simple case of the heat equation.

We propose the following approach:

continuous kinetic system	$\Longleftrightarrow$	continuous heat eq.
($\varepsilon =$ "collision time")	$\varepsilon \ll 1$	(fluid limit when $\varepsilon \ll 1$)
$\downarrow$		$\updownarrow$
$\downarrow$		links with finite differences ?
discretization with $\varepsilon \ll 1$		stability, convergence in L_∞ ?
$\downarrow$		$\uparrow$
LBM scheme	$\longrightarrow$	discretization of
		the heat eq. since $\varepsilon \ll 1$?

We can summerize this approach **(which is the standard approach in num. anal.)** with:

Continuous EDP → discretization → LBM scheme → stability, convergence ?

instead of:

LBM scheme as a "physical" model → discretization → continuous EDP

2 - Fluid limit of a simple kinetic system

Construction of a simple kinetic system:

We firstly define the "maxwellian" distribution

$$M_q := \frac{\rho}{2}\left[1 + \frac{u(x)}{v_q}\right] = \frac{\rho}{2}\left[1 + (-1)^q \frac{u(x)}{c}\right] \qquad (v_q = (-1)^q c)$$

where $u(x)$ is a given function and $c \in \mathbb{R}^+$. It verifies

$$\sum_{q=1,2} \begin{pmatrix} 1 \\ v_q \end{pmatrix} M_q = \begin{pmatrix} \rho \\ \rho u \end{pmatrix}.$$

Proposition 1 *Let $f_q(t,x)$ be solution of the kinetic system*

$$\partial_t f_q + (-1)^q c\partial_x f_q = \frac{1}{\varepsilon}(M_q - f_q) \qquad (q = 1, 2) \tag{1}$$

where $M_q := \frac{f_1+f_2}{2}\left[1 + (-1)^q \frac{u(x)}{c}\right]$. Thus, the density $\rho := f_1 + f_2$ is solution up to the order ε^2 of

$$\partial_t \rho + \partial_x(u\rho) = \nu\partial^2_{xx}\rho \qquad \text{with} \qquad \boxed{\nu = \varepsilon c^2} \tag{2}$$

when $|u(x)| \ll c$ and $\varepsilon \ll 1$. Moreover, we have

$$f_q(t,x) = \frac{\rho}{2}\left[1 + (-1)^q \frac{u(x)}{c} + \varepsilon(-1)^q \left(\frac{\frac{du^2}{dx}(x)}{2c} - c\frac{\partial_x \rho}{\rho}\right)\right] + \mathcal{O}(\varepsilon^2).$$

Proof : We use an Hilbert or Chapman-Enskog expansion.□

When $u = 0$:

Corollary 1 *Let $f_q(t,x)$ be solution of the kinetic system*

$$\partial_t f_q + (-1)^q c \partial_x f_q = \frac{1}{\varepsilon}(M_q - f_q) \qquad (q = 1,2) \tag{3}$$

with $M_q := \frac{f_1+f_2}{2}$. Thus, the density $\rho := f_1 + f_2$ is solution up to the order ε^2 of

$$\partial_t \rho = \nu \partial_{xx}^2 \rho \qquad \text{with} \qquad \boxed{\nu = \varepsilon c^2} \tag{4}$$

when $\varepsilon \ll 1$. Moreover, we have

$$f_q(t,x) = \frac{\rho}{2}\left[1 + (-1)^{q+1} c\varepsilon \frac{\partial_x \rho}{\rho}\right] + \mathcal{O}(\varepsilon^2).$$

Let us note that $\varepsilon \ll 1$ means $\varepsilon \ll t_{fluid}$ where $t_{fluid} = \mathcal{O}(1)$.

3 - Construction of two LBM schemes

3.1 - Integration of the kinetic system

Proposition 2 *Let* $\{f_q(t,x)\}_{q=1,2}$ *be solution of*

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

and let

$$\boxed{g_q(t,x) := f_q(t,x) - \tfrac{\Delta t}{2} \mathcal{Q}_q(f)(t,x).}$$

Thus

$$g_q[t+\Delta t, x+(-1)^q c\Delta t] = g_q(t,x)(1-\eta) + M_q(t,x)\eta + \boxed{\mathcal{O}(\tfrac{\Delta t^3}{\varepsilon})} \quad (5)$$

where

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

Since $g_1 + g_2 = f_1 + f_2 := \rho$, it is possible to propose a LBM scheme **by using the discrete version of (5)** *i.e.* by using the variable $g_{q,i}^n$ **instead of** $f_{q,i}^n$.

Proof of the proposition 2:

The solution of the continuous EDP

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

is given by

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

A classical numerical integration would give

$$f_q[t+\Delta t, x+(-1)^q c\Delta t] \quad = \quad f_q(t,x) + \Delta t \mathcal{Q}_q(f)(t,x) + \mathcal{O}(\tfrac{\Delta t^2}{\varepsilon}).$$

But $\mathcal{O}(\frac{\Delta t^2}{\varepsilon}) = \mathcal{O}(\Delta t)$ (since $\varepsilon = \mathcal{O}(\Delta t)$: see the sequel ...).

Thus, we use the integration formula

$$\begin{aligned} f_q[t+\Delta t, x+(-1)^q c\Delta t] \quad &= \quad f_q(t,x) + \tfrac{\Delta t}{2}[\mathcal{Q}_q(f)(t,x) \\ &+ \quad \mathcal{Q}_q(f)(t+\Delta t, x+(-1)^q c\Delta t)] \\ &+ \quad \mathcal{O}(\tfrac{\Delta t^3}{\varepsilon}). \end{aligned}$$

But, the relation

$$
\begin{aligned}
f_q[t+\Delta t, x+(-1)^q c\Delta t] &= f_q(t,x) + \tfrac{\Delta t}{2}[\mathcal{Q}_q(f)(t,x) \\
&+ \mathcal{Q}_q(f)(t+\Delta t, x+(-1)^q c\Delta t)] \\
&+ \mathcal{O}(\tfrac{\Delta t^3}{\varepsilon})
\end{aligned}
$$

is equivalent to

$$
g_q[t+\Delta t, x+(-1)^q c\Delta t] = g_q(t,x) + \frac{\varepsilon}{\frac{\varepsilon}{\Delta t}+\frac{1}{2}}\mathcal{Q}_q(g)(t,x) + \mathcal{O}(\frac{\Delta t^3}{\varepsilon})
$$

where $g_q(t,x) := f_q(t,x) - \frac{\Delta t}{2}\mathcal{Q}_q(f)(t,x).\square$

Remark: The previous proof is based on an idea that we can find in:

• He et al – *A Novel Thermal Model for the LBM in Incompressible Limit* – JCP, **146**, p. 282-300, 1998.

• Karlin et al – *Elements of the Lattice Boltzmann Method I: Linear advection Equation* – Comm. In Comp. Phys., **1**(4), p. 616-655, 2006.

3.2 - A first LBM scheme

We choose:

$$\begin{cases} c = \frac{\Delta x}{\Delta t}, \\ \varepsilon = \frac{\nu}{c^2} \end{cases} \Longrightarrow \quad \boxed{\varepsilon = C_d \Delta t} \quad \text{with} \quad \Delta t := C_d \frac{\Delta x^2}{\nu} > 0$$

($C_d > 0$). We deduce from the estimate (*cf.* proposition 2)

$$g_q[t + \Delta t, x + (-1)^q c \Delta t] = g_q(t,x)(1-\eta) + M_q(t,x)\eta + \mathcal{O}(\frac{\Delta t^3}{\varepsilon})$$

(where $\eta = \frac{1}{\frac{\varepsilon}{\Delta t} + \frac{1}{2}}$) a first LBM scheme:

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

By noting that $M_q = \frac{g_1+g_2}{2}$, we see that the LBM scheme is equivalent to

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

We will use this formulation in the sequel.

Let us remark that $\eta \in]0,2[$ when C_d (*i.e.* Δt) $\in \mathbb{R}_*^+$.

The "magic" formula: It is possible to writte the previous LBM scheme with

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

where $\widehat{\varepsilon}$ is such that $\nu = \left(\widehat{\varepsilon} - \frac{\Delta t}{2}\right)\left(\frac{\Delta x}{\Delta t}\right)^2$.

To simplify the situation, most of the LBM schemes are written with $\boxed{\Delta x = \Delta t = 1}$ and without the function g:

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

where $\boxed{\boxed{\nu = \left(\widehat{\varepsilon} - \frac{1}{2}\right) c_s^2} \text{ with } c_s := \text{“sound velocity”}(= 1 \text{ here}).}$

For example: D. Wolf-Gladrow – *A Lattice Bolzmann Equation for Diffusion* – J. of Stat. Phys., **79**(5,6), p. 1023-1032, 1995.

A last remark:

By noting that

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

we can rewrite the LBM scheme

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

with the f_q variable. We obtain the LBM scheme:

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

3.3 - A second LBM scheme

We choose:

$$\left\{ \begin{array}{l} c = |\frac{\Delta x}{\Delta t}|, \\ \varepsilon = \frac{\nu}{c^2} \end{array} \right. \quad \Longrightarrow \quad \boxed{\varepsilon = C_d |\Delta t|} \quad \text{with} \quad \Delta t := -C_d \frac{\Delta x^2}{\nu} < 0$$

($C_d > 0$). We deduce from the estimate (*cf.* proposition 2)

$$g_q[t + \Delta t, x + (-1)^q c\Delta t] = g_q(t,x)(1 - \widehat{\eta}) + M_q(t,x)\widehat{\eta} + \mathcal{O}(\frac{\Delta t^3}{\varepsilon})$$

(where $\widehat{\eta} = \frac{1}{\frac{\varepsilon}{\Delta t} + \frac{1}{2}}$) the **second** LBM scheme:

$$\boxed{\left\{ \begin{array}{l} g^{n-1}_{1,i+1} = g^n_{1,i}(1 - \widehat{\eta}) + M^n_{1,i}\widehat{\eta}, \\ g^{n-1}_{2,i-1} = g^n_{2,i}(1 - \widehat{\eta}) + M^n_{2,i}\widehat{\eta}, \\ \rho^n_i = g^n_{1,i} + g^n_{2,i} \end{array} \right. \quad \text{where} \quad \widehat{\eta} = \frac{1}{-C_d + \frac{1}{2}}.}$$

We have the property:

Property 1 *The LBM scheme*

$$\left\{\begin{aligned} g_{1,i+1}^{n-1} &= g_{1,i}^{n}(1-\widehat{\eta}) + M_{1,i}^{n}\widehat{\eta}, \\ g_{2,i-1}^{n-1} &= g_{2,i}^{n}(1-\widehat{\eta}) + M_{2,i}^{n}\widehat{\eta}, \\ \rho_i^n &= g_{1,i}^n + g_{2,i}^n \end{aligned}\right. \qquad \textit{where} \quad \widehat{\eta} = \frac{1}{-C_d + \frac{1}{2}}$$

is equivalent to the LBM scheme

$$\left\{\begin{aligned} g_{1,i}^{n+1} &= g_{1,i+1}^{n}(1-\tfrac{\eta}{2}) + g_{2,i-1}^{n}\tfrac{\eta}{2}, \\ g_{2,i}^{n+1} &= g_{2,i-1}^{n}(1-\tfrac{\eta}{2}) + g_{1,i+1}^{n}\tfrac{\eta}{2}, \\ \rho_i^{n+1} &= g_{1,i}^{n+1} + g_{2,i}^{n+1} \end{aligned}\right. \qquad \textit{where} \quad \eta = \frac{1}{C_d + \frac{1}{2}}$$

with $\Delta t := C_d \frac{\Delta x^2}{\nu}$. *We name this scheme* **LBM* scheme**.

QUESTIONS:

- LBM = LBM* ?
- initial conditions $g_{1,i}^{n=0}$ and $g_{2,i}^{n=0}$?
- boundary conditions ?
- stability and convergence ?
- probabilistic interpretation (not treated in this talk) ?

4 - Links with a finite-difference type scheme

Les us recall the two LBM schemes:

- **LBM scheme:**

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

- **LBM* scheme:**

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

Here, we only study the LBM* scheme which is more simple to study than the LBM scheme. Nevertheless, all the properties verified by the LBM* scheme are also verified by the LBM scheme.

Dirichlet boundary conditions

$\rho(t, x_{\min}) = \rho_{x_{\min}}$ and $x_i = x_{\min} + i\Delta x$ $(i = 1, \ldots)$.

Lemma 1 *The LBM* scheme with the boundary condition*

$$\begin{cases} g_{2,i=0}^{n+1} = \rho_{x_{\min}} - g_{1,i=1}^{n} + \eta(g_{1,i=1}^{n} - \tfrac{1}{2}\rho_{x_{\min}}), \\ g_{2,i=0}^{0} = \alpha\rho_{x_{\min}} \end{cases} \quad (n \in \{0, \ldots\})$$

and with the initial condition $\begin{cases} g_{1,i}^{0} = (1-\alpha)\rho_i^0, \\ g_{2,i}^{0} = \alpha\rho_i^0 \end{cases} \quad (i \in \{1, \ldots\})$

is equivalent to the Du Fort-Frankel scheme

$$\begin{cases} \frac{\rho_i^{n+1} - \rho_i^{n-1}}{2\Delta t} = \frac{\nu}{\Delta x^2}(\rho_{i+1}^{n} - \rho_i^{n+1} - \rho_i^{n-1} + \rho_{i-1}^{n}), \\ \rho_0^n = \rho_{x_{\min}} \end{cases} \tag{6}$$

when $\rho_i^{n=1}$ in (6) is defined with

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

Remarks:

• We have a similar result for Neumann B.C. when

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

and we recover the **bounce-back** B.C. $g_{2,i=0}^{n} = g_{1,i=1}^{n}$ when $\alpha = 1/2$.

• This equivalence between a LBM scheme and a finite-difference scheme was firstly **mentioned** in:

Ancona M.G. – *Fully-Lagrangian and Lattice-Boltzmann Methods for Solving Systems of Conservation Equations* – JCP, **115**, p. 107-120, 1994.

Nevertheless, the importance of the initial and boundary conditions was not studied.

• the Robin B.C. has not been studied.

5 - Some properties: convergence and maximum principle

5.1 - Convergence in L_∞

Proposition 3 *For any* $C_d > 0$ $(\Delta t := C_d \frac{\Delta x^2}{\nu})$ *and any* $\alpha \in \mathbb{R}$:

i) the LBM schemes with periodic, Neumann or Dirichlet B.C. and with the initial condition*

$$\begin{cases} g^0_{1,i} = (1-\alpha)\rho^0_i, \\ g^0_{2,i} = \alpha \rho^0_i \end{cases} \qquad (i \in \{1, \ldots\})$$

converge in L_∞*;*

ii) the Du Fort-Frankel scheme

$$\frac{\rho_i^{n+1} - \rho_i^{n-1}}{2\Delta t} = \frac{\nu}{\Delta x^2}(\rho^n_{i+1} - \rho^{n+1}_i - \rho^{n-1}_i + \rho^n_{i-1})$$

with periodic, Neumann or Dirichlet B.C. converges in L_∞ *when* $\rho_i^{n=1} := \alpha \rho^0_{i-1} + (1-\alpha)\rho^0_{i+1}$*;*

iii) the convergence order is equal to 2 $\iff \alpha = \frac{1}{2}$.

Basic idea of the proof:

unconditional L_∞ stability of the LBM* scheme [**due to convexity**]

+ **equivalence lemma** (*i.e.* lemma 1)

$\Downarrow$

unconditional L_∞ stability of the Du Fort-Frankel scheme

AND

Lax theorem (stability + consistency)

$\Downarrow$

unconditional L_∞ convergence of the Du Fort-Frankel scheme

AND

equivalence lemma (*i.e.* lemma 1)

$\Downarrow$

unconditional L_∞ convergence of the LBM* schemes.

Some comments: Recall that $\Delta t := C_d \frac{\Delta x^2}{\nu}$.

• It is known since 1953 that the Du Fort-Frankel scheme is unconditionally stable in L_2 under periodic B.C. (*cf.* Fourier analysis).

• But, since the Du Fort-Frankel scheme may be written with

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

we have also the L_∞ stab. **under the stab. cond.** $0 \leq C_d \leq 1/2$

(since the maximum principle is verified in that case).

• Here, we have obtained the unconditional L_∞ stability of the Du Fort-Frankel scheme **when**

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

5.2 - Maximum principle with periodic and Neumann B.C.

Lemma 2 *For any $C_d \geq 0$ ($\Delta t := C_d \frac{\Delta x^2}{\nu}$), the LBM* scheme with the initial condition*

$$\begin{cases} g^0_{1,i} = (1-\alpha)\rho^0_i, \\ g^0_{2,i} = \alpha \rho^0_i \end{cases} \qquad (i \in \{1, \dots\})$$

verifies the maximum principle

$$\min_j \rho^0_j \leq \rho^n_i \leq \max_j \rho^0_j$$

i) for any $\alpha \in [0,1]$ in the periodic case;
ii) when $\alpha = \frac{1}{2}$ in the Neumann case.

Thus, this is also the case for the Du Fort-Frankel scheme with periodic or Neumann B.C. when the first iterate is defined with $\rho^{n=1}_i := \alpha \rho^0_{i-1} + (1-\alpha)\rho^0_{i+1}$.

Remark: for the periodic B.C. (*cf.* point *i*), the result is also valid for the LBM sch.. Nevertheless, for the Neumann B.C. (*cf.* point *ii*), the result has still to be proved for the LBM scheme.

Remark:

The Du Fort-Frankel scheme is equivalent to

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

(with $\eta := \frac{1}{\frac{\nu \Delta t}{\Delta x^2} + \frac{1}{2}} \in [0, 2]$). Thus, when $\rho_i^{n=1} := \alpha\rho_{i-1}^0 + (1-\alpha)\rho_{i+1}^0$:

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

This proves that: $\boxed{\min_j \rho_j^0 \le \rho_i^2 \le \max_j \rho_j^0 \text{ for any } \Delta t > 0}$

for the **periodic** case when $\alpha \in [0, 1]$.

Nevertheless, it is *a priori* more difficult to obtain a similar result for $\rho_i^{n\ge 3}$ **without using the LBM equivalence** !!!

5.3 - Maximum principle with modified Dirichlet B.C.

In the Dirichlet case

$$\begin{cases} g_{2,i=0}^{n+1} = \rho_{x_{\min}} - g_{1,i=1}^{n} + \eta(g_{1,i=1}^{n} - \frac{1}{2}\rho_{x_{\min}}), \\ g_{2,i=0}^{0} = \alpha\rho_{x_{\min}} \end{cases} \tag{7}$$

(*idem* in $x = x_{\max}$), the maximum principle

$$\min(\rho_{x_{\min}}, \rho_{x_{\max}}, \min_j \rho_j^0) \leq \rho_i^n \leq \max(\rho_{x_{\min}}, \rho_{x_{\max}}, \max_j \rho_j^0)$$

is verified when $0 \leq C_d \leq \frac{1}{2}$.

We would like this maximum principle to be **unconditionally** satisfied (as for the periodic and Neumann cases),
to be able to treat the case $C_d > \frac{1}{2}$ and *cells number* $= \mathcal{O}(1)$**.**

$\rightarrow$ We have to modify the Dirichlet B.C. (7).

$\rightarrow$ We will lose the equivalence LBM / Du Fort-Frankel !!!

Lemma 3 *For any* $C_d \geq 0$ $(\Delta t := C_d \frac{\Delta x^2}{\nu})$*, the LBM* scheme with the modified Dirichlet boundary condition*

$$\begin{cases} g^n_{2,i=0} = \frac{1}{2}\rho_{x_{\min}}, \\ g^n_{1,i=N+1} = \frac{1}{2}\rho_{x_{\max}} \end{cases} \tag{8}$$

and with the initial condition

$$g^0_{1,i} = g^0_{2,i} = \frac{\rho^0_i}{2}$$

verifies the maximum principle

$$\min(\rho_{x_{\min}}, \rho_{x_{\max}}, \min_j \rho^0_j) \leq \rho^n_i \leq \max(\rho_{x_{\min}}, \rho_{x_{\max}}, \max_j \rho^0_j).$$

Some comments: With the modified Dirichlet B.C. (8) →

- *i)* **loss of the equivalence** LBM - Du Fort-Frankel;
- *ii)* convergence ?
- *iii) a priori*, loss of the order 2 (verified with numerical experiments);
- *iv)* but **ROBUST** on **ROUGH** mesh because of the maximum principle !!!

6 - Numerical results

We test the LBM* scheme

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

where

$$\eta = \frac{1}{C_d + \frac{1}{2}} = \frac{1}{\frac{\nu \Delta t}{\Delta x^2} + \frac{1}{2}}.$$

We choose $[x_{\min}, x_{\max}] = [-10, 10]$ and $\nu = 1$.

Test-case 1: **Maximum principle with order 2 or (order 1 ?) modified Dirichlet B.C.**

We study the influence of the order 2 Dirichlet B.C.

$$\begin{cases} g_{2,i=0}^{n+1} = \rho_{x_{\min}} - g_{1,i=1}^{n} + \eta(g_{1,i=1}^{n} - \frac{1}{2}\rho_{x_{\min}}), \\ g_{2,i=0}^{0} = \frac{1}{2}\rho_{x_{\min}} \end{cases}$$

and of the (order 1 ?) modified Dirichlet B.C. $\begin{cases} g_{2,i=0}^{n} = \frac{1}{2}\rho_{x_{\min}}, \\ g_{1,i=N+1}^{n} = \frac{1}{2}\rho_{x_{\max}} \end{cases}$

on the maximum principle **when the mesh is ROUGH**

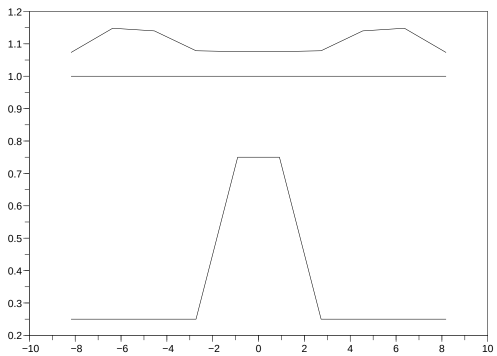
(we think that this is an important test for porous medium).

Here, *cells number* $= 10$ and the initial condition is given by

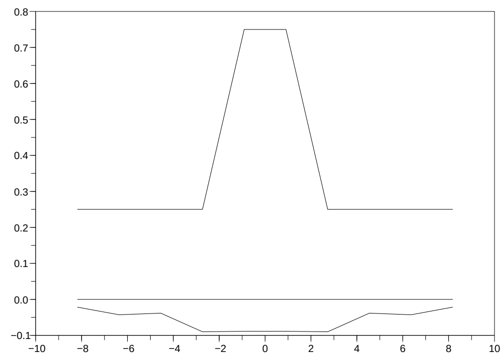
$$\begin{aligned} \rho_i^0 &= \tfrac{1}{4} \text{ if } i \notin \{5,6\} \\ &= \tfrac{3}{4} \text{ if } i \in \{5,6\}. \end{aligned}$$

We choose $C_d = 4$ and $t_{final} = t^{n=10}$.

$\rho_i^{n=4}$ with order 2 Dirichlet B.C. $(C_d = 4)$

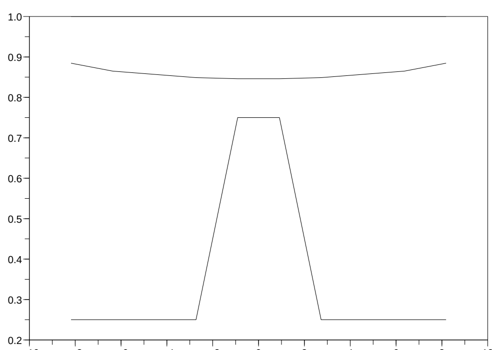


$\rho_{x_{\min}} = \rho_{x_{\max}} = 1$

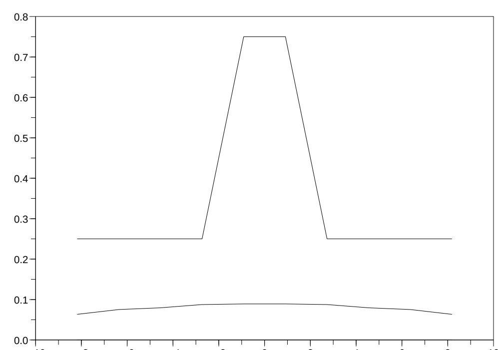


$\rho_{x_{\min}} = \rho_{x_{\max}} = 0$

$\rho_i^{n=4}$ with (order 1 ?) modified Dirichlet B.C. $(C_d = 4)$



$\rho_{x_{\min}} = \rho_{x_{\max}} = 1$



$\rho_{x_{\min}} = \rho_{x_{\max}} = 0$

<u>Test-case 2:</u> instat. analyt. sol. with order 2 or (order 1 ?) modified Dirichlet B.C. and with a fine mesh

We compare the results with the analytical solution

$$\phi(t,x) = erf\left[\frac{x_i - x_{\min}}{\sqrt{4\nu(t+t_0)}}\right]$$

(with $t_0 = 1$).

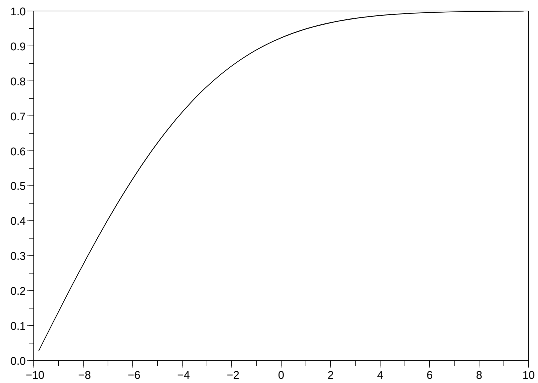
We impose the order 2 or (order 1 ?) modified Dirichlet B.C. with

$$\begin{cases} \rho^n_{x_{\min}} = \phi(t^n, x_{\min}), \\ \rho^n_{x_{\max}} = \phi(t^n, x_{\max}). \end{cases}$$

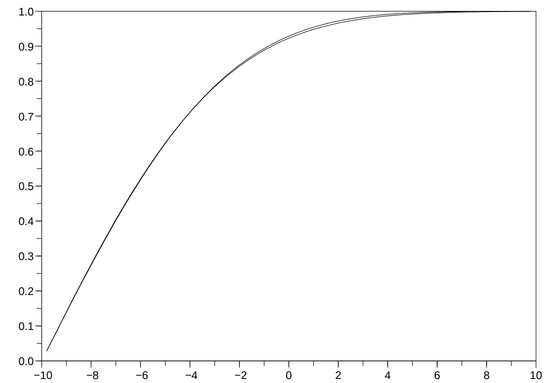
We choose *cells number* $= 100$, $C_d \in \{2,4,8,16\}$ and $t_{final} = 15$.

Order 2 Dirichlet B.C.

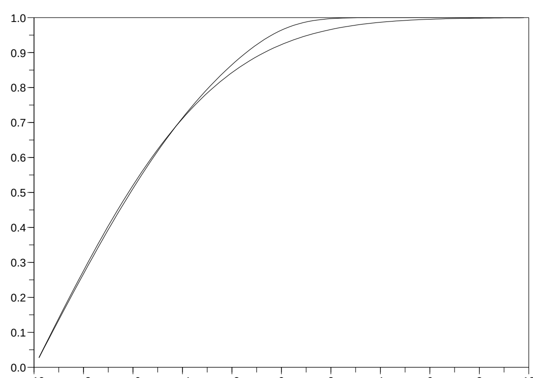
ρ_i^n and $\rho_{exact}(t^n, x_i)$ ($t^n = 15$)



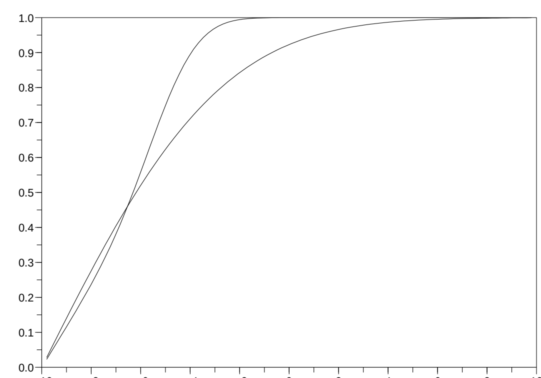
$C_d = 2$



$C_d = 4$



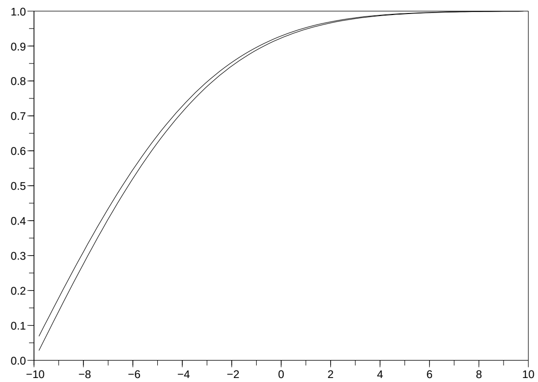
$C_d = 8$



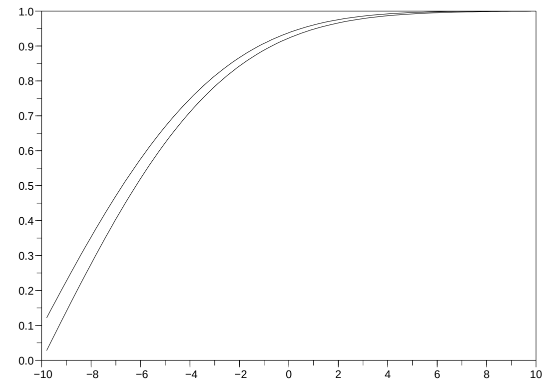
$C_d = 16$

(Order 1 ?) modified Dirichlet B.C.

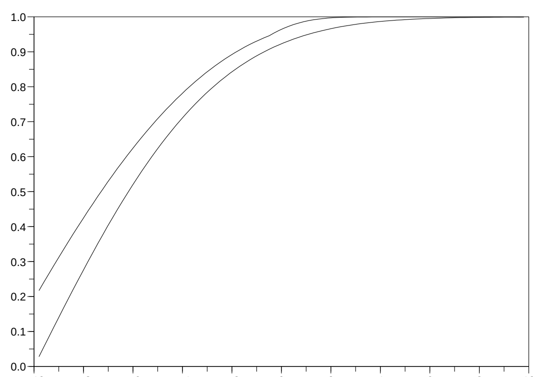
ρ_i^n **and** $\rho_{exact}(t^n, x_i)$ **(**$t^n = 15$**)**



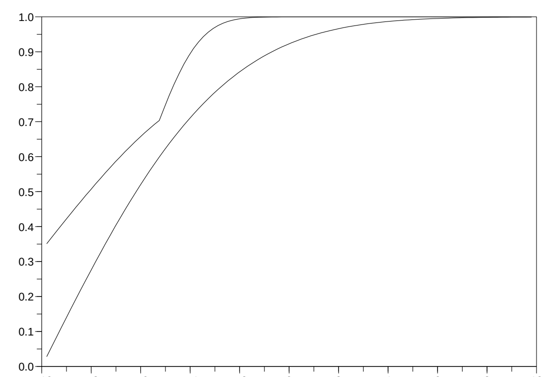
$C_d = 2$



$C_d = 4$

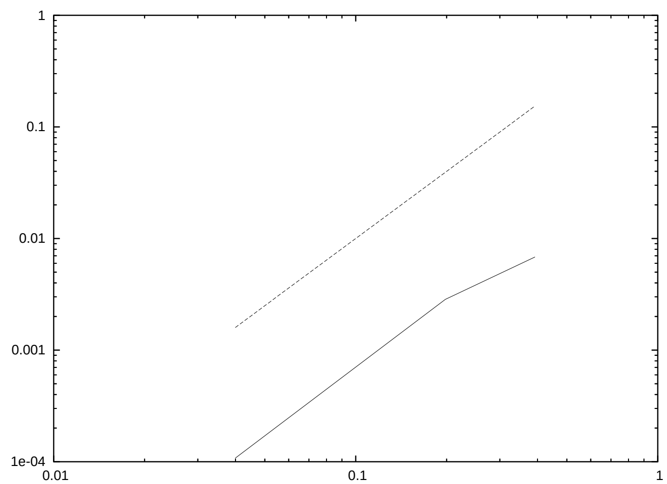


$C_d = 8$

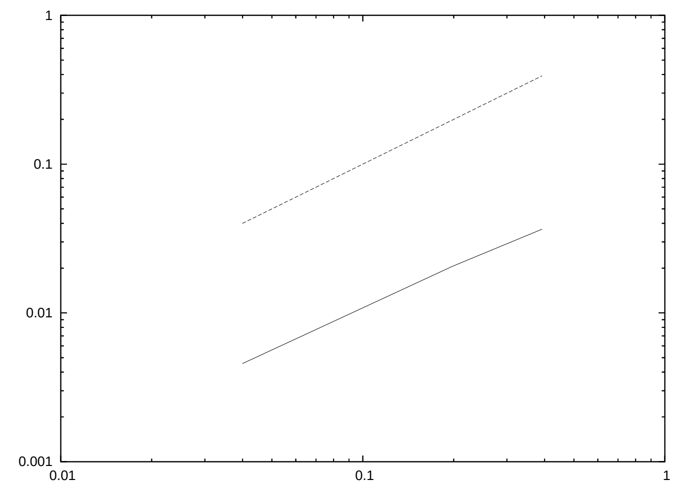


$C_d = 16$

Convergence (LBM* scheme)
Erreur $L_2(\Delta x)$ (—) et $y = x^{1 \text{ ou } 2}$ (- - -)
pour $N \in \{50, 100, 500\}$ ($C_d = 2$)



Order 2 Dirichlet B.C.



(Order 1 ?) modified Dirichlet B.C.

Thus, the modified Dirichlet B.C. seems to be of order 1. This B.C. is adapted when the mesh is rough (*cf.* porous medium) since the **max. principle is verified** (ROBUST code). But, when the mesh is fine, the order 2 is better.

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

We impose periodic boundary condition.

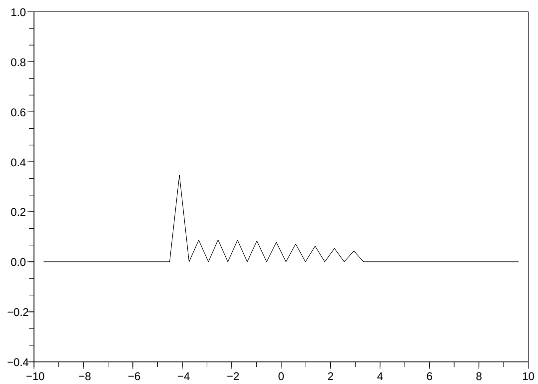
We choose *cells number* $= 100$ and $C_d = 4$.

We choose the initial condition

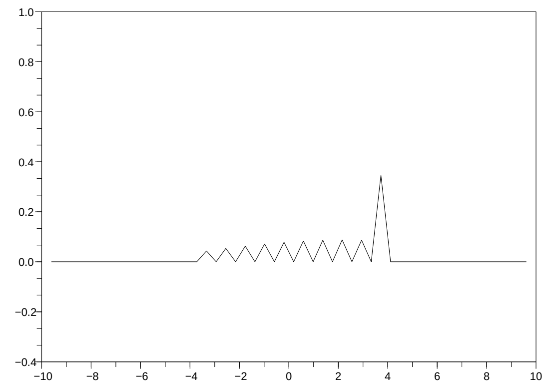
$$\begin{aligned} \rho_i^0 &= 0 \text{ si } i \neq 50 \\ &= 1 \text{ si } i = 50 \end{aligned}$$

($i.e.$ $\rho_i^0 =$ Dirac in $x = 0$).

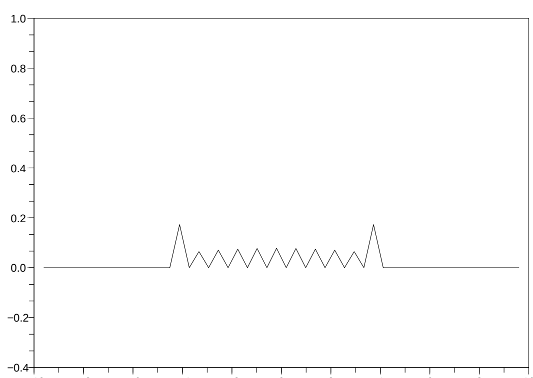
Influence of $\rho_i^{n=1}$ on the positivity of the DFF scheme



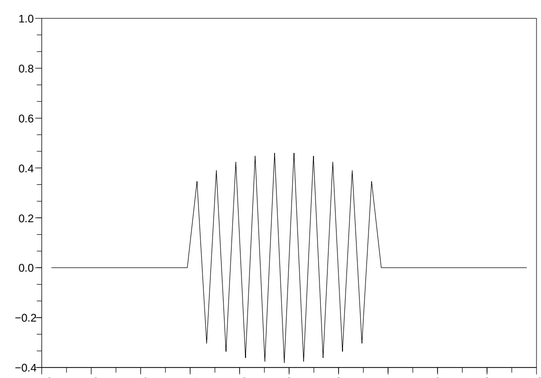
$$\rho_i^{n=1} = \rho_{i+1}^0$$
(= LBM with $\alpha = 0$)



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



$$\rho_i^{n=1} = \frac{1}{2}(\rho_{i-1}^0 + \rho_{i+1}^0)$$
(= LBM with $\alpha = \frac{1}{2}$)



$$\rho_i^{n=1} = \rho_i^0$$
($\neq$ LBM)

7 - Two strange properties

$(\Delta t = C_d \frac{\Delta x^2}{\nu})$

• $C_d = 0$:

Lemma 4 *When $C_d = 0$ (i.e. $\Delta t = 0$), the LBM* scheme preserves the initial condition in the sense*

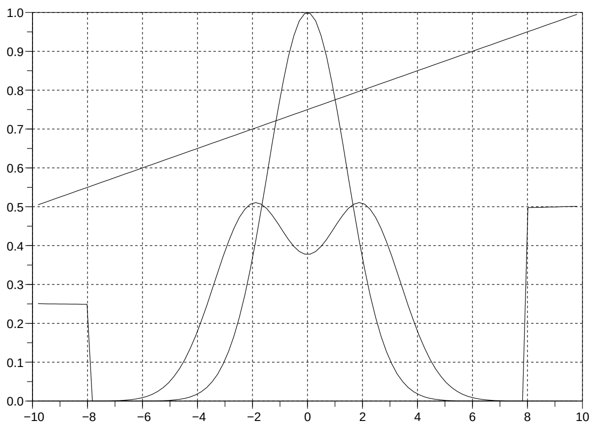
$$C_d = 0 \qquad \Longrightarrow \qquad \forall n \in \mathbb{N} : \quad \rho_i^n = \rho_i^{n+2}.$$

Thus, the Du Fort-Frankel scheme verifies the same property when the first iterate is defined with $\rho_i^{n=1} := \alpha \rho_{i-1}^0 + (1-\alpha)\rho_{i+1}^0$.

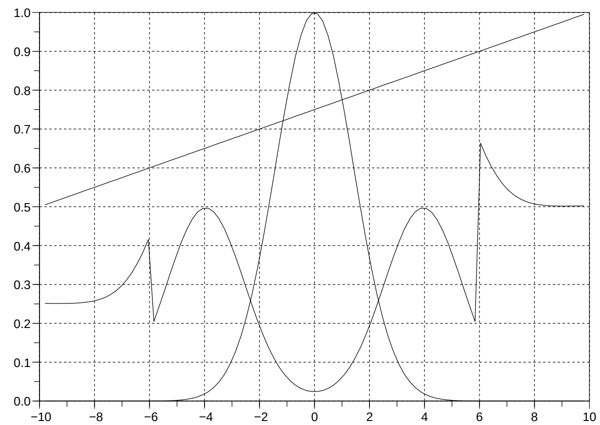
• $C_d = +\infty$:

When $C_d \to +\infty$, we observe waves and discontinuities !!!

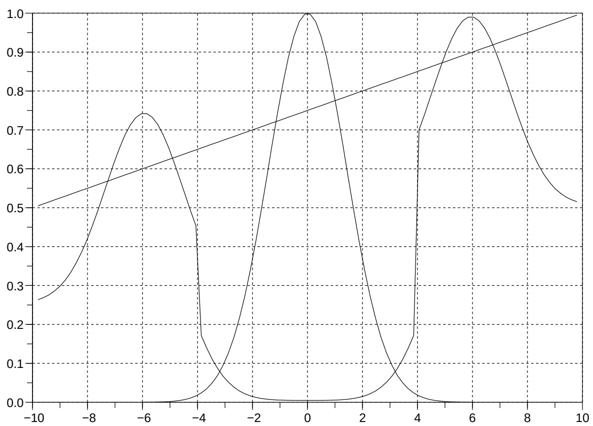
Dirichlet B.C. and $C_d = 1000$



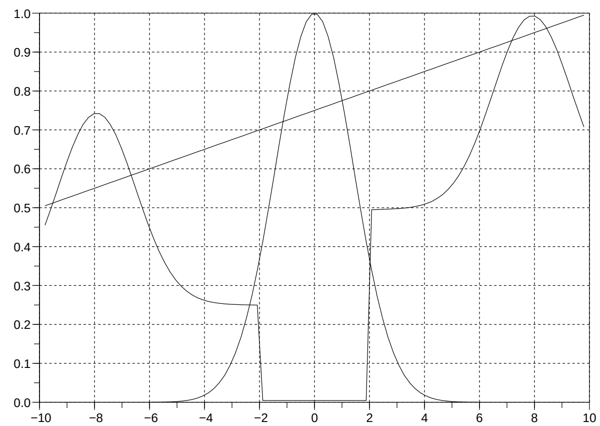
$t^{n=10}$



$t^{n=20}$

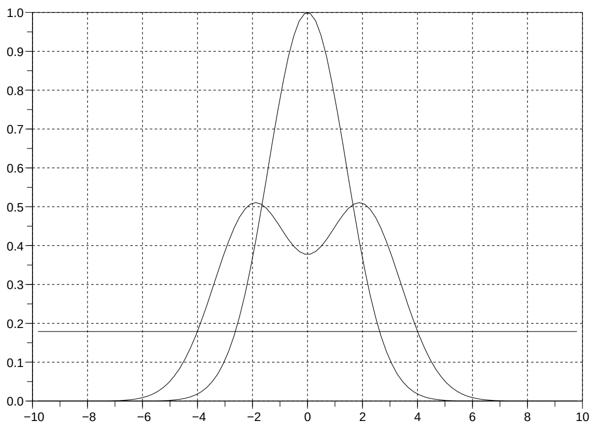


$t^{n=30}$

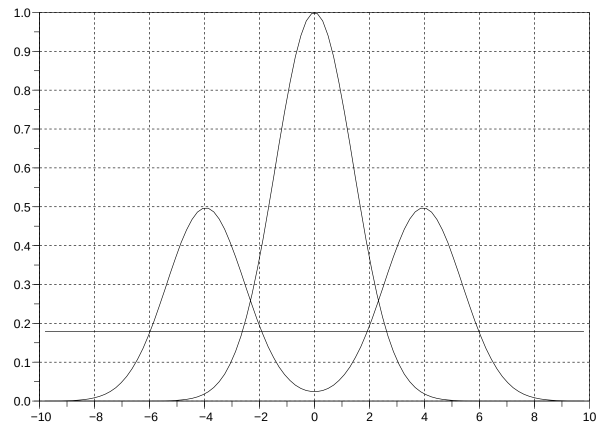


$t^{n=40}$

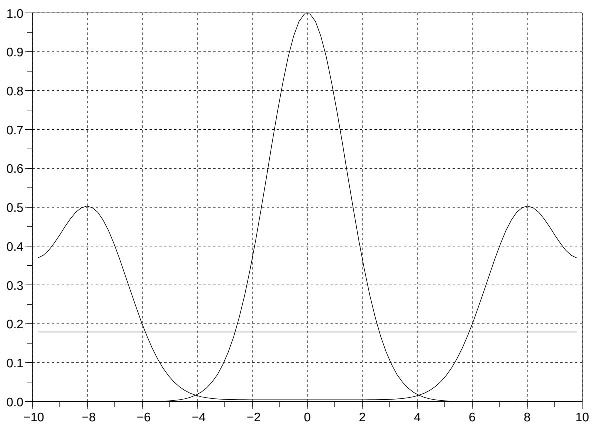
Neumann B.C. and $C_d = 1000$



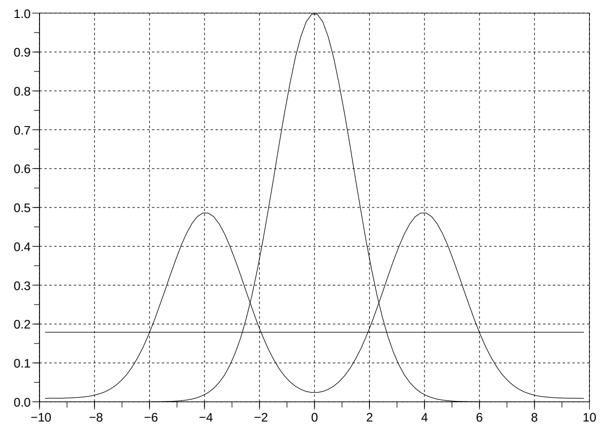
$t^{n=10}$



$t^{n=20}$



$t^{n=40}$



$t^{n=80}$

We can explain this phenomena:

When $C_d \to +\infty$ (i.e. $\Delta t \to +\infty$), the LBM and LBM is given by*

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

The distributions g_q are advected with the velocity $v_q = (-1)^q \frac{\Delta x}{\Delta t}$. Thus, ρ_i^n cannot converge toward the stationary solution of the heat equation when $\Delta t \to +\infty$.

More precisely, we can prove that the consistency error $\mathbb{E}$ of the Dufort-Frankel scheme is given by $\mathbb{E} = -\nu \frac{\Delta t^2}{\Delta x^2} \partial^2_{tt}\rho + \mathcal{O}(\Delta x^2)$. Thus, the equivalent equation is given by

$$\boxed{\partial_t \rho = \nu(\partial^2_{xx}\rho - \tfrac{1}{c^2}\partial^2_{tt}\rho)} + \mathcal{O}(\Delta x^2) \qquad \text{with} \qquad c = \frac{\Delta x}{\Delta t}$$

(telegraph equation).

$\rightarrow$ This means that the Du Fort-Frankel scheme is consistent under the **consistency condition** $\Delta t = C_d \frac{\Delta x^2}{\nu}$.

Thus, when $C_d \rightarrow +\infty$ or when $\Delta t = C^{st}\Delta x$, the LBM scheme solves the wave equation

$$\partial^2_{tt}\rho - c^2 \partial^2_{xx}\rho = 0 \qquad \text{with} \qquad c = \frac{\Delta x}{\Delta t}.$$

This explains why there are waves and discontinuities when $C_d \rightarrow +\infty$.

Thus: although the LBM scheme is unconditionally stable,
we do not have to choose a large C_d.
More precisely, the LBM scheme is consistent
under the condition $\Delta t = C^{st} \Delta x^{\alpha}$ $(\alpha > 1)$.

But, from a practical point of view, how to choose C_d ?

It depends on the test-case and on the mesh.

9 - Conclusion

• construction of two LBM schemes for $\partial_t \rho = \nu \partial^2_{xx} \rho$;

• equivalence with a particular class of Du Fort-Frankel schemes for periodic, Neumann and Dirichlet B.C.;

• convergence of this particular class of Du Fort-Frankel schemes in L_∞ for any $\Delta t := C_d \frac{\Delta x^2}{\nu} \in \mathbb{R}^+$;

• maximum principle for any $\Delta t \in \mathbb{R}^+$ with periodic and order 2 Neumann B.C., **but not with the order 2 Dirichlet B.C.**;

• modification of the order 2 Dirichlet B.C. $\rightarrow$ LBM scheme with a order 1 Dirichlet B.C.;

$\Longrightarrow$ maximum principle for any $\Delta t \in \mathbb{R}^+$ for the LBM scheme with this new order 1 Dirichlet B.C.;

• it is possible to propose a probabilistic interpretation of the LBM scheme and of the Du Fort-Frankel scheme: **could it be a general tool to analyse LBM schemes for other equations** ?